Doctoral Thesis

Optimization of Kinematic Dynamos Using Variational Methods

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Optimization of kinematic dynamos using variational methods

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presented by

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Abstract

The Earth possesses a magnetic field that is generated by the fluid motion in a conducting outer core. This system that converts kinetic energy into long lasting magnetic energy is called a dynamo. Not only found on the Earth, a dynamo is a fundamental mechanism that also exists in astrophysical bodies, and various research groups have reproduced dynamos with computer simulations and experiments. Despite extensive studies there is no general recipe to guarantee dynamo action. One important question is therefore: how to generate a dynamo most efficiently? In this thesis, we adapt a variational method to search numerically for the most efficient dynamos and the corresponding optimal flow fields. This method covers a large parameter space that in theory represents infinitely many field configurations, something conventional methods cannot achieve.

Our optimization scheme combines existing dynamo models with adjoint modelling and subsequent updates using variational derivatives. We start with a kinematic dynamo model and update iteratively the initial conditions of both a steady flow field and a magnetic field. We use the enstrophy based magnetic Reynolds number ($Rm$) as an input parameter. For a given $Rm$, the asymptotic growth of the magnetic energy needs to be non-negative in order to maintain a dynamo. When the asymptotic growth is precisely zero in an optimized model, we identify the corresponding value of $Rm$ as the lower bound for dynamo action, denoted by the minimal critical magnetic Reynolds number $Rm_{c,min}$. For some non-dynamo configurations the magnetic energy can grow during a transient period but eventually decays. The critical transient magnetic Reynolds number for which the magnetic energy cannot grow in any time window, even a very narrow one, is denoted by $Rm_t$.

Using this method, we study kinematic dynamos in three main categories: unconstrained dynamos in a cube, unconstrained dynamos in a full sphere and dynamos with symmetries in a full sphere. All models are implemented numerically using a spectral Galerkin method. In the cubic model, we study optimized dynamos at $Rm_{c,min}$ with four sets of magnetic boundary conditions: NNT, NTT, NNN and TTT (T denotes superconducting boundary conditions and N denotes pseudo-vacuum boundary conditions on opposite sides of the cube), meanwhile keeping the flow field satisfying impermeable boundary conditions. Numerically swapping the magnetic boundary conditions from T to N leaves the magnetic energy growth nearly unchanged, and if $u$ is an optimal flow field, then $-u$ is the new optimum after swapping. For the mixed cases, we can represent the dominant optimal flow field at $Rm_{c,min}$ with three Fourier modes that each describe a 2D flow field.
In the unconstrained spherical models, we impose electrically insulating boundary conditions on the magnetic field while we let the flow field satisfy either no-slip or free-slip boundary conditions. For the no-slip case, we find the optimal flow at $Rm_{c,\text{min}}$ is spatially localized near the centre of the sphere. The dominant optimal flow is well-represented by the first three spherical harmonic degrees $l \leq 3$ and contains only even spherical harmonic order $m$. We also find that the corresponding optimal flow field at $Rm_t$ is equatorially symmetric ($E^S$). For the free-slip case, we get similar results as in the no-slip case, which suggests that the boundary condition of the flow field does not play a significant role in this kinematic model.

Previous studies have used symmetry as a guide to categorize dynamo solutions with a simple spectral representation ($O(10)$ spectral coefficients). We extend this approach here using our large-scale optimizations. We study in total five different set-ups: (1) dynamos generated by axisymmetric flows, (2) dynamos with an equatorially anti-symmetric ($E^A$) magnetic field (the dipole family) generated by $E^S$ flows, (3) dynamos with an $E^S$ magnetic field (the quadrupole family) generated by $E^S$ flows, (4) dynamos generated by axisymmetric $E^S$ flows, (5) dynamos generated by axisymmetric $E^A$ flows. All models in this part satisfy electrically insulating and no-slip boundary conditions. Ranking them by the associated value of $Rm_{c,\text{min}}$ from low to high, we find the order (2), (3), (1), (4) and (5). Both set-ups (2) and (3) have the same $Rm_t$ as in the unconstrained case. The most unstable magnetic eigenmode at $Rm_t$ in set-up (4) is $m = 0$, but in set-up (5) it is $m = 1$. 

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Résumé

La Terre possède un champ magnétique généré par l’écoulement de métal liquide dans son noyau externe. Ce système, qui convertit l’énergie cinétique en énergie magnétique, est appelé une dynamo. Non seulement trouvé sur la Terre, une dynamo est un mécanisme fondamental qui existe également dans les corps astrophysiques, et divers groupes de recherche ont tenté de reproduire ces dynamos avec des simulations et des expériences. Malgré des études approfondies, il n’y a pas de recette générale pour garantir une dynamo. Une question importante est donc : comment générer une dynamo de manière optimale ? Dans cette thèse, nous adaptons une méthode variationnelle pour rechercher numériquement les dynamos les plus efficaces et les champs de vitesse optimum correspondants. Cette méthode couvre un grand espace de paramètres qui, en théorie, représente une infinité de configurations de champ, un avantage que les méthodes conventionnelles ne possèdent pas.

Notre schéma d’optimisation combine les modèles de dynamo existants avec la modélisation adjointe et les mises à jour ultérieures à l’aide de dérivées variationnelles. Nous commençons par un modèle de dynamo cinématique et mettons à jour itérativement les conditions initiales d’un champ de vitesse stationnaire et d’un champ magnétique. Nous utilisons le nombre de Reynolds magnétique basé sur l’enstrophy ($Rm$) comme paramètre d’entrée. Pour un $Rm$ donné, la croissance asymptotique de l’énergie magnétique doit être négative afin de maintenir une dynamo. Lorsque la croissance asymptotique est précisément nulle dans un modèle optimisé, nous identifions ce paramètre $Rm$ comme limite inférieure pour l’action de la dynamo, que nous appellerons le nombre de Reynolds magnétique critique minimum $Rm_{c,min}$. Pour certaines configurations non dynamo, l’énergie magnétique peut se développer pendant une période transitoire mais finit par se dégrader. Le nombre de Reynolds magnétique transitoire critique pour lequel l’énergie magnétique ne peut pas croître dans une fenêtre temporelle, même très étroite, est désigné par $Rm_t$.

En utilisant cette méthode, nous étudions les dynamos cinématiques dans trois catégories principales : les dynamos sans contrainte dans un cube, les dynamos sans contrainte dans une sphère et les dynamos avec des symétries dans une sphère. Tous les modèles sont réalisés numériquement à l’aide d’une méthode Galerkin spectrale. Dans le modèle cubique, nous étudions des dynamos optimisées à $Rm_{c,min}$ avec quatre ensembles de conditions aux limites magnétiques : NNT, NTT, NNN et TTT (T désigne les conditions aux limites supraconductrices et N désigne les conditions aux limites pseudo-nulles sur le côté opposé), tout en gardant le champ de vitesse satisfaisant les conditions aux limites imperméables. Numériquement,
l'échange des conditions aux limites magnétiques de T à N laisse la croissance de l'énergie magnétique quasiment inchangée, et si $\mathbf{u}$ est un champ de vitesse optimal, alors $-\mathbf{u}$ est le nouvel optimum après l'échange. Pour les cas mixtes, nous pouvons représenter le champ de vitesse optimal dominant à $Rm_{c,min}$ avec trois modes de Fourier qui décrivent chacun un champ de vitesse 2D.

Dans les modèles sphériques non contraints, nous imposons des conditions aux limites électriquement isolantes sur le champ magnétique tout en laissant le champ de vitesse satisfaire des conditions de non-glissement ou de glissement libre. Pour la condition de non-glissement, le champ de vitesse optimal à $Rm_{c,min}$ est localisé près du centre de la sphère. Le flux optimal dominant est bien représenté par les trois premiers degrés harmoniques sphériques $l \leq 3$ et ne contient que l'ordre harmonique sphérique pair $m$. Nous trouvons également que le champ de vitesse optimal correspondant à $Rm_t$ est équatorialement symétrique ($E^S$). Pour le cas du glissement libre, nous obtenons des résultats similaires à ceux de la condition de non-glissement, ce qui suggère que la condition limite du champ de vitesse ne joue pas un rôle important dans ce modèle cinématique.

Des études antérieures ont utilisé la symétrie comme critère pour classer les solutions de dynamo avec une représentation spectrale simple (nombre de coefficients spectral $O(10)$). Nous étendons cette approche ici en utilisant nos optimisations à grande échelle. Nous étudions au total cinq configurations différentes : (1) dynamos générées par flux axisymétriques, (2) dynamos avec un champ magnétique équatorialement anti-symétrique ($E^A$) (la famille dipolaire) généré par un champ de vitesse $E^S$, (3) dynamos avec un champ magnétique $E^S$ (la famille quadrupolaire) généré par un champ de vitesse $E^S$, (4) dynamos générées par un champ de vitesse axisymétrique $E^S$, (5) dynamos générées par un champ de vitesse axi-symétrique $E^A$. Tous les modèles de cette partie satisfont aux conditions aux limites électriquement isolantes et de non-glissement. Par valeur croissante de $Rm_{c,min}$, on a (2), (3), (1), (4) et (5). Les deux configurations (2) et (3) ont le même $Rm_t$ que dans le cas non contraint. Le mode propre magnétique le plus instable à $Rm_t$ dans la configuration (4) est $m = 0$, mais dans la configuration (5) c'est $m = 1$. 

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Chapter 1

Introduction

1.1 Motivation

The Earth has a dynamical and enduring magnetic field. Based on measurements from ancient crystals, the geomagnetic field has existed at least 3.4 billion years [Tarduno et al., 2010]. The magnetic field strength and spatial distributions change with time. For example, there are irregular magnetic reversals on the scale of millions of years [Cox, 1973], and secular variations measured in years [Jackson et al., 2000]. This geomagnetic field is generated in the liquid outer core, a layer primarily consisting of iron and a few percent of light elements, shown in Figure 1.1. Consequently, the dynamics of the geomagnetic field is influenced by fluid motions inside the core. As the Earth cools down, the iron-nickel alloy crystallizes in the centre of the Earth to form a growing inner core. The fluid is then driven by thermal convection, chemical convection [Roberts & King, 2013], and possibly procession [Lin, 2015]. The area of study that combines fluid dynamics and magnetism is referred to as magnetohydrodynamics (MHD). In particular, if motions of the conducting fluid in a simply-connected domain generate and sustain a magnetic field, then this system is a magnetic generator, or a dynamo. A dynamo is a fundamental phenomenon that occurs in various environments. In the solar system the Sun, Mercury, Jupiter, Saturn, Uranus and Neptune all have dynamos, yet they have distinct conducting interiors.

There are two common paths to study a dynamo: numerical simulations and experiments. Both are supported by dynamo theory, a mathematical framework first postulated by Larmor [1919]. The numerical models are able to reproduce known features such as magnetic reversals but some parameters cannot reach the estimated range as in a natural dynamo [Sheyko et al., 2016]. In general, self-consistent dynamo models are very complex and computationally expensive. Instead, a reduced kinematic model can be used. Many known dynamo solutions in the literature are based on kinematic models. Numerical studies have also led to proposals for specific dynamo models and to theoretical bounds that rule out spurious solutions, but as yet there is still no simple physical law that guarantees dynamo action. In a parallel path, three dynamo experiments have verified the dynamo effect in the lab: the Riga dynamo [Gailitis et al., 2000], the Karlsruhe dynamo [Muller & Stieglitz, 1999] and the VKS dynamo [Monchaux et al., 2007].
In general dynamo experiments are very difficult to perform, involving a large and complex apparatus, potential hazards with liquid metals, enormous power consumption, etc. The three working dynamo experiments are also limited due to a very constrained type of flow or unnatural ferromagnetic materials.

One may ask, if it is difficult to produce a dynamo in general, can we identify the best field configurations in order to get a dynamo as easily as possible? What would the corresponding dynamo properties be? To answer these questions, one must search over a large number of candidate models due to the lack of analytical solutions, a task that is difficult to complete using conventional methods. We call this the large scale optimization problem. A variational method has been developed specifically for large scale optimization problems based on research in fluid dynamics. In Willis [2012] this variational method was used first to optimize kinematic dynamos in a periodic cube. The aim of this thesis project is to further develop variational methods in order to identify optimal kinematic dynamos with different boundary conditions and geometry.

The plan of this thesis is as follows: Chapter 1 introduces the dynamo theory and gives a brief overview of some of the latest developments in dynamo studies, Chapter 2 reviews kinematic dynamo solutions and their optimizations in a cube and a sphere, Chapter 3 reviews the variational method, which is the main method for optimization in this thesis, Chapter 4 presents the optimization of unconstrained dynamos in a cube, Chapters 5 and 6 present the optimization of unconstrained dynamos in a sphere with no-slip and free-slip boundary conditions respectively, and Chapter 7 presents the optimization of dynamos with imposed symmetries in a sphere. This is then followed by a summary and discussion in Chapter 8.
1.2 Kinematic dynamo theory

1.2.1 Maxwell’s equations

One of the fundamental forces in nature is the electromagnetic force. It corresponds to interactions of particles that carry charges and is mediated by a magnetic field $\mathbf{B}$ and an electric field $\mathbf{E}$. In a classical system, these two fields are described by the four Maxwell’s equations listed below.

1. Gauss’s law:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \quad (1.1)$$

$\rho$ is the charge density, $\epsilon_0$ is the electric constant.

2. Gauss’s law for magnetism:

$$\nabla \cdot \mathbf{B} = 0. \quad (1.2)$$

3. Ampere’s law:

$$\nabla \times \mathbf{B} = \mu_0 (\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}), \quad (1.3)$$

$\mu_0$ is the vacuum permeability, $\mathbf{J}$ is the current.

4. Faraday’s law:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \quad (1.4)$$

If we assume the material that the charges pass through has a uniform conductivity $\sigma$, the current is related to the electrical field by Ohm’s law,

$$\mathbf{J} = \sigma \mathbf{E}. \quad (1.5)$$

If the medium that carries charges is moving, (1.5) needs corrections; we need to consider what are $\mathbf{E}$ and $\mathbf{B}$ as seen by the observer. A standard Lorentz boost considers field transformations with uniform relative velocity $\mathbf{u}$, and transforms field components parallel ($\parallel$) or perpendicular ($\perp$) to the velocity $\mathbf{u}$ as:

$$\mathbf{E}'_{\perp} = \gamma (\mathbf{E}_{\perp} + (\mathbf{u} \times \mathbf{B})_{\perp}), \quad \mathbf{E}'_{\parallel} = \mathbf{E}_{\parallel}, \quad (1.6)$$

$$\mathbf{B}'_{\perp} = \gamma (\mathbf{B}_{\perp} - c^{-2} (\mathbf{u} \times \mathbf{E})_{\perp}), \quad \mathbf{B}'_{\parallel} = \mathbf{B}_{\parallel}, \quad (1.7)$$

where $\gamma = 1/\sqrt{1-u^2/c^2}$ is the Lorentz factor, $c$ is the speed of light, and $u = |\mathbf{u}|$ is the relative speed. If the relative motion has a spatially dependent distribution $\mathbf{u}(\mathbf{x})$, (1.6)-(1.7) still hold at each spatial point [Roberts, 2007]. Consequently the Lorentz factor $\gamma(\mathbf{x})$ must be spatially dependent. For Lorentz transformations in an accelerated frame, the velocity $\mathbf{u}(t)$ and Lorentz factor $\gamma(t)$ become time-dependent [Nelson, 1987]. Thus the most general form we have are (1.6)-(1.7) with $\mathbf{u}(\mathbf{x},t)$ and

$$\gamma(\mathbf{x},t) = \frac{1}{\sqrt{1-u(\mathbf{x},t)^2/c^2}}. \quad (1.8)$$

---

1. Technically it is unified with the so-called weak force at subatomic distances.
In the low speed limit \( u(x, t) \ll c \), the Lorentz factor \( \gamma(x, t) \approx 1 \) regardless of the precise form of \( u \), so \( \mathbf{E}'_\perp \) and \( \mathbf{E}'_\parallel \) can be combined into one expression. Assuming the amplitude of electric field \( |\mathbf{E}| \) is small compared to \( c^2 \), we can ignore the corrections to the magnetic field \( \mathbf{B} \). At such limits, the transformed fields can be written as

\[
\mathbf{E}' = \mathbf{E} + \mathbf{u} \times \mathbf{B}, \quad \mathbf{B}' = \mathbf{B}
\]  
(1.9)

This then explains the corrections on \( \mathbf{E} \) and \( \mathbf{B} \) which we will use. On top of field transformations, we need a few more details for non-relativistic dynamo modelling. First of all, when the time change in the electrical field is small, equation (1.3) simplifies to:

\[
\frac{1}{\mu_0} (\nabla \times \mathbf{B}) = \mathbf{J}.
\]  
(1.10)

Second, if the electromagnetic field needs to cross two media of different conductivity, by integrating Maxwell’s equations over a closed loop intersecting the two sides, we get the interface conditions:

\[
[n \cdot \mathbf{E}] = \rho_s, \quad [n \cdot \mathbf{B}] = 0, \quad [n \times \mathbf{B}] = \mu_0 J_s, \quad [n \times \mathbf{E}] = 0.
\]  
(1.11)

Here \( \rho_s \) and \( J_s \) stand for the surface charge density and the surface current respectively. We will see in the next section that by combining these equations, we get the mathematical description of how a magnetic field can be generated. The interface conditions are also useful when we consider boundary effects.

### 1.2.2 A kinematic dynamo

A kinematic model uses a prescribed flow field, and ignores the feedback from the magnetic field to the flow field. The time evolution of the magnetic field is described by the induction equation:

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) + \eta \nabla^2 \mathbf{B},
\]  
(1.12)

which is derived by substituting (1.9) into (1.5), and then combining (1.4), (1.5) and (1.10). Here \( \eta = 1/(\mu_0 \sigma) \) is the magnetic diffusivity. The rate of change in the magnetic field is the result of a combination of two terms: the magnetic induction and the magnetic diffusion. The fluid is assumed to be incompressible,

\[
\nabla \cdot \mathbf{u} = 0
\]  
(1.13)

and the magnetic field always satisfies the solenoidal condition (1.2). These are the three equations of a kinematic model.

We non-dimensionalize the equations using typical scales. Let us use \( L \) as the typical length and \( u^* \) as the typical velocity scale (we will discuss more about typical velocity scales in §1.2.4). Using a diffusion time scale \( t^* = L^2/\eta \), we get

\[
\frac{\partial \mathbf{B}}{\partial t^*} = Rm \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla^2 \mathbf{B}.
\]  
(1.14)
The **magnetic Reynolds number** is then

\[ Rm = \frac{u^* L}{\eta} \]  

(1.15)

Alternatively one can write the induction equation on the advection time scale \( t^* = L/u^* \),

\[ \frac{\partial B}{\partial t} = \nabla \times (u \times B) + \frac{1}{Rm} \nabla^2 B. \]  

(1.16)

Both equations have been used in the literature. The difference is merely a convention and does not change the physics in the model.

For a fixed \( Rm \), we prescribe a velocity field \( u \) and calculate how much the magnetic field changes at later times. If the flow fields are steady, \( u = u(x) \), then by the linearity of the induction equation in \( B \) we get exponential solutions,

\[ B(x,t) = \sum_i a_i b_i(x) e^{\alpha_i t} \]  

(1.17)

where \( a_i \) are coefficients, \( \alpha_i \) are the eigenvalues and \( b_i \) are the corresponding eigenvectors of the induction equation. The real part \( \gamma = \Re(\alpha) \) denotes the growth rate, the imaginary part \( \Omega = \Im(\alpha) \) denotes the oscillation frequency. As \( t \to \infty \), only the eigenmode with the largest \( \Re(\alpha) \) survives. If the largest real eigenvalue

\[ \max_i \Re(\alpha_i) \geq 0, \]  

(1.18)

then we have a **kinematic dynamo**. If \( \max_i \Re(\alpha_i) = 0 \) at a particular magnetic Reynolds number, then this number is called the **critical** magnetic Reynolds number, denoted by \( Rm_c \). If we measure the magnetic norm over a volume \( V \) as a function of time, denoted by \( \langle B_t^2 \rangle \), where

\[ \langle \cdots \rangle = \frac{1}{V} \int \cdots dV, \]  

(1.19)

we can easily trace what is the asymptotic growth rate \( \gamma \). For example, suppose we have a solution at \( Rm_c \):

\[ B(x,t) = \frac{1}{\sqrt{2}} b_1(x) e^{-7t} + \frac{2}{\sqrt{2}} b_2(x) \]  

(1.20)

where the \( b_i(x), i = 1, 2 \) are eigenvectors to the induction equation for a given \( u(x) \) such that \( \langle b_i^2 \rangle = \langle b_2^2 \rangle = 1 \), and \( \langle b_1 \cdot b_2 \rangle = -3/4 \). There are two eigenvalues, \(-7\) and \(0\). The eigenvalue with largest real part dominates at later times, Figure 1.2 shows the change in magnetic norm with time.

### 1.2.3 Transient growth

We can decide on the presence of a kinematic dynamo by looking at the behaviour of the magnetic field as the time window grows infinitely long: \( t \to \infty \). What happens at a short time window? If magnetic eigenmodes are not orthogonal
we may get a short-term growth that does not match with the asymptotic growth of the least decaying magnetic eigenmode. This intermediate stage is referred to as the transient period. The transient growth could be positive, negative, or zero depending on the initial condition of $\mathbf{B}$ and the flow field $\mathbf{u}$. Let us consider one simple example: suppose we have a solution at a particular $Rm$ such that the magnetic field is described by two non-orthogonal eigenvectors,

$$\mathbf{B}(\mathbf{x}, t) = \frac{1}{\sqrt{2}} \mathbf{b}_1(\mathbf{x}) e^{-7t} + \frac{2}{\sqrt{2}} \mathbf{b}_2(\mathbf{x}) e^{-t}$$  \hspace{1cm} (1.21)$$

where $\langle \mathbf{b}_1^2 \rangle = \langle \mathbf{b}_2^2 \rangle = 1$, and $\langle \mathbf{b}_1 \cdot \mathbf{b}_2 \rangle = -3/4$. We see there is a short term positive transient growth followed by a negative asymptotic growth in magnetic norm $\langle \mathbf{B}^2 \rangle$ in Figure 1.3. In this way, a time-dependent flow may sustain the magnetic field for a brief period. In fact, the instantaneous magnetic energy growth generated by arbitrary flows can be studied using the same kinematic model as in §1.2.2. This is because if we limit the time window to be infinitesimally small, and choose time $t = 0$ to be at any instant we like, we can use a steady flow $\mathbf{u}(\mathbf{x})$ to approximate a dynamical flow at that instant,

$$\lim_{t \to 0} \tilde{\mathbf{u}}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}),$$  \hspace{1cm} (1.22)$$

and use the induction equation to compute the magnetic eigenmodes. For a given set of initial conditions, the critical $Rm$ at which the instantaneous growth of $\mathbf{B}$
is zero,
\[
\lim_{t \to 0} \frac{\partial (B(x,t)^2)}{\partial t} = 0,
\]  
(1.23)
is denoted as \( Rm_t \). Below this critical value \( Rm_t \), there is no positive magnetic energy growth due to insufficient magnetic induction.

### 1.2.4 Definition of \( Rm \)

In the induction equation, the magnetic Reynolds number gives the ratio of magnetic induction to magnetic diffusion, based on an estimate of typical scales:
\[
\frac{\left| \nabla \times (u^* \times B^*) \right|}{\left| \eta \nabla^2 B^* \right|} \sim \frac{u^* L}{\eta}. \tag{1.24}
\]
There are multiple definitions of the magnetic Reynolds number in the literature, due to different definitions of \( u^* \) and \( L \). If not specified, the convention for length scale is to use domain length in a cube, radius in a sphere or shell thickness in a spherical shell. As for the typical velocity scale \( u^* \), we list here three common measures. The kinetic energy based based magnetic Reynolds number is
\[
Rm_u = \frac{U L}{\eta} \tag{1.25}
\]
where \( U = \sqrt{\frac{1}{V^*} \int u^*^2 \, dV^*} \) is the dimensional root mean square (rms) speed, \( V^* \) is the dimensional volume. The typical scale \( u^* \) here is the rms speed \( U \). The enstrophy based magnetic Reynolds number is
\[
Rm_\omega = \frac{\omega^* L^2}{\eta} \tag{1.26}
\]
where \( \omega^* = \sqrt{\frac{1}{V^*} \int (\nabla \times u^*)^2 \, dV^*} \) is the dimensional root mean enstrophy, and the typical scale \( u^* \) is given by \( \omega^* L \). The maximum strain rate based magnetic Reynolds number is
\[
Rm_s = \frac{S_{max} L^2}{\eta} \tag{1.27}
\]
where \( S_{max} \) is the dimensional absolute maximum eigenvalue of the strain rate tensor \( S_{ij} \),
\[
S_{ij} = \frac{1}{2} (\nabla_i u_j + \nabla_j u_i), \tag{1.28}
\]
and the typical scale \( u^* \) is given by \( S_{max} L \). In Cartesian coordinates, \( \nabla_i = \partial_i \), \( i = x, y, z \),
\[
S_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i). \tag{1.29}
\]
In spherical coordinates, \( \nabla_i \) is more complicated, each component of the strain rate tensor is given as follows:

\[
S_{rr} = \frac{\partial u_r}{\partial r},
\]

\[
S_{\theta\theta} = \frac{1}{r} \left( \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r} \right),
\]

\[
S_{\phi\phi} = \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \phi} + \frac{u_r}{r} + \cot \theta u_\theta,
\]

\[
S_{r\theta} = S_{\theta r} = \frac{1}{2} \left( \frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} \right),
\]

\[
S_{r\phi} = S_{\phi r} = \frac{1}{2} \left( \frac{1}{r \sin \theta} \frac{\partial u_r}{\partial \phi} + \frac{\partial u_\phi}{\partial r} - \frac{u_\phi}{r} \right),
\]

\[
S_{\theta\phi} = S_{\phi\theta} = \frac{1}{2} \left( \frac{1}{r \sin \theta} \frac{\partial u_\phi}{\partial \theta} + \frac{1}{r} \frac{\partial u_\theta}{\partial \phi} - \frac{\cot \theta u_\phi}{r} \right).
\]

For the derivation of \( S_{ij} \) in spherical coordinates, see Appendix C.1. The global measure of shear is

\[
S = \sqrt{\left( \frac{1}{V} \int_{V} 2S_{ij}S_{ij} \, dV \right)}.
\]

In special cases, when the flow field \( u \) satisfies either

\[
u |_{\Sigma} = 0,
\]

or

\[
u \cdot \hat{n} |_{\Sigma} = 0, \quad (\nabla \times \nu) \times \hat{n} |_{\Sigma} = 0,
\]

where \( \Sigma \) denotes the boundary and \( \hat{n} \) denotes the unit normal vector pointing outward, the global shear is equivalent to root mean enstrophy, then \( S = \omega^* \). This property is useful when we want to limit the global shear \( S \), we can use \( \omega^* \) which can be easily computed.

**1.2.5 Theoretical bounds**

The value of magnetic Reynolds number needs to be sufficiently large to support dynamo action, i.e. the magnetic induction has to be strong enough to overcome the magnetic diffusion. In addition, dynamo action also depends on the spatial profile of the velocity field and the magnetic field. Some combination of fields can never produce a dynamo. Theoretical bounds then quantify which condition is required, i.e. the necessary but not sufficient condition for dynamo action. Some bounds impose limits on how low \( Rm \) can be:

1. Backus bound [Backus, 1958]. This bound is based on the absolute maximum strain rate \( S_{max} \) in region \( V \) filled with conducting fluid,

\[
\frac{S_{max}}{\eta} \geq \frac{\int_V \nabla \times B^2 \, dV}{\int_V B^2 \, dV}.
\]
In a sphere with electrical insulating boundary conditions, this gives

\[ Rm_s \geq \pi^2. \]  

(1.40)

For more details, see §A.1.1.

2. Childress bound [Childress, 1969]. This bound is based on the maximum speed \( u_{\text{max}} \) and states that in a sphere with electrical insulating boundary conditions,

\[ \frac{u_{\text{max}} L}{\eta} \geq \pi \]  

(1.41)

For more details, see §A.1.2. Note here \( u_{\text{max}} \) is non-dimensionalized using the same scale \( u^* \) as in the definition of \( Rm \). Another way to write it is to use the dimensional maximum speed \( u_{\text{max}}^* \), so the bound is \( u_{\text{max}}^* L/\eta > \pi \).

3. Busse bound [Busse, 1975]. This bound is based on the maximum speed in the radial direction \( \max u_r \) in spherical coordinates,

\[ \max_V u_r \geq \eta \left( \frac{2M_p}{M_t + M_p} \right)^{\frac{1}{2}} \]  

(1.42)

where \( M_p \) is the magnetic energy for poloidal field \( B^p = \nabla \times \nabla \times P(r, \theta, \phi) \hat{r} \), and \( M_t \) is the magnetic energy for toroidal field \( B^t = \nabla \times T(r, \theta, \phi) \hat{r} \).

4. Proctor bound [Proctor, 1977]. This is an improved analytic result over the Backus bound,

\[ \frac{S_{\text{max}}}{\eta} > \frac{\int_V \nabla \times B^2 \, dV}{\int_{V + \hat{V}} B^2 dV} \]  

(1.43)

where \( V \) is a conducting sphere, \( \hat{V} \) is the electrical insulating region outside. By matching the magnetic field from two regions \( V \) and \( \hat{V} \), the least decaying mode of \( B \) gives

\[ Rm_s \geq 12.29, \]  

(1.44)

For more details, see §A.1.3.

Other bounds limit the spatial distribution of a dynamo:

1. In Cartesian coordinates, no field independent of one coordinate which vanishes at infinity can be maintained by dynamo action [Jones, 2011].

2. Planar velocity theorem [Zeldovich, 1957]: No dynamo can be maintained by a planar flow in an unbounded domain. In a bounded domain, however, it is shown that a kinematic dynamo may be generated by a planar flow [Bachtiar et al., 2006; Li et al., 2010].

3. Cowling’s theorem [Cowling, 1933]: An axisymmetric magnetic field vanishing at infinity cannot be maintained by dynamo action.

4. Toroidal velocity theorem [Bullard & Gellman, 1954]: A purely toroidal flow \( u = \nabla \times T(r, \theta, \phi) \hat{r} \) in spherical coordinates cannot maintain a dynamo.

Some impose limits that are related to spatial distributions:
1. Upper bounds on the product of suprema of the toroidal and poloidal velocities [Proctor, 2004]:

2. Bounds on viscous dissipation [Proctor, 1979].

There are also assertions that certain bounds do not exist:

1. No generic bound on growth rate $\gamma$ can be formulated using the $L^{-p}$ norm for the velocity field $u$ with $p \leq N$, where $N$ is the spatial dimension, proven by counterexamples [Nunez, 2002].

2. No lower bound can exist on $Rm_u$ for dynamo action [Proctor, 2015].

These theoretical bounds on $Rm$ do not directly correspond to the critical value $Rm_c$ for the onset of a dynamo. Known dynamo solutions can have an $Rm_c$ that is one order of magnitude higher than the lower bounds given above. It is then natural to search numerically for an actual dynamo solution with the lowest possible $Rm_c$. At the same time, these dynamo solutions have to avoid the spatial distributions that are forbidden for dynamo action.

1.3 Self-consistent dynamo models

With recent development in numerics, the self-consistent magnetohydrodynamics (MHD) models are able to take into account the fluid dynamics and other possible effects in direct numerical simulations (DNS). This should be contrasted to the kinematic model we discussed in previous sections with a prescribed flow field. A common form of MHD model, as is used for planetary dynamo studies, is described by three coupled equations plus two solenoidal conditions. In addition to the kinematic model there are two other coupled equations. One is the Navier-Stokes (NS) equation that describes the fluid motion, the other is the heat equation. For the NS equation, the Boussinesq approximation is widely used so the density difference in the fluid only results in the buoyancy force. A general dimensional NS equation written in the rotating frame is

$$\frac{\partial u}{\partial t} + (u \cdot \nabla) u + \nabla \times u = \frac{1}{\rho_0} \nabla P + \frac{1}{\rho_0} \mathbf{J} \times \mathbf{B} + \nu \nabla^2 u - \frac{\alpha}{\rho_0} \Delta T \mathbf{g}$$

where $\Omega$ is a constant angular velocity, $\rho$ is the fluid density, $\nabla P$ is the pressure gradient, $\nu$ is the kinematic viscosity, $\alpha$ is the coefficient of thermal expansion, $\Delta T$ is the temperature variation, and $\mathbf{g}$ is the gravitational acceleration. For the heat equation, the radiative heating from internal sources is usually ignored for

2. The $L^{-p}$ norm of $u$ is defined as $||u||_p = (\int_X |u|^p dV)^{1/p}$ over a domain $X$. It remains unclear if a bound exists for dynamo solutions that do not behave the same way as illustrated in the counterexamples, where the velocity field scales as $||u||_p \sim h L^{-N/p}$ for $p < N$ and $||u||_p \sim \log L^{-1}$ for $p = N$. Here $h$ is the magnitude of the magnetic field $B$ at the origin and $L$ is the typical scale of the fluid domain.

3. The proof of Proctor [2015] does not rely on counterexamples. Given an existing dynamo solution, a new solution with a smaller $Rm_u$ can always be found so that there is no lower bound.
planetary dynamo studies in spherical shells. The heat equation then has the form:

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \kappa \nabla^2 T \]  (1.46)

where \( T \) is the temperature and \( \kappa \) is the thermal diffusivity. In general multiple physical parameters need to be tuned and relevant dynamical regimes are difficult to reach. For example, a parameter study by Christensen & Aubert [2006] found the lowest \( Rm_u \) for dynamo action in a group of self-consistent dynamo models is about 40, where the fluid is confined in a spherical shell that has the same inner/outer radius ratio as the Earth’s core. At the same time the Ekman number \( (E_k) \), which is another dimensionless number that gives the ratio of viscosity to Coriolis forces, is in reality many orders of magnitude lower, see Table 1.1. In this thesis, we will focus on kinematic models with only one dimensionless number \( Rm \) to worry about.

<table>
<thead>
<tr>
<th>[Christensen &amp; Aubert, 2006]</th>
<th>( Rm_u )</th>
<th>( E_k = \nu / (\Omega L^2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Earth’s core</td>
<td>( &gt; 40, O(10^2) )</td>
<td>( 10^{-4} \sim 10^{-6} )</td>
</tr>
</tbody>
</table>

Table 1.1. A comparison of \( Rm \) and \( E_k \) between the geodynamo and self-consistent dynamo models. †: estimated value using rms speed at the core mantle boundary as the typical scale \( u^* \). Note here the typical length scale \( L \) is the shell thickness, and the volume \( V \) used to calculate rms speed in Christensen & Aubert [2006] is the volume of a spherical shell.

### 1.4 Dynamo experiments

As we mentioned earlier in §1.1, another way to study dynamos is through experiments. Experiments offer direct testing whether imposed conditions make a dynamo. To give an estimate of what we need in a dynamo experiment, let us suppose the maximum speed a mechanical device can drive is \( \sim 1 \text{ m/s} \), and the typical length scale is \( \sim 1 \text{ m} \) in the lab, then the Childress bound gives the lower bound on the dynamo effect to be \( (1 \text{ m}^2/\text{s})/\eta \sim O(1) \). Taking the magnetic permeability of free space \( \mu_0 = 1.257 \times 10^{-6} \text{ H/s} \), this requires the electrical conductivity to be \( \sim 10^6 \text{ S/m} \). Such a high conductivity limits the choice of conducting fluid and usually liquid metals or plasma are used. There are three working dynamos generated by liquid sodium, the experimental apparatuses are shown in Figures 1.4-1.6:

1. Riga dynamo
   A cylindrical dynamo experiment with a restricted spiral flow field [Gailitis et al., 2000]. The flow profile has been optimized by Stefani et al. [1999].

---

4. We note however in a full sphere an internal heat source is required.
Figure 1.4. Riga dynamo experiment. Left picture shows the dominant flow profile, right picture shows main components of the cylindrical apparatus [Gailitis et al., 2000].

2. Karlsruhe dynamo
A cylindrical tank with duct pipes to mimic convection rolls, also has a restricted flow field [Muller & Stieglitz, 1999].

Figure 1.5. Karlsruhe dynamo experiment. The size of the tank and direction of the flow are shown here [Muller & Stieglitz, 1999].

3. VKS dynamo
A cylindrical dynamo experiment with two impellers rotating in opposite directions, has an unrestricted highly turbulent flow field [Monchaux et al., 2007]. VKS needs both a soft-iron blade and a lid on the propellers to get a dynamo. From material selection to flow profile optimization, there are several optimization studies for VKS, e.g. Faranda et al. [2014]; Marie et al. [2003]; Ravelet et al. [2005].

There are also three spherical dynamo experiments that use a conducting fluid, the experimental apparatuses are shown in Figures 1.7-1.9:

1. Maryland 3 m
A 3-meter-diameter spherical shell filled with liquid sodium. The differential
rotation at the inner sphere and outer sphere stirs the fluid [Zimmerman et al., 2014].

   A spherical tank with two counter rotating propellers in the middle [Nornberg et al., 2006].
3. Madison plasma experiment
   A plasma filled spherical tank controlled by strong magnets at the boundary
Figure 1.8. Madison sodium experiment. A spherical tank with two counter rotating propellers inside. This figure shows the apparatus as seen from outside with connecting pipes and motor.

[Cooper et al., 2014].

Figure 1.9. Madison plasma experiment. Strong magnets installed at the boundary of a sphere stirs the plasma filled inside. The spherical tank is shown here.

Just as the other dynamo experiments, for each member of this group of spherical experiments there exists a series of associated studies aimed at improving the design to create a dynamo. One example is the flow profile study by Khalzov et al. [2012]. They use an axisymmetric dynamical MHD model to study what is the optimal driving boundary velocity. They compared three profiles of boundary flows, shown in Figure 1.10. Only profile III results in dynamo action. Identifying the optimal flow field is an important step towards better understanding the dynamo action. We list in Table 1.2 the order of magnitude of $Rm$ in these six dynamo experiments. Although the reported value of $Rm$ uses different conventions of velocity scale $u^*$ and length scale $L$, the range of $Rm$ stays approximately at $10 \sim 10^2$. It is difficult to increase $Rm$ further as the power consumption to drive the fluid is huge. This technical bottleneck raises interesting questions concerning dynamos in the low $Rm$ range. Also from a theoretical point of view, finding dynamo solutions with a low critical magnetic Reynolds number $Rm_c$ is an interesting, and at times challenging, mathematical problem.
Figure 1.10. Three driving boundary flow profiles in polar angle studied for the Madison plasma dynamo experiment [Khalzov et al., 2012].

<table>
<thead>
<tr>
<th></th>
<th>$Rm$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Riga</td>
<td>$\sim 20$</td>
</tr>
<tr>
<td>Karlsruhe</td>
<td>$\sim 3$</td>
</tr>
<tr>
<td>VKS</td>
<td>$\sim 30$</td>
</tr>
<tr>
<td>Madison sodium</td>
<td>$&lt; 180$</td>
</tr>
<tr>
<td>Madison plasma</td>
<td>$\sim 300$</td>
</tr>
<tr>
<td>Maryland (3m)</td>
<td>up to 715</td>
</tr>
</tbody>
</table>

Table 1.2. Comparison of magnetic Reynolds numbers in dynamo experiments. The first three experiments have confirmed dynamo effects. Note these are the originally reported values each using their own velocity scale $u^*$ and length scale $L$. Due to differences in the experimental setup, it may be difficult to find a standard formula that fits all experiments.

In the literature, numerical models with a low critical magnetic Reynolds number already exist. Taking one step further, we ask: are these existing models the most efficient set-ups, i.e. can we find a solution with the lowest possible $Rm_c$ for the onset of a dynamo? Experiments alone cannot answer this question, and neither can specific MHD models nor existing theoretical bounds. We need optimizations for a general type of dynamo solutions. In the next chapter, we will discuss known dynamos and their optimizations in two commonly used domains: a cube and a sphere.
Chapter 2

Dynamos and optimizations

In this chapter, we review some selected dynamos solutions and their optimizations. Some of the known dynamos represent examples from a specific class of solutions, and we will use them later in Chapter 4 and 5 for comparison of dynamos. We choose to study dynamo models in a cube due to their simple geometry and a sphere due to their relevance in the geophysical and astrophysical applications.

2.1 Optimizations in a cube

In this section, we review existing optimizations of kinematic dynamo models in Cartesian coordinates. Usually the geometry of the fluid domain is a cube for simplicity. Optimizations of both a specific type of solutions and a general type of solutions will be discussed.

2.1.1 Optimization of ABC type

ABC flows are named after three authors: Arnold, Beltrami and Childress [Arnold & Korkina, 1983; Childress, 1969]. The flow field is prescribed in a $2\pi$ periodic domain and has the form:

$$u(x, y, z) = (B \cos y + C \sin z, A \sin x + C \cos z, A \cos x + B \sin y), \quad (2.1)$$

where $A, B, C$ are constants. They have a special Beltrami property such that

$$\nabla \times u = u. \quad (2.2)$$

ABC flows represent a family of dynamo solutions. Different values of $A, B, C$ correspond to different $Rm_c$. A well-known case is when $A = B = C = 1$, the reported critical magnetic Reynolds number is $Rm_c \approx 8.93$ [Arnold & Korkina, 1983] and the rms speed is $U = \sqrt{3}$. If $u$ is rescaled to have unit rms speed and the typical length scale is the side length of the periodic cube, the critical value for the kinetic norm based magnetic Reynolds number becomes $Rm_u \approx 15L^*$ where $L^* = 2\pi$ is the periodicity. The Roberts flow is a special case of ABC flows with $A = B = 1, C = 0$:

$$u(x, y, z) = (\cos y, \sin x, \cos x + \sin y). \quad (2.3)$$
The critical value for the onset of a dynamo is $Rm_u = 8.79 L^*$ [Willis, 2012]. A parameter study by Alexakis [2011] found the Roberts flow and its permutations have the lowest critical $Rm_u$ among all ABC flows.

Another parameter study of ABC type includes the ABC forcing in an MHD model [Sadek et al., 2016]. The time variation of the flow field in the NS equation is determined by advection, pressure gradient, diffusion and a forcing term $f$,

$$f = \begin{bmatrix}
A \sin(k_f z) + C \cos(k_f y) \\
B \sin(k_f x) + A \cos(k_f z) \\
C \sin(k_f y) + B \cos(k_f x)
\end{bmatrix},$$

with $A = B = C = 1$, and $k_f$ is the dimensional forcing wavenumber. The authors found $k_f \approx 4/L$ gives the lowest critical $Rm_u$, where $L$ is the dimensional side length. These two studies identify the optimal solution within a specific class (ABC type) using a grid search method. The advantage of this approach is that it covers all parameters on the grid; the disadvantages is that when the parameter space becomes large, it is not feasible to compute all models. To optimize general dynamo solutions, we need other methods.

### 2.1.2 Large scale optimizations

For a general class of periodic solutions, Willis [2012] (henceforth called W12) has found the optimal dynamo in a cube generated by steady flows. This study uses a variational method that is applicable to large scale optimization problems, i.e. the ones that cannot be solved using a grid search method. The optimal dynamo has critical $Rm_u \approx 1.737 L^*$ and $Rm_\omega \approx 2.48(L^*)^2$ with normalized rms speed and root mean enstrophy respectively, where $L^* = 2\pi$ is the periodicity. Figure 2.1 shows the results of optimization as a function of iterations at $Rm_u = L^*$, and the inset shows result from perturbation study at the critical $Rm_u = 1.737 L^*$. The optimal solution is robust against perturbation and converges to the same optimum with different random initial conditions. W12 also optimized the transient growth using steady flows in a short $T = 0.05$ convection time window. The lower bound for any positive growth in magnetic energy is $Rm_\omega = 2.12(L^*)^2$. Recall from §1.2.3 that some flows may not support long term dynamo solutions but can create short term transient growth. The ultimate lower bound $Rm_t$ eliminates any solution with a lower critical $Rm$ for the onset of dynamo.

### 2.1.3 Outlook

Inspired by W12, the same method can be used to search for the most efficient dynamo solutions with different boundary conditions and geometry. The question we asked, namely “what is the most efficient dynamo?”, can thereby be answered using the mathematical framework of W12. In chapter 3, we will review the variational method of W12 in detail, which provides the starting point for our subsequent analyses. Another related question, namely “what is the lower bound of $Rm$ below which all dynamos will fail?”, can also be tackled following the transient growth study of W12. One thing to keep in mind though is that the
optimal transient solution is not equivalent to a kinematic dynamo solution at $Rm_t$. This can be easily verified by extending the time window $T$. In W12, at the same $Rm_t$, the optimal transient solution produces a magnetic field that decays faster as $t \to \infty$ than that produced by the optimal kinematic dynamo solution, so it cannot be optimal in the long term.

2.2 Optimizations in a sphere

Planetary and stellar dynamos occur in a spherical geometry. We want to better understand how dynamos operate in spherical coordinates. In this chapter, we review some well-known spherical dynamo solutions and existing small scale optimizations.

2.2.1 The KR and DJ types

In this section, we review two well known classes of dynamo solutions in a sphere and their optimization studies. There was no known optimization for a general type of spherical dynamos before our project started. There were, however, small scale optimizations within specific classes of dynamo solutions, as well as transient growth optimizations for selected flows. We use these results as a reference for our optimal model. We list eight dynamo solutions here and present their spatial structures. The flow field has the form

$$\mathbf{u} = \sum_{l,m} t_l^m + s_l^m$$

(2.5)
in a poloidal-toroidal decomposition, where the toroidal field component $t$ and poloidal field component $s$ are given by

$$t_{l}^{m(s,c)} = \nabla \times \left[ t_{l}^{m(s,c)}(r) P_{l}^{m}(\cos \theta) \{ \sin, \cos \}(m\phi) \hat{\mathbf{r}} \right],$$

$$s_{l}^{m(s,c)} = \nabla \times \nabla \times \left[ s_{l}^{m(s,c)}(r) P_{l}^{m}(\cos \theta) \{ \sin, \cos \}(m\phi) \hat{\mathbf{r}} \right],$$

and $P_{l}^{m}$ are the Schmidt quasi-normalized associated Legendre functions, $l$ is spherical harmonic degree, $m$ is spherical harmonic order. The magnetic field always satisfies insulating boundary conditions.

2.2.1.1 KR flow

Kumar & Roberts [1975] found a dynamo solution with a critical $Rm_u \approx 900$ generated by a flow field that contains both azimuthal differential rotation and meridional circulation, two effects thought to be present in dynamos in nature. The radial profile of the flow is given by

$$t_{0}^{1}(r) = K r^{2}(1 - r^{2}),$$

$$s_{0}^{2}(r) = K \epsilon_{1} r^{6}(1 - r^{2})^{3},$$

$$s_{2}^{2}(r) = K \epsilon_{2} r^{4}(1 - r^{2})^{2} \cos(3\pi r),$$

$$s_{2}^{2c}(r) = K \epsilon_{3} r^{4}(1 - r^{2})^{2} \sin(3\pi r),$$

(2.7)

$\epsilon_{1} = 0.03, \epsilon_{2} = \epsilon_{3} = 0.04$, and $K = 4.40$ is a normalization factor that has been used later in Love & Gubbins [1996b] to get rms speed $U = 1$. The spatial profile of differential rotation given by $t_{0}^{1}$ and the spatial profile of meridional circulation given by $s_{0}^{2}$ are simple, but it is not always clear how the flow field looks like when we combine all four components. So we plot the kinetic energy $u^{2}$ isocontours in Figure 2.2 a) b), which allows us to see immediately in which regions the fluid moves faster. We also plot the local maximum strain rate, i.e. the maximum eigenvalue of the strain rate tensor at a given location, in Figure 2.2 c) d). This shows how the shear in the flow is distributed; the spiral pattern caused by differential rotation is evident.

Figure 2.2. KR flow [Kumar & Roberts, 1975]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isocontours in the meridional plane at $\phi = 0$. c) Maximum strain rate isocontours the in the equatorial plane. d) Maximum strain rate isosurfaces in 3D.
2.2.1.2 GKR flow

The KR flow was developed later into a family of flows with variable coefficients $\epsilon_0, \epsilon_1, \epsilon_2, \epsilon_3$. One of the generalized dynamo solutions is given by Gubbins et al. [2000a] (GKR) and verified by Li et al. [2010]. The critical value is $Rm_u \approx 131$. The flow field has the form

\begin{align}
    t_1^0(r) &= \epsilon_0 \, r^2(1 - r^2), \\
    s_2^0(r) &= \epsilon_1 \, r^6(1 - r^2)^3, \\
    s_2^c(r) &= \epsilon_2 \, r^4(1 - r^2)^2 \sin(3\pi r), \\
    s_2^s(r) &= \epsilon_3 \, r^4(1 - r^2)^2 \cos(3\pi r),
\end{align}

where $\epsilon_0 = \sqrt{315/32}$, $\epsilon_1 = -4.6325$, $\epsilon_2 = \epsilon_3 = 1.41446$. The spatial properties are shown in Figure 2.3. Compared to the KR flow in Figure 2.2, the GKR flow is much more concentrated in small regions.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{gkr_flow.png}
\caption{GKR flow [Gubbins et al., 2000a]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isosurfaces the meridional plane at $\phi = 0$. c) Maximum strain rate isocontours in the equatorial plane. d) Maximum strain rate isosurfaces in 3D.}
\end{figure}

2.2.1.3 STW flow

This is a dynamo solution that satisfies the so-called thermal wind equation, see Sarson [2003] for details. The critical value is $Rm_u = 479$. The flow field has the form

\begin{align}
    t_1^0(r) &= K \, r^2(1 - r^2), \\
    s_2^s(r) &= K \, \epsilon_2 \, r^4(1 - r^2)^2 \cos(3\pi r), \\
    s_2^c(r) &= K \, \epsilon_3 \, r^4(1 - r^2)^2 \sin(3\pi r), \\
    t_3^2(r) &= - K \, \epsilon_3 \, \frac{4}{\sqrt{5}} \left( \frac{\partial}{\partial r} - \frac{3}{r} \right) r^4(1 - r^2)^2 \sin(3\pi r), \\
    t_3^c(r) &= K \, \epsilon_2 \, \frac{4}{\sqrt{5}} \left( \frac{\partial}{\partial r} - \frac{3}{r} \right) r^4(1 - r^2)^2 \cos(3\pi r),
\end{align}

where $\epsilon_2 = 0.04$ and $\epsilon_3 = -0.04$. Here $K = 4.2449$ is a normalization factor chosen so the rms speed of the non-dimensionalized flow is 1. The kinetic energy and maximum strain rate are shown in Figure 2.4.

We see again the prominent differential rotation component. The level of flow concentration (the contrast between high and low speed regions) is in between KR
and GKR flow. Coincidentally, the critical magnetic Reynolds number for STW flow also lies in between that of KR and GKR flow. However, in order to identify the lowest \( Rm_c \) among KR flows, we need a more systematic approach.

2.2.1.4 Parameter study of KR flows

There are a series of papers dedicated to the optimization of KR flows [Gubbins et al., 2000a,b; Love & Gubbins, 1996a]. The lowest critical value from a complete parameter space study by Gubbins et al. [2000a] is \( Rm_u \approx 44 \), which is given by a poloidal only flow field that was also discussed by Holme [1997]; Love & Gubbins [1996b]. The phase space of KR flows shows several dynamo regions as isolated islands, see Figure 2.5.

![Figure 2.4. STW flow [Sarson, 2003]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isocontours in the meridional plane at \( \phi = 0 \). c) Maximum strain rate in the equatorial plane. d) Maximum strain rate in isosurfaces in 3D](image)

![Figure 2.5. Map of critical magnetic Reynolds number \( Rm_u \) for KR type of flows [Gubbins et al., 2000b]. The rms speed is always normalized to 1. \( M \) stands for meridional circulation, \( D \) stands for differential rotation, letters from A to G indicate dynamo regions.](image)
They blend smoothly into non-dynamo solutions. There is no obvious pattern in these solutions. An earlier study used a variational method to optimize KR flows [Love & Gubbins, 1996a]. The result improved the original KR model but was not converged to the optimum. It could be that the program prematurely converged to a local optimum.

2.2.1.5 DJ flows

The original DJ flows are three axisymmetric flows found by Dudley & James [1989], each is named after their corresponding spherical harmonic modes. They are given by

\[
\begin{align*}
\text{DJ } t_1 s_1 & : t_1^0(r) = r \sin(\pi r), \quad s_1^0(r) = 0.17 \ r \sin(\pi r), \quad (2.10) \\
\text{DJ } t_1 s_2 & : t_1^0(r) = r \sin(\pi r), \quad s_2^0(r) = 0.13 \ r^2 \sin(\pi r), \quad (2.11) \\
\text{DJ } t_2 s_2 & : t_2^0(r) = r^2 \sin(\pi r), \quad s_2^0(r) = 0.14 \ r^2 \sin(\pi r). \quad (2.12)
\end{align*}
\]

With these examples the authors have shown that simple flows are capable of generating dynamos. The reported critical values are \( t_1 s_1 \) flow: \( Rm_c \approx 55 \), \( t_1 s_2 \) flow: \( Rm_c \approx 155 \), \( t_2 s_2 \) flow: \( Rm_c \approx 54 \). Note here the values of \( Rm \) are not equivalent to the kinetic energy based \( Rm_u \) due to unnormalized rms speed. The kinetic energy distribution is dictated by spherical harmonic degree \( l \). The spatial properties of \( t_1 s_1 \) flow, \( t_1 s_2 \) flow, \( t_2 s_2 \) flow are shown in Figure 2.6, Figure 2.7 and Figure 2.8 respectively. Interestingly, even simple axisymmetric flows can have

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{DJ_t1s1.png}
\caption{DJ \( t_1 s_1 \) flow [Dudley & James, 1989]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isocontours in the meridional plane at \( \phi = 0 \). c) Maximum strain rate in the equatorial plane. d) Maximum strain rate in the meridional plane at \( \phi = 0 \).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{DJ_t1s2.png}
\caption{DJ \( t_1 s_2 \) flow [Dudley & James, 1989]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isocontours in the meridional plane at \( \phi = 0 \). c) Maximum strain rate in the equatorial plane. d) Maximum strain rate in the meridional plane at \( \phi = 0 \).}
\end{figure}
asymmetric properties. The DJ \( t_2 s_2 \) flow has an asymmetry the other two DJ flows do not have: the absolute value of local min strain rate over all angles \( \theta, \phi \) as a function of radius \( r \) exceeds that of local maximum strain rate for \( 0.5 \leq r \leq 1 \), see Figure 2.9.

![Figure 2.8](image1.png)

**Figure 2.8.** DJ \( t_2 s_2 \) flow [Dudley & James, 1989]. a) Kinetic energy isocontours in the equatorial plane. b) Kinetic energy isocontours in the meridional plane at \( \phi = 0 \). c) Maximum strain rate in the equatorial plane. d) Maximum strain rate in the meridional plane at \( \phi = 0 \).

![Figure 2.9](image2.png)

**Figure 2.9.** Absolute value of local max and local min strain rate for DJ \( t_2 s_2 \) flow [Dudley & James, 1989] over all angles \( \theta, \phi \) as a function of radius.

### 2.2.1.6 MDJ flows

A modified Dudley James flow which satisfies the no-slip boundary conditions is discussed by Holme [1997]; Livermore & Jackson [2004] and verified by Li \textit{et al.} [2010]. The flow field is given by

\[
t_1^0(r) = Kr^2(1 - r^2), \quad s_2^0(r) = K0.19 r^3(1 - r^2)^2,
\]

where \( K = 3.96155 \) to the make rms speed \( U = 1 \). The critical \( Rm_u = 55 \) and the spatial properties are shown in Figure 2.10. The spatial profile of MDJ \( t_1 s_2 \) is quite similar to DJ \( t_1 s_2 \). The main difference is in the boundary conditions, as seen by comparing Figure 2.10 b) and Figure 2.7 b). The MDJ \( s_2 \) is another variation of DJ type, given by

\[
s_2^0(r) = Kr^3(1 - r^2)^2,
\]

where \( K = 3.96155 \) to the make rms speed \( U = 1 \). The critical \( Rm_u = 55 \) and the spatial properties are shown in Figure 2.10. The spatial profile of MDJ \( t_1 s_2 \) is quite similar to DJ \( t_1 s_2 \). The main difference is in the boundary conditions, as seen by comparing Figure 2.10 b) and Figure 2.7 b). The MDJ \( s_2 \) is another variation of DJ type, given by

\[
s_2^0(r) = Kr^3(1 - r^2)^2,
\]
where $K = \sqrt{\frac{115}{16}}$. It is not a confirmed dynamo solution, but it promotes strong transient growth [Livermore & Jackson, 2004]. So we also show its spatial properties here in Figure 2.11. Even though the kinetic energy distribution just shows two convection rolls in Figure 2.11 b), the maximum strain rate shows more complex spatial variations in Figure 2.11 d).

2.2.1.7 Optimizing DJ flows

Holme [2003] optimized the three DJ flows using the absolute maximum strain rate based magnetic Reynolds number $Rm_s$. The spatial distributions of DJ flow field is adjusted using spline functions. This is the only known optimization of kinematic dynamos that lowers the absolute maximum strain rate. The lowest critical value is $Rm_s = 108$ for DJ $t_2 s_2$ type flow with free-slip boundary conditions, which improved the original critical value $Rm_s = 152$ for DJ $t_2 s_2$ flow by a third.

2.2.2 Optimal transient growth for selected flows

Livermore & Jackson [2004, 2006] studied the magnetic energy instability in a sphere for several prescribed steady flows. The magnetic instability is a necessary but not sufficient condition for the dynamo action. Over all eigenmodes for the magnetic field, the authors optimize the instantaneous magnetic energy growth
rate,

$$\max \frac{dM}{dt} = \max \langle (L^\dagger + L)B_0, B_0 \rangle$$

(2.15)

where $B_0 = B(x,0)$ is the initial magnetic field, $M = \langle B^2 \rangle / 2$ is the magnetic energy, $L$ is the induction operator:

$$\frac{\partial B}{\partial t} = L \cdot B$$

(2.16)

that replaces the right-hand side of the induction equation (5.4), and $L^\dagger$ is the adjoint induction operator. Recall from §1.2.3, there is a critical transient magnetic Reynolds number $Rm_t$ at which the magnetic instability can occur, i.e. above which positive transient growth is possible. The lowest value among the models studied is $Rm_s = 61.2$ for an equatorially symmetric MDJ $s_2$ flow. The associated most unstable eigenmode is axisymmetric and equatorially anti-symmetric ($E^A$) for the magnetic field.
Chapter 3

Methods

In this chapter we introduce the variational method based on Willis [2012], and the numerical methods needed for dynamo modelling. The variational principle behind it forms the foundation of our approach to dynamo optimizations. Note that in this chapter we work with time non-dimensionalized by the advective time scale.

3.1 The variational method

3.1.1 The Lagrangian formulation

The variational method is an optimization method based on a variational principle. An overall measure of a system at a given point in its phase space is given by the Lagrangian. Such a Lagrangian consists of an objective minus/plus one or more constraints that each is multiplied by a Lagrange multiplier. The sign is determined as to cause penalties in the system. In other words, violating constraints will move the solution away from the extremum we want to achieve. The maximal/minimal solution lies where all variational derivatives with respect the Lagrangian vanish. This is analogous to searching for the maximum or minimum of a function: at the extremal point, the gradient is zero.

3.1.1.1 A toy problem

Let us start with a simple example: we want to find the maximum of an objective function \( f(x, y) = 2x - y^2 \) subject to the constraint \( x + y = 4 \) for any \( x, y \in \mathbb{R} \). This constraint means the value of \((x, y)\) has to lie on a straight line that passes through \((0, 4)\) and \((4, 0)\). The isocontours of allowed \( f(x, y) \) have to intersect the constraint line, see Figure 3.1. We can write down a Lagrangian:

\[
L(x, y, \lambda) = 2x - y^2 - \lambda(x + y - 4), \tag{3.1}
\]

\( \lambda \) is a Lagrange multiplier. The Lagrange multiplier has no physical meaning, it is a strategy used in constrained optimizations. We want to find a set of solutions such that the total derivative of the Lagrangian vanishes, i.e.

\[
dL = 0 \tag{3.2}
\]
Figure 3.1. An illustration of the objective function and the constraint. The constraint \(x + y = 4\) limits the values of \((x, y)\) to a straight line. Three examples of isocontours of \(f(x, y)\) show that as the value of \(f(x, y)\) increases, it will violate the constraint so there will be no common points with the line \(x + y = 4\). We want to find the maximum value of \(f(x, y)\) that still intersects the constraint line.

with
\[
dL = \frac{\partial L}{\partial x} dx + \frac{\partial L}{\partial y} dy + \frac{\partial L}{\partial \lambda} d\lambda. \tag{3.3}
\]

We find the partial derivative with respect to each variable as:

\[
\frac{\partial L}{\partial x} = 2 - \lambda, \tag{3.4}
\]

\[
\frac{\partial L}{\partial y} = -2y - \lambda, \tag{3.5}
\]

\[
\frac{\partial L}{\partial \lambda} = -x - y + 4. \tag{3.6}
\]

One derivative can be directly set to zero,

\[
x + y = 4. \tag{3.7}
\]

This equation is the constraint we initially imposed. To illustrate our method we will not set the other two derivatives immediately to zero but use an iterative approach to arrive at

\[
\frac{\partial L}{\partial x} \rightarrow 0, \quad \frac{\partial L}{\partial y} \rightarrow 0. \tag{3.8}
\]

We start with any solution \(x, y\) (could be random) satisfying the constraint (3.7). We use the steepest ascent (to reach the maximum) method to update \(x, y\) iteratively:

\[
x := x + \Delta_1 \frac{\partial L}{\partial x} = x + \Delta_1 (2 - \lambda),
\]

\[
y := y + \Delta_2 \frac{\partial L}{\partial y} = y + \Delta_2 (-2y - \lambda). \tag{3.9}
\]
Let us fix the step size $\Delta_1 = \Delta_2 = 1$. $\lambda$ is solved such that the updated $x$ and $y$ still satisfy (3.7), which gives

$$\lambda = \frac{x - y - \frac{2}{2}}{2}. \quad (3.10)$$

We can track the convergence process by following a measure called the **residue**. It is usually a weighted average of gradient magnitudes. In this case, let us use

$$r_{tot} = \sqrt{\left(\frac{\partial L}{\partial x}\right)^2 + \left(\frac{\partial L}{\partial y}\right)^2}. \quad (3.11)$$

The optimization process is stopped when $r_{tot}$ is below a small cut-off number.

— iteration 1

Suppose we start from an initial point $(x, y) = (3, 1)$, we get $\lambda = 0$, and then $\left(\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}\right) = (2, -2)$ by substitute the value of $\lambda$ back into (3.4)-(3.5). This gives a residue $r_{tot} = 2\sqrt{2}$, the result is not converged. We update the value of $(x, y)$ using (3.9), this gives us $(x, y) = (5, -1)$.

— iteration 2

The new initial point in iteration 2 is $(x, y) = (5, -1)$, we get $\lambda = 2$, then find that $\left(\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}\right) = (0, 0)$ and $r_{tot} = 0$. The result is converged. This would give the maximal solution of $f(x, y) = 24$.

We can verify this solution using conventional methods. Substituting $x = 4 - y$ into $f(x, y)$, we get the reduced function $f(y) = 2(4 - y) - y^2$ with a maximum given by solving $df(y)/dy = 0$, resulting again in $(x, y) = (5, -1)$.

### 3.1.1.2 The analysis of W12

Let us return to the kinematic dynamo model. The flow fields and magnetic fields are represented by elements in a vector space of functions. We need to extend the variational principle from a 2D real domain to a vector space. Each variable now is an element in the vector space of functions, and the objective is now a **functional** – a map from functions to numbers. The constraints are also more complex. Besides normalization constraints, they also include the three equations from a kinematic dynamo model. The flow field $\mathbf{u}(\mathbf{x})$ is taken to be steady and we trace the time evolution of magnetic field $\mathbf{B}(\mathbf{x}, t)$ to search for the best initial conditions that can maximize the magnetic energy growth. In W12, the flow field $\mathbf{u}$ lives in a vector space $\mathcal{E}_U$ that satisfies

$$\nabla \cdot \mathbf{u} = 0, \quad \mathbf{x} \in V, \quad (3.12)$$

and satisfies the periodic boundary conditions in a cube,

$$\mathbf{u}|_{x=0} = \mathbf{u}|_{x=2\pi},$$
$$\mathbf{u}|_{y=0} = \mathbf{u}|_{y=2\pi},$$
$$\mathbf{u}|_{z=0} = \mathbf{u}|_{z=2\pi}. \quad (3.13)$$
The magnetic field $B \in \mathcal{E}_B$ satisfies
\[ \nabla \cdot B = 0, \quad x \in V, \quad (3.14) \]
and also has the periodic boundary conditions
\[
\begin{align*}
B|_{x=0} &= B|_{x=2\pi}, \\
B|_{y=0} &= B|_{y=2\pi}, \\
B|_{z=0} &= B|_{z=2\pi}.
\end{align*}
\quad (3.15)
\]
The initial conditions $u$ and $B_0$, are always normalized so subsequent updates only change the spatial distributions of fields. The scale of magnetic field is arbitrary in a kinematic dynamo model, usually $\langle B_0^2 \rangle = 1$ for simplicity. In W12, two normalization schemes for the flow field are used: unit kinetic norm and unit enstrophy norm. The kinetic norm normalized flow field has unrestricted shear; the optimization fails for $Rm_u > 2L^*$, where $L^* = 2\pi$ is the periodicity. Later Proctor [2015] proved the kinetic norm based $Rm_u$ has no lower bound precisely due to unlimited shear. In the following sections, we will discuss the Lagrangian formulation with unit enstrophy norm. In this case, the global shear equals to the root mean enstrophy $S = \omega^*$ due to periodic boundary conditions. The Lagrangian $\mathcal{L}$ is
\[
\mathcal{L} = \langle B_T^2 \rangle - \lambda_1 \left( \langle (\nabla \times u)^2 \rangle - 1 \right) - \lambda_2 \left( \langle B_0^2 \rangle - 1 \right) - \langle \Pi_1 \nabla \cdot u \rangle - \langle \Pi_2 \nabla \cdot B_0 \rangle - \int_0^T \left\langle B_{\hat{T}} \cdot \left[ \frac{\partial B}{\partial t} - \nabla \times (u \times B) - \frac{1}{Rm} \nabla^2 B \right] \right\rangle dt \quad (3.16)
\]
The first term is the objective functional to be maximized: the magnetic norm at time $T$. The second and the third term impose the normalization constraints. The fourth term and fifth term impose solenoidal conditions, and the last term imposes the induction equation as a constraint; $\lambda_1$, $\lambda_2$, $\Pi_1(x)$, $\Pi_2(x)$ and $B_{\hat{T}}(x,t)$ are all Lagrange multipliers. Here the magnetic Reynolds number $Rm$ is related to the enstrophy norm based $Rm_\omega$ as
\[
Rm(L^*)^2 = Rm_\omega, \quad (3.17)
\]
in a fluid domain with periodicity $L^*$. We want to find a solution such that the objective is maximized while all the constraints are satisfied. This implies all the variational derivatives with respect to the Lagrangian vanish at the maximum. Therefore, the next step is to derive these variational derivatives. A small variation in the Lagrangian is a sum of variations from each variable:
\[
\delta \mathcal{L} = \frac{\delta \mathcal{L}}{\delta \lambda_1} \delta \lambda_1 + \frac{\delta \mathcal{L}}{\delta \lambda_2} \delta \lambda_2 + \left\langle \frac{\delta \mathcal{L}}{\delta \Pi_1} \delta \Pi_1 \right\rangle + \left\langle \frac{\delta \mathcal{L}}{\delta \Pi_2} \delta \Pi_2 \right\rangle + \left\langle \frac{\delta \mathcal{L}}{\delta u} \delta u \right\rangle + \left\langle \frac{\delta \mathcal{L}}{\delta B_0} \delta B_0 \right\rangle + \left\langle \frac{\delta \mathcal{L}}{\delta B_T} \delta B_T \right\rangle + \int_0^T \left\langle \frac{\delta \mathcal{L}}{\delta B} \delta B \right\rangle dt + \int_0^T \left\langle \frac{\delta \mathcal{L}}{\delta B_{\hat{T}}} \delta B_{\hat{T}} \right\rangle dt \quad (3.18)
\]
The general definition of a functional derivative is

\[
\frac{\delta F[f(x)\big]}{\delta f(x)} = \lim_{\epsilon \to 0} \frac{F[f(x) + \epsilon \delta f(x)] - F[f(x)]}{\epsilon}.
\]  

(3.19)

In this case, the list of all variational derivatives is

\[
\begin{align*}
\frac{\delta L}{\delta \lambda_1} &= -\langle (\nabla \times u)^2 \rangle + 1 \\
\frac{\delta L}{\delta \lambda_2} &= -\langle B_0^2 \rangle + 1 \\
\frac{\delta L}{\delta \Pi_1} &= -\nabla \cdot u \\
\frac{\delta L}{\delta \Pi_2} &= -\nabla \cdot B_0 \\
\frac{\delta L}{\delta B_T} &= \frac{\partial B}{\partial t} - \nabla \times (u \times B) - \frac{1}{Rm} \nabla^2 B \\
\frac{\delta L}{\delta B_0} &= \int_0^T B \times (\nabla \times B) \, dt - 2\lambda_1 \nabla \times \nabla \times u + \nabla \Pi_1 \\
\frac{\delta L}{\delta B_T} &= B_T^\dagger - 2\lambda_2 B_0 + \nabla \Pi_2 \\
\frac{\delta L}{\delta B} &= \frac{\partial B}{\partial t} + (\nabla \times B) \times u + \frac{1}{Rm} \nabla^2 B \\
\end{align*}
\]  

(3.20-3.28)

3.1.2 Boundary terms

When we calculate variational derivatives, we may get boundary terms after integration by parts. For example, when we evaluate the variation of the velocity field \(\delta u\), we need to isolate \(\delta u\). This gives three boundary terms. Part of the variation in \(\delta u\) is related to the solenoidal constraint,

\[
\langle \Pi_1 \nabla \cdot \delta u \rangle = \frac{1}{V} \int \nabla \cdot (\Pi_1 \delta u) \, dV - \frac{1}{V} \int_v \nabla \Pi_1 \cdot \delta u \, dV
\]

\[
= \frac{1}{V} \int_{\Sigma} (\Pi_1 \delta u) \cdot dS - \langle \nabla \Pi_1 \cdot \delta u \rangle.
\]  

(3.29)

The first term in the last line is a boundary term. Another part of the variation in \(\delta u\) that comes from the normalization condition is:

\[
\langle (\nabla \times u) \cdot (\nabla \times \delta u) \rangle = \langle \nabla \cdot (\delta u \times (\nabla \times u)) \rangle + \delta u \cdot (\nabla \times \nabla \times u)
\]

\[
= \frac{1}{V} \int_{\Sigma} \delta u \times (\nabla \times u) \cdot dS + \langle \delta u \cdot (\nabla \times \nabla \times u) \rangle
\]

(3.30)
which gives the second boundary term. For the variation in \(\delta u\) related to the magnetic induction term we have:

\[
\langle B^\dagger \cdot \nabla \times (\delta u \times B) \rangle = \langle \nabla \cdot ((\delta u \times B) \times B^\dagger) \rangle + \langle (\delta u \times B) \cdot \nabla \times B^\dagger \rangle
\]

\[
= \frac{1}{V} \int_{\Sigma} [(\delta u \times B) \times B^\dagger] \cdot dS + \langle (\delta u \times B) \cdot \nabla \times B^\dagger \rangle
\]

(3.31)

Using the vector identity:

\[
\langle (u \times B) \cdot \nabla \times B^\dagger \rangle = \langle u \cdot (B \times (\nabla \times B^\dagger)) \rangle = \langle B \cdot ((\nabla \times B^\dagger) \times u) \rangle
\]

(3.32)

we get variations

\[
\langle B^\dagger \cdot \nabla \times (\delta u \times B) \rangle = \frac{1}{V} \int_{\Sigma} [(\delta u \times B) \times B^\dagger] \cdot dS + \langle \delta u \cdot (B \times (\nabla \times B^\dagger)) \rangle
\]

(3.33)

This gives the third and last boundary term related to \(\delta u\). For the variation of \(B\) in the magnetic induction term,

\[
\langle B^\dagger \cdot \nabla \times (u \times \delta B) \rangle = \frac{1}{V} \int_{\Sigma} [(u \times \delta B) \times B^\dagger] \cdot dS + \langle \delta B \cdot ((\nabla \times B^\dagger) \times u) \rangle
\]

(3.34)

and we can again isolate \(\delta B\) using (3.32). There are also variations from the magnetic diffusion term,

\[
\langle B^\dagger \cdot \frac{1}{Rm} \nabla^2 \delta B \rangle = \langle \delta B \cdot \frac{1}{Rm} (\nabla^2 B^\dagger - \nabla (\nabla \cdot B^\dagger)) \rangle + \left( \frac{1}{Rm} B^\dagger (\nabla \cdot B) \right)
\]

\[
+ \frac{1}{V} \int_{\Sigma} \frac{1}{Rm} [B^\dagger \times (\nabla \times \delta B) - \delta B \times (\nabla \times B^\dagger)] \cdot dS
\]

\[
= \langle \delta B \cdot \frac{1}{Rm} \nabla^2 B^\dagger \rangle + \frac{1}{V} \int_{\Sigma} \frac{1}{Rm} [B^\dagger \times (\nabla \times \delta B) - \delta B \times (\nabla \times B^\dagger)] \cdot dS,
\]

where we assumed that \(B^\dagger\) also satisfies the solenoidal condition

\[
\nabla \cdot B^\dagger = 0.
\]

(3.35)

Collecting all the boundary terms \(BT\) we get

\[
BT = -\frac{1}{V} \int_{\Sigma} \Pi_1 (n \cdot \delta u) dS - \frac{1}{V} \int_{\Sigma} 2\lambda_1 [(\delta u \times (\nabla \times u)] \cdot n dS
\]

\[
- \frac{1}{V} \int_{\Sigma} \Pi_2 (n \cdot \delta B_0) dS + \int_0^T \frac{1}{V} \int_{\Sigma} \left[ \frac{1}{Rm} (\nabla \times B^\dagger) \times \delta B \right] \cdot n dS dt
\]

\[
+ \int_0^T \frac{1}{V} \int_{\Sigma} \left[ B^\dagger \times (\frac{1}{Rm} \nabla \times \delta B - u \times \delta B - \delta u \times B) \right] \cdot n dS dt
\]

\[
= 0,
\]

(3.36)
where we used $dS = n\, dS$. All boundary terms sum to zero in a periodic box. In
general, we need to get $BT = 0$ for any stationary solution of a Lagrangian, so
the boundary conditions of the scalar fields and vector fields have to be defined in
a way such that the sum of all boundary terms vanish. In other words, we derive
the allowed boundary conditions by following the variational derivatives.

### 3.1.3 Euler-Lagrange equations

When the variational derivatives are zero, we get the corresponding Euler-
Lagrange (EL) equations. There are nine variational derivatives in total in $W12$.
Seven of the EL equations can be obtained immediately. Five of them are just the
constraints we want to impose initially. There are four time-independent condi-
tions:

$$
\langle (\nabla \times \mathbf{u})^2 \rangle = 1, \quad \langle \mathbf{B}_0^2 \rangle = 1, \quad \nabla \cdot \mathbf{u} = 0, \quad \nabla \cdot \mathbf{B}_0 = 0, \quad (3.37)
$$

plus one dynamical equation (the direct induction equation):

$$
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) - \frac{1}{Rm} \nabla^2 \mathbf{B} = 0. \quad (3.38)
$$

We get another EL equation that links $\mathbf{B}_T$ and $\mathbf{B}_T^\dagger$,

$$
2\mathbf{B}_T - \mathbf{B}_T^\dagger = 0. \quad (3.39)
$$

through integration by parts. This is because time derivative of $\mathbf{B}$ inside the time
integral in $\mathcal{L}$ is transferred to $\mathbf{B}_T^\dagger$ as

$$
\int_0^T \left\langle \mathbf{B}_T^\dagger \cdot \frac{\partial (\delta \mathbf{B})}{\partial t} \right\rangle \, dt = \left\langle \mathbf{B}_T^\dagger \cdot \delta \mathbf{B}_T - \mathbf{B}_0^\dagger \cdot \delta \mathbf{B}_0 \right\rangle - \int_0^T \left\langle \frac{\partial \mathbf{B}_T^\dagger}{\partial t} \cdot \delta \mathbf{B} \right\rangle \, dt. \quad (3.40)
$$

The second dynamical EL equation comes from the variational derivative with
respect to $\mathbf{B}$,

$$
\frac{\partial \mathbf{B}_T^\dagger}{\partial t} = \mathbf{u} \times (\nabla \times \mathbf{B}_T^\dagger) - \frac{1}{Rm} \nabla^2 \mathbf{B}_T^\dagger. \quad (3.41)
$$

This is referred to as the adjoint induction equation. The final two variational
derivatives need to approach zero iteratively in our method,

$$
\frac{\delta \mathcal{L}}{\delta \mathbf{u}} = \int_0^T \mathbf{B} \times (\nabla \times \mathbf{B}_T^\dagger) \, dt - 2\lambda_1 \nabla \times \nabla \times \mathbf{u} + \nabla \Pi_1 \rightarrow 0, \quad (3.42)
$$

$$
\frac{\delta \mathcal{L}}{\delta \mathbf{B}_0} = \mathbf{B}_0^\dagger - 2\lambda_2 \mathbf{B}_0 + \nabla \Pi_2 \rightarrow 0. \quad (3.43)
$$

When deriving the adjoint induction equation (3.41), we used the assumption in
(3.35) that $\mathbf{B}_T^\dagger$ is solenoidal. This constraint is in practice not enforced at every time
step, because the Lagrange multiplier $\Pi_2$ is used to project out the non-solenoidal
part in $\delta \mathcal{L}/\delta \mathbf{B}_0$. The value of $\Pi_2$ is obtained by solving a Poisson equation,

$$
\nabla^2 \Pi_2 = -\nabla \cdot \mathbf{B}_0^\dagger. \quad (3.44)
$$
3.2 Time stepping method

One could solve the direct/adjoint induction equations as an eigenvalue problem or using a time stepping method. The eigenvalue method can identify all the eigenvalues within a finite dimensional vector space, but it gets more difficult with large dimensions. For the rest of this thesis, we will use the time stepping methods described below.

The right-hand sides of the direct/adjoint induction equations have two terms: the non-linear direct/adjoint induction term \( I \) and the linear diffusion term \( D \). The precise form of \( I_i \) and \( D_i \) at time step \( i \) depend on the representation of the vector fields, for now we just use this abstract notation. We usually treat \( I \) and \( D \) differently so the resulting time step method is a combination of the two parts.

3.2.1 Second order Adams Bashforth method

We can use the second order Adam-Bashforth as follows. Ignoring the magnetic diffusion \( D \) for now, the first time step uses a first order Euler method,

\[
B_1 = B_0 + I_0 \Delta t.
\]  

(3.45)

Here \( \Delta t \) is the time step size. For the second time step and all timesteps afterwards, we use

\[
B_{i+1} = B_i + \left( \frac{3}{2} I_i - \frac{1}{2} I_{i-1} \right) \Delta t.
\]  

(3.46)

The diffusion term is solved using an implicit Crank-Nicolson method, which without the magnetic advection \( I \) gives

\[
\frac{B_{i+1} - B_i}{\Delta t} = \frac{1}{2} (D_{i+1} + D_i).
\]  

(3.47)

In the end, the combined time stepping scheme becomes

\[
\frac{B_1 - B_0}{\Delta t} = \frac{1}{2} (D_1 + D_0) + I_0,
\]  

(3.48)

\[
\frac{B_{i+1} - B_i}{\Delta t} = \frac{1}{2} (D_{i+1} + D_i) + \left( \frac{3}{2} I_i - \frac{1}{2} I_{i-1} \right), \quad i > 0.
\]  

(3.49)

The value of \( B_i \) at time step \( i \) is a solution of the equations above. The adjoint problem uses the same time stepping scheme with backward time integration from step \( i \) to \( i - 1 \).

3.2.2 Predictor-corrector method

Again let \( I \) denote the magnetic induction term and \( D \) denote the magnetic diffusion term. The induction equation (3.38) can be written as

\[
(\partial_t - D)B = I,
\]  

(3.50)
then we multiply both side by $e^{-Dt}$,

$$\partial_t (Be^{-Dt}) = I e^{-Dt}, \quad (3.51)$$

so the diffusion term is solved using an integrating factor. Let us define a new variable $A_i = B_i e^{-Di\Delta t}$ at time step $i$ and use the forward time integration as an example. The induction term is calculated in two steps using a predictor-corrector method. First is the predictor step,

$$A'_{i+1} = A_i + I e^{-Di\Delta t} \Delta t, \quad (3.52)$$

then the corrector step,

$$A_{i+1} = A'_{i+1} + \frac{1}{2} (I'_{i+1} e^{-D(i+1)\Delta t} - I_i e^{-Di\Delta t}) \Delta t. \quad (3.53)$$

Finally, we rewrite (3.53) with the original variable $B$. The time stepping scheme for $B$ is then finally

$$B_{i+1} = B'_{i+1} + \frac{1}{2} (I'_{i+1} e^{-D\Delta t} - I_i) \Delta t. \quad (3.54)$$

### 3.2.3 CFL condition

Courant–Friedrichs–Lewy (CFL) conditions are necessary conditions for stable numerical solutions. CFL conditions give an estimated limit on the time step size $\Delta t$ based on flow speed. In Cartesian coordinates, we use

$$\max u_i < \frac{d}{\Delta t}, \quad (3.55)$$

where $\max u_i$ is the max speed along $i = x, y, z$ direction, $d$ is the spacing between grid points. In spherical coordinates, the velocity can be separated into the horizontal part $u_\theta, u_\phi$ and the radial part $u_r$. CFL conditions [Glatzmaier, 1984] require the minimal time step size $\Delta t$ to satisfy

$$\Delta t < \min \frac{r}{\sqrt{l(l+1)(u_\theta^2 + u_\phi^2)}}, \quad \Delta t < \min \frac{\Delta r}{u_r}, \quad (3.56)$$

where $l$ is the spherical harmonic degree, and $\Delta r$ is the spacing between radial grids. In this thesis, the time step size $\Delta t$ is fixed for a given model. We check the CFL conditions at each iteration to ensure the numerical solution is reliable.

### 3.3 Galerkin method in Cartesian coordinates

#### 3.3.1 Fourier decomposition

To compute the direct/adjoint induction term ($I$) and the diffusion term ($D$) we use a Galerkin method. The vector fields of $u$ and $B$ are decomposed into a sum of Fourier modes in Cartesian coordinates. The Fourier modes form a complete
orthogonal basis over the interval $[-L^*/2, L^*/2]$ with periodicity $L^*$. The Fourier decomposition for a vector field $u$ in a 3D domain is

\[
\begin{align*}
    u_x(x, y, z) &= \sum_{k_x, k_y, k_z} a_x(k_x, k_y, k_z) \exp \left[ \frac{2\pi i}{L^*} (k_x x + k_y y + k_z z) \right], \\
    u_y(x, y, z) &= \sum_{k_x, k_y, k_z} a_y(k_x, k_y, k_z) \exp \left[ \frac{2\pi i}{L^*} (k_x x + k_y y + k_z z) \right], \\
    u_z(x, y, z) &= \sum_{k_x, k_y, k_z} a_z(k_x, k_y, k_z) \exp \left[ \frac{2\pi i}{L^*} (k_x x + k_y y + k_z z) \right],
\end{align*}
\]

where $k_x, k_y, k_z$ are the wavenumbers. In spectral space, only the spectral coefficients $a(k_x, k_y, k_z)$ are stored. In physical space, the field values $u(x, y, z)$ on grid points $(x_n, y_n, z_n)$ are stored. A forward transform from spectral space to physical space is

\[
\begin{align*}
    u(k_x, k_y, k_z) &= \sum_{x_n, y_n, z_n} u(x_n, y_n, z_n) \exp \left[ -\frac{2\pi i}{L^*} (k_x x_n + k_y y_n + k_z z_n) \right],
\end{align*}
\]

and the backward transform from physical space to spectral space is

\[
\begin{align*}
    u(x_n, y_n, z_n) &= \sum_{k_x, k_y, k_z} u(k_x, k_y, k_z) \exp \left[ \frac{2\pi i}{L^*} (k_x x_n + k_y y_n + k_z z_n) \right].
\end{align*}
\]

We use FFTW library for the Fourier transforms and call the subroutines for discretized Fourier transformation of real data. The actual array size in spectral space is reduced from $N_x \times N_y \times N_z$ to $(N_x/2 + 1) \times N_y \times N_z$ due to the symmetry property of a periodic function $f(k_x, k_y, k_z) = f^*(N_x - k_x, N_y - k_y, N_z - k_z)$.

### 3.3.2 Optimization loop

The initial conditions $u$ and $B_0$ are updated interactively in an optimization loop using $\delta L/\delta u$ and $\delta L/\delta B_0$ until the two variational derivatives are sufficiently small. This loop consists of (0) an initialization of $u$ and $B_0$, then (1) the evolution of the $B$ field forward in time until a fixed time $T$, (2) then mapped to the adjoint field $B_T^\dagger$, followed by (3) the evolution of $B^\dagger$ backward in time in an adjoint model, and finally (4) using information from both forward and adjoint model to update the initial conditions $u$ and $B_0$. An illustration of the steps is shown in Figure 3.2, more details are discussed below.

#### 3.3.2.1 Initialization

In this stage, the vector field $u$ and $B_0$ need to be normalized and solenoidal as in (3.37). For the first iteration, we use a projection to remove the non-solenoidal part. Let us take the velocity field $u$ as an example. Suppose an additional pressure term $\nabla g'$ will remove the non-solenoidal part from field $u'$,

\[
\nabla \cdot (u' + \nabla g') = 0
\]

(3.60)
In spectral space, this translates to:

\[ \mathbf{k} \cdot \mathbf{u}' - \mathbf{k}^2 g' = 0 \]  \hspace{1cm} (3.61)

where \( \mathbf{k} = (k_x, k_y, k_z) \) is the wave vector. The projection is then

\[ \mathbf{u} = \mathbf{u}' + \frac{\mathbf{k}(\mathbf{k} \cdot \mathbf{u}')}{k^2} \]  \hspace{1cm} (3.62)

after which the flow field \( \mathbf{u} \) will satisfy the solenoidal condition. In addition, the root mean enstrophy and initial magnetic norm must equal 1. Numerically, this can be done easily in spectral space with a Fourier basis. The differential operator acts on the Fourier basis as

\[ \nabla_i = \frac{2\pi i}{L^* k_i} \]  \hspace{1cm} (3.63)

where \( i = x, y, z \). We first compute \( \nabla \times \mathbf{u} \) in spectral space, then normalize the spectral coefficients so that \( \langle (\nabla \times \mathbf{u})^2 \rangle = \langle B_0^2 \rangle = 1 \).

### 3.3.2.2 Forward model

In the forward part we need to solve the time evolution of a magnetic field according to the (direct) induction equation (3.38) from time \( t = 0 \) to \( t = T \). The right-hand side of the induction equation requires two main operations: calculating the diffusion of \( \mathbf{B} \) and the curl of \( \mathbf{u} \times \mathbf{B} \). The diffusion term is calculated directly by a matrix multiplication in spectral space,

\[ \langle \mathbf{B}_i \cdot \nabla^2 \mathbf{B}_j \rangle = a_i M_{ij} a_j \]  \hspace{1cm} (3.64)

where \( i, j \) represent wavenumber \( k \), \( a \) is the spectral coefficient. The diffusion matrix in Fourier basis is a diagonal matrix, \( M_{ij} = -(2\pi)^2 k^2 / L^* \mathbf{1} \), \( \mathbf{k} = (k_x, k_y, k_z) \) is the wave vector. The cross product \( \mathbf{u} \times \mathbf{B} \) is calculated in physical space on grid points, then transferred back to spectral space by a backward Fourier transform. The curl of \( \mathbf{u} \times \mathbf{B} \) is calculated in spectral space.
3.3.2.3 Adjoint model

In the adjoint model, the initial condition $B_T^\dagger$ is related to $B_T$ as in (3.39). We must then calculate $B^\dagger$ by evolving backward in time from $t = T$ until $t = 0$. The diffusion of $B^\dagger$ is calculated in the same way as in the forward model. $\nabla \times B^\dagger$ is calculated in spectral space. The cross product $u \times (\nabla \times B^\dagger)$ is calculated in physical space on grid points, followed by a backward Fourier transform to spectral space.

We also compute the integral term in $\delta L/\delta u$ during backward time evolution of $B^\dagger$. We need information on $u(x), B(x, t), B^\dagger(x, t)$ for the entire time window $T$. When the total number of time steps becomes too large, a check point strategy is used to reduce the memory load. The total time window $T$ is divided into several segments. When the magnetic field is evolving forward, its value at the beginning of each time segment, or at a checkpoint, is written to disk. Later when we evaluate the adjoint model, we recalculate $B$ for each time segment from the checkpoints. The time integral term $\int_0^T B \times (\nabla \times B^\dagger) \, dt$ in $\delta L/\delta u$ is then computed segment by segment. For an illustration, see Figure 3.3. The downside is that the forward routine is evaluated twice in total. Therefore a whole forward and adjoint calculation is $3/2$ more expensive than when everything can be stored in memory.

![Figure 3.3](image)

Figure 3.3. An illustration of the checkpoint strategy. Black dots represent $B$ at each discretized time step, red circle indicate check points where $B$ is written to disk. The red dots represent $B$ stored in memory when we compute the convolution product $B \times (\nabla \times B^\dagger) \, dt$ for one time segment. The arrow indicates the direction of forward time evolution.

3.3.2.4 Updates

After the preceding two steps we have solved the time evolution of both the magnetic field $B$ and the adjoint magnetic field $B^\dagger$. We can now use this to make an update of $B_0$ and $u$ towards the optimal solution. The update in $B_0$ is:

$$B_0 := B_0 + \Delta_B \frac{\delta L}{\delta B_0}$$

$$= B_0 + \Delta_B \left( B_0^\dagger - 2\lambda_2 B_0 + \nabla \Pi_2 \right)$$

(3.65)
where the step size $\Delta_B$ can be adjusted depending on the optimization algorithm. Similarly, the update in $u$ is:

$$ u := u + \Delta_U \frac{\delta L}{\delta u} $$

$$ = u + \Delta_U \left( \int_0^T B \times (\nabla \times B^t) \, dt - 2\lambda_1 \nabla \times \nabla \times u + \nabla \Pi_1 \right) \tag{3.66} $$

and $\Delta_U$ is the corresponding step size. $\Pi_1$ and $\Pi_2$ are used to project out the non-solenoidal part of $\delta L/\delta u$ and $\delta L/\delta B_0$ as in (3.44). Finally, we calculate the values of $\lambda_1$ and $\lambda_2$ by demanding that the enstrophy and initial magnetic norm remain normalized. Then we are ready to launch the next iteration.

### 3.4 Galerkin method in spherical coordinates

#### 3.4.1 Poloidal-toroidal decomposition

In spherical coordinates, a solenoidal vector field can be decomposed into a poloidal part and a toroidal part [Backus, 1958]. We now review this decomposition and some of its consequences for the induction equation. Taking the magnetic field $B$ for example, we write

$$ B = B^p + B^t, \tag{3.67} $$

where a poloidal magnetic field $B^p$ and a toroidal magnetic field $B^t$ are defined as

$$ B^t(r, \theta, \phi) = \sum_{l,m} \nabla \times \left( t_m^l(r)Y_m^l(\theta, \phi)\hat{r} \right), \tag{3.68} $$

$$ B^p(r, \theta, \phi) = \sum_{l,m} \nabla \times \nabla \times \left( p_m^l(r)Y_m^l(\theta, \phi)\hat{r} \right), \tag{3.69} $$

and the $Y_m^l$ are the spherical harmonics with degree $l$, $l \geq 1$, and order $m$, $|m| \leq l$. $t(r)$ and $p(r)$ are scalar functions of $r$. One can further use a discrete set of radial basis functions to represent the scalar functions:

$$ t_m^l(r) = \sum_n a_{nm} t_n^l(r), \quad p_m^l(r) = \sum_n b_{nm} p_n^l(r), \tag{3.70} $$

$a$ and $b$ are spectral coefficients. In this part, we use fully normalized real spherical harmonics which are defined as

$$ Y_m^l(\theta, \phi) = N_{lm} \begin{cases} \cos(m\phi) \hat{P}_l^{|m|}(\cos \theta), & \text{if } m \geq 0, \\ \sin(|m|\phi) \hat{P}_l^{-|m|}(\cos \theta), & \text{if } m < 0, \end{cases} \tag{3.71} $$

where $\hat{P}_l^m(\cos \theta)$ are the associated Legendre functions of $\cos \theta$. These are defined by $\hat{P}_l^m(x) = (-1)^m (1 - x^2)^{\frac{|m|}{2}} \frac{d^{|m|}}{dx^{|m|}} P_n(x)$, where $P_n(x)$ is the Legendre function of $x$. We have chosen this notation so we have a simple formula for the derivatives of $Y_l^m$. With the normalization factor

$$ N_{lm} = \sqrt{\frac{(2 - \delta_{bm})(2l + 1)(l - |m|)!}{4\pi(l + |m|)!}}, \tag{3.72} $$
we have the orthonormality condition for the spherical harmonics:

\[ \int_0^{2\pi} \int_0^\pi Y_{l,m}^*(\theta, \phi) Y_{l,m}(\theta, \phi) \sin \theta \, d\theta d\phi = \delta_{ll} \delta_{mm}. \]  

(3.73)

The derivative of spherical harmonics satisfies

\[ \frac{dY_{l,m}}{d\phi} = -m Y_{l,-m}, \]  

(3.74)

\[ \sin \theta \frac{dY_{l,m}}{d\theta} = -(l + 1) \hat{a}_{l+1}^m \hat{Y}^m_{l-1} + l \hat{a}_{l+1}^m \hat{Y}^m_{l+1}, \]  

(3.75)

where \( \hat{a}_{l+1}^m = \sqrt{\frac{(l+|m|)!}{l!(l-|m|)!}} \). With the definitions above the explicit form for the magnetic field is

\[ \mathbf{B}^t(r, \theta, \phi) = \sum_{l,m,n} c_{nml} \left[ \frac{1}{r \sin \theta} t^l_n(r) \nabla \times \hat{r} + \frac{1}{r} t^l_n(r) \nabla \times \hat{\theta} \right], \]  

(3.76)

\[ \mathbf{B}^p(r, \theta, \phi) = \sum_{l,m,n} d_{nml} \left[ \frac{1}{r} \left( \frac{l(l+1)}{r^2} p^l_n(r) Y_{l,m}\hat{r} + \frac{1}{r} \frac{\partial p^l_n(r)}{\partial r} \frac{\partial Y_{l,m}}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial p^l_n(r)}{\partial r} \frac{\partial Y_{l,m}}{\partial \phi} \hat{\phi} \right) \right]. \]  

(3.77)

The curl of the magnetic field is then

\[ \nabla \times \mathbf{B}^t = \sum_{l,m,n} a_{nml} \left[ \frac{1}{r \sin \theta} \nabla^2 Y_{l,m} \hat{r} + \frac{1}{r} \frac{\partial Y_{l,m}}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial Y_{l,m}}{\partial \phi} \hat{\phi} \right], \]  

(3.78)

\[ \nabla \times \mathbf{B}^p = \sum_{l,m,n} b_{nml} \left[ -\frac{1}{r \sin \theta} \nabla^2_1 p^l_n \frac{\partial Y_{l,m}}{\partial \phi} \hat{\theta} + \frac{1}{r \sin \theta} \nabla^2_1 p^l_n \frac{\partial Y_{l,m}}{\partial \phi} \hat{\phi} \right], \]  

(3.79)

where \( \nabla^2_1 = \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} \), and the double curl of the magnetic field is

\[ \nabla \times (\nabla \times \mathbf{B}^t) = \sum_{l,m,n} a_{nml} \left[ -\frac{1}{r \sin \theta} \nabla^2_1 Y_{l,m} \hat{r} + \frac{1}{r} \nabla^2_1 Y_{l,m} \hat{\theta} \right], \]  

(3.80)

\[ \nabla \times (\nabla \times \mathbf{B}^p) = \sum_{l,m,n} b_{nml} \left[ -\frac{1}{r^2} \nabla^2_1 p^l_n \frac{\partial Y_{l,m}}{\partial \phi} \hat{\theta} \right]. \]  

(3.81)
3.4.2 Selection rules

By looking at the spherical harmonic decomposition of fields, one can find out which modes of \(u\) and \(B\) are interacting. Bullard & Gellman [1954] give the selection rules for non-zero interacting modes for the magnetic induction term,

\[
\langle B_\gamma \cdot \nabla \times (u_\alpha \times B_\beta) \rangle
\]  

(3.82)

where \(\alpha, \gamma, \beta\) are spherical harmonic degrees, \(B_\gamma = \sum_{n,m} B_{nm\gamma}\) is a partial sum of spectral modes. Using \(T_\alpha T_\beta P_\gamma\) as a short notation for \(B_{\gamma}\) interacting with \(u_t\alpha\) and \(B_t\beta\) we can list three groups of rules.

First of all, for \(P_\alpha P_\beta P_\gamma\), \(P_\alpha T_\beta T_\gamma\), \(T_\alpha P_\beta T_\gamma\) interactions the amplitude vanishes unless all of the following conditions are satisfied:

1. \(\alpha + \beta + \gamma\) is even
2. \(\alpha, \beta, \gamma\) satisfy a triangle inequality, \(|\alpha - \gamma| \leq \beta \leq |\alpha + \gamma|\)
3. At least one of \(m_\alpha \pm m_\beta \pm m_\gamma\) is zero
4. Either one or all three spherical harmonics contains \(\cos(m\phi)\)

For \(P_\alpha T_\beta P_\gamma\), \(P_\alpha P_\beta T_\gamma\), \(T_\alpha P_\beta T_\gamma\), \(T_\alpha T_\beta T_\gamma\) interactions, the amplitude vanishes unless

1. \(\alpha + \beta + \gamma\) is odd
2. \(\alpha, \beta, \gamma\) satisfy a triangle inequality
3. At least one of \(m_\alpha \pm m_\beta \pm m_\gamma\) is zero
4. Either none or two spherical harmonics contains \(\cos(m\phi)\)
5. One cannot have two identical spherical harmonics

For \(T_\alpha T_\beta P_\gamma\) interactions the amplitude is always zero. We will see later in chapters 5, 6 and 7 that these rules help us to analyse the symmetry of the optimal solution, as well as to select different classes of solutions.

3.4.3 Symmetry properties

Gubbins & Zhang [1993] gave a detailed analysis on symmetry separations in a spherical geometry. There are several symmetry operations:

1. Reflection. This can be used to separate a solenoidal vector field into an equatorially symmetric (\(E^S\)) or an equatorially anti-symmetric (\(E^A\)) part. Written in terms of spherical harmonic modes, \(E^S\) symmetry requires \(l - m\) to be odd for a toroidal field and even for a poloidal field; \(E^A\) requires \(l - m\) to be even for a poloidal field and odd for a toroidal field.
2. Inversion through origin, which maps the radial function \(r \rightarrow -r\).
3. Rotation. Rotate by angle \(2\pi/N\) where \(N\) is an integer. The field is axisymmetric when \(m = 0\).

These symmetry properties can be used to analyze dynamo solutions. Which symmetry class has a lower \(Rm_c\)? Which structure is most unstable at a short time scale? Is an \(E^S\) field easier to generate than an \(E^A\) field? There are many interesting questions waiting to be answered. Chapter 7 is dedicated to the study of dynamo solutions within a fixed symmetry class.
3.4.4 Forward model

The implementation of the iteration scheme in spherical coordinates is discussed for the different models in the next chapters. Here we therefore only briefly discuss one method for the forward part of the model.

When we apply the Galerkin method to solve the induction equation, the induction term $I$ is projected onto the vector basis of $B$ [Glatzmaier, 1984; Li et al., 2010]. This method uses the property that a toroidal field has no radial component, and the radial component of a poloidal field is relatively simple. The diffusion term $D$ is directly calculated in spectral space using a matrix multiplication. We postpone the discussion of the representation for the diffusion term to §5.2.5 since the precise form depends on the radial basis functions. Due to the orthogonality of the spherical harmonics, the diffusion matrix in spherical coordinates is block diagonal in $(l, n)$ space so each spherical harmonic degree $l$ is decoupled from any other $l$. Each block of the diffusion matrix is then denoted by $T_{nm}$ for the toroidal part or by $P_{nm}$ for the poloidal part. In terms of toroidal spectral coefficients $c_{nml}$ and poloidal spectral coefficients $d_{nml}$ the induction equation, using diffusion time scale, becomes

$$\partial_t c_{nml} = Rm I_{nml} + \sum_{n'} T_{nm} c_{n'ml},$$

$$\partial_t d_{nml} = Rm I_{nml} + \sum_{n'} P_{nm} d_{n'ml}. \quad (3.83)$$

We can then extract the radial functions $\tilde{t}^m_l(r)$ and $\tilde{p}^m_l(r)$ corresponding to the induction term $I$ by using

$$\frac{r^2}{l(l+1)} \tilde{t}^m_l(r) = [\hat{r} \cdot \nabla \times (u \times B)]^m_l, \quad \frac{r^2}{l(l+1)} \tilde{p}^m_l(r) = [\hat{r} \cdot \nabla \times \nabla \times (u \times B)]^m_l. \quad (3.84)$$

These radial functions are then projected onto the radial basis functions of $B$ to get the spectral coefficients of the induction term $I$. A more detailed description with a slightly different derivation is given in §5.5.1.3.

3.5 Summary

This ends the methods section. We have covered the variational method, the optimization loop and relevant numerical methods. Most tools are now in place. Recall from §2.1.3 that the central questions in this thesis are to find the most efficient dynamo, identify its properties and search for the lower bounds on $Rm$, either for dynamo action or for magnetic instability. In the next Chapter 4 we describe the implementation of these ideas in a cubic model with impermeable boundary conditions, and in Chapter 5 we describe their use in a sphere with no-slip boundary conditions. In Chapter 6 and 7 we extend the spherical model of Chapter 5 with different boundary conditions and symmetry restrictions. These four chapters contain the main results of this thesis.
Chapter 4
Optimal kinematic dynamos in a cube


4.1 Introduction

W12 has demonstrated large scale optimization is possible for kinematic models. In a periodic cube, W12 identified the optimal kinematic dynamo and the lower bound on the magnetic Reynolds number, already a significant step in dynamo optimizations. In the real world, periodic boundary conditions in 3D are however difficult to achieve. We want to further develop this optimization scheme to study dynamo action with physical boundary conditions. In this chapter, we present our optimization results for a cube with two types of magnetic boundary conditions that represent two extreme cases. On opposite faces of the cube, the boundary can be either superconducting (in the limit when electrical resistance $1/\sigma \to 0$) or pseudo-vacuum (in the limit when magnetic permeability $\mu \to \infty$). The flow field $u$ satisfies impermeable boundary conditions which confine the fluid inside the cube for all four combinations. In 3D, this setting splits into four combinations, i.e. four unordered arrangements. The advantages of choosing this kind of boundary conditions for $u$ and $B$ is that solutions for the magnetic field then naturally fall into two pairs of complementary vector spaces. We found some quite interesting results in our models that match pairwise.

The general procedure used in this chapter is illustrated in Figure 4.1. We fix the input parameters such as the size of 3D physical grids $N \times N \times N$, the magnetic Reynolds number $Rm$, time step size $\Delta t$, and total time window $T$, we then create fields $u(x)$ and $B(x,0)$ in spectral space from random values or restart from previously stored spectral coefficients. The output from the optimization loop are the two variational derivatives $\delta L/\delta u$, $\delta L/\delta B_0$, and the updated field $u$ and $B_0$. We keep updating $u$, $B_0$ until the magnitudes of the two variational derivatives are sufficiently small.

We show below the test run results and highlight some adjustments to the
Figure 4.1. An illustration of the general procedure of optimization. Inputs are shown in the green box, the optimization process is shown in the red box, and the output is shown outside. \( \Delta t \) is the time step size, \( T \) is the total time window, \( N \) is the number of grids in each direction in physical space, \( \lambda_1 \) is a Lagrange multiplier that used to adjust the enstrophy norm of the updated velocity field \( u \), and \( \lambda_2 \) is used to adjust the norm of the updated initial magnetic field \( B_0 \).

procedure we made, some of which were crucial to the success of this project. A more detailed description of the methodology is given in the methods section §4.2, followed by the results and analysis section §4.3.

### 4.1.1 Preliminary tests

To ensure we have a robust code, we want to reproduce the results of W12 before we start any new optimization. The first one we tried was a Matlab code provided by Dr. Herreman. This test code uses the kinetic energy normalization and Adam-Bashforth second order time stepping method. We use a flexible update scheme to improve the convergence rate. The value of the stepsize \( \Delta_1 \) for the update of \( u \) is adjusted based on the correlation of \( \delta L/\delta u \) from two consecutive steps, and the stepsize \( \Delta_2 \) for the update of \( \delta B_0 \) is adjusted similarly. We use two separate stepsize values because \( u \) and \( B_0 \) generally have different rates of convergence.

For a value below the critical \( Rm_u \), the optimization algorithm converges quickly within \( \sim 30 \) iterations from a random initial data. For simulations at the critical \( Rm_u \), the convergence becomes very slow. This difficulty of convergence is also mentioned in W12. Recall from the work subsequently performed by Proctor [2015], there is no lower bound on a kinetic energy based \( Rm_u \) due to unlimited shear. Numerically the program is likely to crash before reaching such a limit. We then switched to a more flexible Fortran code with enstrophy normalization provided by Dr. Herreman. The time stepping method combines an exponential integrator for the diffusion term and a predictor-corrector for the induction term. We show in Figure 4.2 the test run results with \( \Delta t = 0.02 \) for
Figure 4.2. Two examples of reproduced results of W12 (with periodic boundary conditions): $\Delta t = 0.02$ for $N = 32$ grid and $\Delta t = 0.04$ for $N = 48$ grid; $Rm_\omega = 2.48(L^*)^2$ and the total time window $T = 10$. This value is slightly below the critical value. a) Magnetic norm $\langle B^2 \rangle$ as a function of advective overturn time $t \sim 1/\omega^*$. The two lines almost lie exactly on top of each other. b) Power spectrum of the optimal flow field $u$. We show the first 20 wave numbers; there are small differences in the low energy modes.

grid size $N = 32$ and $\Delta t = 0.04$ for grid size $N = 48$, two resolutions we used for simulations presented in the results section. We could have used $\Delta t = 0.04$ for grid size $N = 32$ as well, but we chose a smaller $\Delta t$ to have better numerical stability. The calculations take about 50 iterations to converge with random initial conditions. The difference in the growth rate from two configurations is small. The power spectrum shows the optimal solution is well converged. We recovered the same threshold of $Rm_c$ as reported by W12.

4.1.2 Modification of the Lagrangian

Instead of maximizing the final magnetic norm directly, we have changed the objective functional in the Lagrangian to maximize its logarithm, $\langle B^2_T \rangle \rightarrow \ln \langle B^2_T \rangle$. The initial conditions for the adjoint magnetic field becomes

$$B^\dagger_T = \frac{2B_T}{\langle B^2_T \rangle}.$$  \hspace{1cm} (4.1)

This helps to stabilize the backward time evolution for $B^\dagger$. Because of this rescaling, the residue (a measure of convergence) now does not depend on the absolute value of $\langle B_T \rangle$. We get a better measure of how far the solution is away from the optimum. For a comparison of the two schemes, see Figure 4.3.

1. In this chapter our times are based on a advective time scale.
Figure 4.3. Comparison of residue and magnetic norm as a function of iterations. Two test runs use random initial start, \( N = 32, \Delta t = 0.02 \). a) Before rescaling the amplitude of residue is related to \( \langle B^2 \rangle_T \), in this test run \( T = 10 \). b) After rescaling the amplitude of residue does not depend on \( \langle B^2 \rangle_T \), in this test run \( T = 9.91 \).

4.1.3 Galerkin basis

We want to test two limiting cases for the magnetic boundary conditions. The superconducting boundary requires

\[
\mathbf{n} \cdot \mathbf{B}|_\Sigma = 0, \quad \mathbf{n} \times \mathbf{J}|_\Sigma = 0,
\]

and the pseudo vacuum boundary requires

\[
\mathbf{n} \times \mathbf{B}|_\Sigma = 0, \quad \mathbf{n} \cdot \mathbf{J}|_\Sigma = 0,
\]

where \( \Sigma \) represents the boundary with unit normal vector pointing outward \( \mathbf{n} \). In this model the Galerkin basis is constructed from a periodic Fourier basis with half of its periodicity. This formulation is discussed in more detail in §4.2.4.1 and §4.6.1. The magnetic field can be be either tangential (T) to a superconducting boundary or normal (N) to a pseudo vacuum boundary. Considering there are three directions, \( \mathbf{n} = \hat{x}, \hat{y}, \hat{z} \), and we do not count the permutations, we get the four combinations of boundary conditions shown in Figure 4.4. We denote the four settings by their boundary conditions along \( \hat{x}, \hat{y}, \hat{z} \) respectively, giving the nomenclature NNT, NTT, NNN and TTT. We tested the field values at the boundary...
and find they match with what is expected. For the flow field we use tangential (T) boundaries in all three directions. This corresponds to the impermeable boundary condition. We furthermore have one additional constraint that is a requirement for optimality that arises from the boundary terms,

\[ \mathbf{n} \times (\nabla \times \mathbf{u})|_{\Sigma} = 0. \]  \hspace{1cm} (4.4)

Effectively this gives the same Galerkin basis for the velocity field \( \mathbf{u} \) as the TTT case for the magnetic field. It turns out when we use this particular TTT basis to represent \( \mathbf{u} \), the additional constraint is equivalent to the stress-free boundary condition \( \mathbf{n} \times (\mathbf{n} \cdot S_{ij})|_{\Sigma} = 0 \), where \( S_{ij} \) is the strain rate tensor, because on each surface \( \mathbf{n} \cdot \partial_i u_j|_{\Sigma} = 0 \).

### 4.1.4 Solving the initial scattering problem in our results

When we ran the numerical simulations, the preliminary results were not satisfactory. As shown below in Figure 4.5, there was quite a lot of scatter in the optimized growth rate as a function of \( \frac{Rm \omega}{(L^*)^2} \) with a time window \( T \) of between 4 and 16 was used. For the rest of this chapter we omit the subscript \( \omega \) and just write \( Rm \). The resolution we use should be sufficient as we already passed the preliminary test. We ultimately found out this scatter is due to transient growth leaking into the asymptotic growth of the magnetic field. After we extended the time window \( T \), we found very clean results as shown in §4.3.2. We also found a symmetry mapping in the optimal solutions that was first mentioned in Favier & Proctor [2013]. This will be discussed in more detail in §4.4.3.
4.2 Problem & method

4.2.1 Objective function

The variational optimization method [Lions, 1970; Talagrand & Courtier, 1987] we use in this chapter is strongly inspired by Willis [2012]. We choose to optimize the asymptotic growth of the magnetic energy in the cube directly to select the most efficient dynamo. More precisely, inside the fluid domain $\mathcal{V}$, which is a cubic box of unit size, we search for the best stationary flows $\mathbf{u}(\mathbf{x})$ and initial magnetic fields $\mathbf{B}_0 = \mathbf{B}(\mathbf{x}, 0)$ that give the maximal magnetic energy growth at a large but finite time $T$. This results in the following objective functional with various constraints:

$$
\mathcal{L} = \ln \langle \mathbf{B}_T^2 \rangle - \lambda_1 \left( \langle (\nabla \times \mathbf{u})^2 \rangle - 1 \right) - \lambda_2 \left( \langle \mathbf{B}_0^3 \rangle - 1 \right) - \langle \Pi_1 \nabla \cdot \mathbf{u} \rangle - \langle \Pi_2 \nabla \cdot \mathbf{B}_0 \rangle - \int_0^T \langle \mathbf{B}^\dagger \cdot [\partial_t \mathbf{B} - \nabla \times (\mathbf{u} \times \mathbf{B}) + Rm^{-1} \nabla \times \nabla \times \mathbf{B}] \rangle \, dt
$$

(4.5)

We denote here $\langle \ldots \rangle = \frac{1}{V} \int_{\mathcal{V}} \ldots \, dV$ as the integral over the box. The first term expresses that we maximize the logarithm of magnetic energy at time $T$, since at large $T$ the magnetic energy can be described by an exponential function. We write as shorthand $\mathbf{B}_T = \mathbf{B}(\mathbf{x}, T)$ for the final magnetic field. In the non-dimensional setting, the fluid flow has to be normalized (constrained by $\lambda_1$), here by an enstrophy or dissipation norm. As noted by Willis, the alternative normalization that fixes the kinetic energy $-\lambda_1 \langle U^2 \rangle$ is problematic as discontinuous flows with unlimited shear may then be picked up by the optimizer. This problem is avoided by using the dissipation norm. The flow also has to be a solenoidal (constrained by $\Pi_1$) field. The magnetic field satisfies the induction equation at all times (constrained by $\mathbf{B}^\dagger$). It is sufficient to impose that the initial magnetic field $\mathbf{B}_0$ is solenoidal (constrained by $\Pi_2$), since solenoidality is preserved by the induction equation, and therefore $\nabla \cdot \mathbf{B} = 0$ is guaranteed at all times. The maximization is not well defined unless the initial magnetic field amplitude is fixed (normalized) (constrained by $\lambda_2$).

The functional was written immediately in non-dimensional form and depends on 2 non-dimensional numbers: $T$, the time-horizon and $Rm$, the magnetic Reynolds number defined as

$$
Rm = SL^2/\eta.
$$

(4.6)

Here $S$ is a measure for the dimensional enstrophy or typical shear magnitude, $L$ is the dimensional box-size and $\eta$ the magnetic diffusivity. Time is measured in units $S^{-1}$, space in units of $L$, velocity in units $SL$ and magnetic field units are arbitrary.

4.2.2 Boundary conditions

The crucial difference with Willis’ work is that we demand that $\mathbf{u}$ and $\mathbf{B}$ satisfy boundary conditions on the walls $\Sigma$ of the cubic box. We can impose these
boundary conditions by adding supplementary constraints to $\mathcal{L}$ or we can limit
the variations to classes of functions that meet a fixed set of boundary conditions.
We choose the second approach.

Flows $\mathbf{u}$ are allowed to slip on the boundary but cannot penetrate it:

$$n \cdot \mathbf{u} |_{\Sigma} = 0 \quad (4.7)$$

where $n$ is the external unit normal everywhere on $\Sigma$.

Magnetic fields $\mathbf{B}$ will satisfy either a perfectly conducting (T, tangential) or
a pseudovacuum (N, normal) boundary condition, on each of the 3 pairs of
parallel end plates. Out of 8 possible configurations, we consider only 4 physically
independent combinations:

\[
\begin{array}{cccc}
\hat{x} \times \mathbf{B} |_{x=0,1} = 0 & \hat{x} \times \mathbf{B} |_{x=0,1} = 0 & \hat{x} \times \mathbf{B} |_{x=0,1} = 0 & \hat{x} \times \mathbf{B} |_{x=0,1} = 0 \\
\hat{x} \cdot \mathbf{J} |_{x=0,1} = 0 & \hat{x} \cdot \mathbf{J} |_{x=0,1} = 0 & \hat{x} \cdot \mathbf{J} |_{x=0,1} = 0 & \hat{x} \cdot \mathbf{J} |_{x=0,1} = 0 \\
\hat{y} \times \mathbf{B} |_{y=0,1} = 0 & \hat{y} \times \mathbf{B} |_{y=0,1} = 0 & \hat{y} \times \mathbf{B} |_{y=0,1} = 0 & \hat{y} \times \mathbf{B} |_{y=0,1} = 0 \\
\hat{y} \cdot \mathbf{J} |_{y=0,1} = 0 & \hat{y} \cdot \mathbf{J} |_{y=0,1} = 0 & \hat{y} \cdot \mathbf{J} |_{y=0,1} = 0 & \hat{y} \cdot \mathbf{J} |_{y=0,1} = 0 \\
\hat{z} \times \mathbf{B} |_{z=0,1} = 0 & \hat{z} \times \mathbf{B} |_{z=0,1} = 0 & \hat{z} \times \mathbf{B} |_{z=0,1} = 0 & \hat{z} \times \mathbf{B} |_{z=0,1} = 0 \\
\hat{z} \cdot \mathbf{J} |_{z=0,1} = 0 & \hat{z} \cdot \mathbf{J} |_{z=0,1} = 0 & \hat{z} \cdot \mathbf{J} |_{z=0,1} = 0 & \hat{z} \cdot \mathbf{J} |_{z=0,1} = 0 \\
\hline
\end{array}
\]

Cases NTN, TNN and TNT, TTN are not studied, because they are identified as
NNT and NTT up to a permutation of $x, y,$ and $z$. We denote $\mathbf{J} = R m^{-1} \nabla \times \mathbf{B}$
as the current density. On perfectly conducting boundaries $\Sigma_T$, one more usually
expresses the condition $n \times \mathbf{E} = 0 |_{\Sigma_T}$, but given Ohm’s law $\mathbf{J} = \mathbf{E} + u \times \mathbf{B}$,
impermeability (4.7) and the fact that $n \cdot \mathbf{B} |_{\Sigma_T} = 0$, this is equivalent to $n \cdot \mathbf{J} = 0 |_{\Sigma_T}$.

### 4.2.3 Euler-Lagrange equations

At the optimal the Lagrangian must be stationary with respect to arbitrary variations, which means that

\[
\delta \mathcal{L} = \frac{\delta \mathcal{L}}{\delta \lambda_1} \delta \lambda_1 + \frac{\delta \mathcal{L}}{\delta \lambda_2} \delta \lambda_2 + \left< \frac{\delta \mathcal{L}}{\delta \Pi_1} \delta \Pi_1 \right> + \left< \frac{\delta \mathcal{L}}{\delta \Pi_2} \delta \Pi_2 \right> + \int_0^T \left< \frac{\delta \mathcal{L}}{\delta \mathbf{B}^1} \cdot \delta \mathbf{B}^1 \right> dt \\
+ \left< \frac{\delta \mathcal{L}}{\delta \mathbf{u}} \cdot \delta \mathbf{u} \right> + \left< \frac{\delta \mathcal{L}}{\delta \mathbf{B}_0} \cdot \delta \mathbf{B}_0 \right> + \left< \frac{\delta \mathcal{L}}{\delta \mathbf{B}_T} \cdot \delta \mathbf{B}_T \right> + \int_0^T \left< \frac{\delta \mathcal{L}}{\delta \mathbf{B}} \cdot \delta \mathbf{B} \right> dt \\
+ BT = 0 \quad (4.9)
\]

Each of the variational derivatives $\delta \mathcal{L}/\delta \cdot$ has to disappear separately, which de-
fines 9 Euler-Lagrange equations for the optimal problem. Boundary terms ($BT$) generated by partial integration should disappear and define boundary conditions
for the fields $\Pi_2, \mathbf{B}^1$ and here a supplementary condition for the flow $\mathbf{u}$.

The 5 variational derivatives with respect to the Lagrange multipliers $\lambda_1, \lambda_2,
\Pi_1, \Pi_2, \mathbf{B}^1$, generate the physical constraints that fix the functional classes for $\mathbf{u}$.
and $B_0$ and produce the “direct” induction equation for $B$. The 4 variational derivatives with respect to $u, B_0, B_T, B$ generate 4 non-trivial equations, that can be obtained by partial integration:

$$
\frac{\delta L}{\delta u} = \int_0^T B \times (\nabla \times B^\dagger) \, dt + 2\lambda_1 \nabla^2 u + \nabla \Pi_1 \to 0 
$$

(4.10)

$$
\frac{\delta L}{\delta B_0} = B_0^\dagger - 2\lambda_2 B_0 + \nabla \Pi_2 \to 0 
$$

(4.11)

$$
\frac{\delta L}{\delta B_T} = \frac{2B_T}{(B_T^\dagger)} - B_T^\dagger = 0 
$$

(4.12)

$$
\frac{\delta L}{\delta B} = \partial_t B^\dagger + (\nabla \times B^\dagger) \times u - Rm^{-1} \nabla \times \nabla \times B^\dagger = 0 
$$

(4.13)

Equations (4.10) and (4.11) will be used to define updates and will only reach zero in an iterative optimization process. Equation (4.12) defines the so-called compatibility condition that allows the adjoint magnetic field $B_T^\dagger$ to be initialized. Equation (4.13) sets the adjoint induction equation.

The partial integration produce the boundary terms that should also disappear at the optimum. Here they are

$$
BT = - \oint_{\Sigma} \Pi_1 (n \cdot \delta u) \, dS 
- \oint_{\Sigma} \Pi_2 (n \cdot \delta B_0) \, dS + \int_0^T \oint_{\Sigma} \left[ (J^\dagger \times \delta B) \cdot n + (B^\dagger \times \delta \mathbf{E}) \cdot n \right] \, dS \, dt 
- \oint_{\Sigma} \left[ \delta u \times (\nabla \times u) \right] \cdot n \, dS = 0 
$$

(4.14)

We abbreviate by

$$
\delta E = Rm^{-1} \nabla \times \delta B - u \times \delta B - \delta u \times B \quad , \quad \mathbf{J}^\dagger = Rm^{-1} \nabla \times \mathbf{B}^\dagger 
$$

(4.15)

the variation of the electrical field and an adjoint current density. We now inspect term per term. The first term always disappears since $n \cdot \delta u|_{\Sigma} = 0$. The second line groups all boundary terms related to the magnetic field. Using the various boundary conditions NNN, NNT, NTT and TTT on $\delta B$ and $\delta \mathbf{J}$ or $\delta \mathbf{E}$, we find that they disappear only when the adjoint boundary conditions

$$
\begin{align*}
\hat{x} \times B^\dagger|_{x=0,1} &= 0 & \hat{x} \times B^\dagger|_{x=0,1} &= 0 & \hat{x} \times B^\dagger|_{x=0,1} &= 0 & \hat{x} \times \mathbf{J}^\dagger|_{x=0,1} &= 0 \\
\Pi_2|_{x=0,1} &= 0 & \Pi_2|_{x=0,1} &= 0 & \Pi_2|_{x=0,1} &= 0 & \Pi_2|_{x=0,1} &= 0 \\
\hat{y} \times B^\dagger|_{y=0,1} &= 0 & \hat{y} \times B^\dagger|_{y=0,1} &= 0 & \hat{y} \times B^\dagger|_{y=0,1} &= 0 & \hat{y} \times \mathbf{J}^\dagger|_{y=0,1} &= 0 \\
\Pi_2|_{y=0,1} &= 0 & \Pi_2|_{y=0,1} &= 0 & \Pi_2|_{y=0,1} &= 0 & \Pi_2|_{y=0,1} &= 0 \\
\hat{z} \times B^\dagger|_{z=0,1} &= 0 & \hat{z} \times B^\dagger|_{z=0,1} &= 0 & \hat{z} \times B^\dagger|_{z=0,1} &= 0 & \hat{z} \times \mathbf{J}^\dagger|_{z=0,1} &= 0 \\
\Pi_2|_{z=0,1} &= 0 & \Pi_2|_{z=0,1} &= 0 & \Pi_2|_{z=0,1} &= 0 & \Pi_2|_{z=0,1} &= 0 \\
\text{NNN} & & \text{NNT} & & \text{NTT} & & \text{TTT} 
\end{align*} 
$$

(4.16)
apply. This entirely sets the boundary conditions for the adjoint problem that need to be fulfilled.

The third and final boundary term does not disappear for all flows that meet the impermeability condition (4.7) and therefore fixes a supplementary constraint. Optimality apparently requires that the flow satisfies

$$n \times (\nabla \times u) \big|_\Sigma = 0 \quad \text{(4.17)}$$

on the boundaries. This necessity of a supplementary requirement on the tangential components of the flow is not really an accident and mainly a consequence of the use of the enstrophy norm. Alternatively, we could also have restricted the flows to those that satisfy the no-slip boundary conditions $u|_\Sigma = 0$. In that case the boundary term automatically disappears and then no extra condition is required, but we will not deal with this case here; it represents an interesting extension to the problem.

### 4.2.4 Numerical method

The analytical solution to the coupled differential equations in this model is unknown and it generally needs to be approximated numerically. In a non-periodic domain, “the natural choice” for the series expansion of a smooth function is to use the Chebyshev method [Boyd, 2000]. This is because the Chebyshev method gives spectral (also called exponential) accuracy. By spectral accuracy, we mean the $n$th coefficient in the series $(a_n)$ has the following property:

$$a_n \sim O(e^{-qn^k}), \quad k, q > 0, \quad n \gg 1. \quad \text{(4.18)}$$

For example, the Fourier series of an infinitely differentiable function $f(x)$ in a periodic domain has spectral convergence because the coefficients $a_n$ must decay faster than $1/n^k$ for any $k > 0$ and $n \gg 1$. The Chebyshev series has the same property, essentially because it gives coefficients identical to the series expansion of a function $f(\cos(x))$. However the boundary conditions for a Chebyshev series expansion have to be added as explicit constraints.

Over the years, many numerical codes have been developed for magnetohydrodynamics (MHD) simulations in Cartesian coordinates. The choice of basis functions varies. For example, a combined Fourier and Chebyshev method by Stellmach & Hansen [2008] provides efficient and accurate results on massively parallel computers for all common boundary conditions, whereas the dynamo study by Calkins et al. [2016] uses the Chebyshev series, and one of the authors Dr. Marti is developing a numerical platform called QuiCC for Cartesian, cylindrical and spherical geometry using the Chebyshev method. The Dedalus project is another example of a very flexible platform [DEDALUS project, 2014-2017]. The users can choose among Fourier series, Chebyshev series, and cosine/sine series, with other types of bases still being developed. Snoopy [Lesur, 2007-2017] is also popular in the MHD community for studies of turbulence involving shear and rotation. It is mainly developed for periodic domains, and employs fast Fourier transform in parallel as much as possible. In this project, we use the Fourier bases in a non-periodic domain due to its simple implementation of boundary conditions. More details are explained in sections below.
4.2.4.1 Galerkin expansions

To implement the boundary conditions, we expand all fields on a complete set of basis-functions that have the boundary conditions built-in and thus use Galerkin expansions. For the flow components we use the Fourier sine/cosine series:

\[
\begin{bmatrix}
U_x(x, y, z) \\
U_y(x, y, z) \\
U_z(x, y, z)
\end{bmatrix} = \sum_{m_x, m_y, m_z \in \mathbb{N}} \begin{bmatrix}
\hat{U}_x(m_x, m_y, m_z) & \sin(m_x \pi x) \cos(m_y \pi y) \cos(m_z \pi z) \\
\hat{U}_y(m_x, m_y, m_z) & \cos(m_x \pi x) \sin(m_y \pi y) \cos(m_z \pi z) \\
\hat{U}_z(m_x, m_y, m_z) & \cos(m_x \pi x) \cos(m_y \pi y) \sin(m_z \pi z)
\end{bmatrix}
\]

(4.19)

Boundary conditions (4.7)-(4.17) are indeed satisfied and the expansion is also complete for all flows satisfying these boundary conditions. We introduce the following shorthand notation:

\[U_x \in \mathcal{E}_{scc}, \quad U_y \in \mathcal{E}_{csc}, \quad U_z \in \mathcal{E}_{css}\]

(4.20)

for the function spaces (e.g. the suffix *scc* means: sine function of \(x\), cosine function of \(y\) and cosine function of \(z\)).

For the direct and adjoint magnetic field components, we use similar expansions:

\[
\begin{align*}
B_x, B_x^\dagger & \in \mathcal{E}_{css} \\
B_y, B_y^\dagger & \in \mathcal{E}_{scs} \\
B_z, B_z^\dagger & \in \mathcal{E}_{ssc} \\
B_x, B_y, B_z, B_x^\dagger & \in \mathcal{E}_{ccc} \\
B_y, B_y^\dagger & \in \mathcal{E}_{csc} \\
B_z, B_z^\dagger & \in \mathcal{E}_{css} \\
B_x, B_y, B_z, B_x^\dagger & \in \mathcal{E}_{scc} \\
B_y, B_y^\dagger & \in \mathcal{E}_{csc} \\
B_z, B_z^\dagger & \in \mathcal{E}_{sss}
\end{align*}
\]

(4.21)

which are again complete expansions for magnetic fields that satisfy the boundary conditions (4.8)-(4.16).

Upon inspection of the direct and adjoint induction equations and regarding the expansions of the flow (4.19) and magnetic field (4.21) it can be verified that

\[
\nabla \times (u \times B), \quad (\nabla \times B^\dagger) \times u
\]

(4.22)

have the same structure as the fields \(B\) and \(B^\dagger\), meaning that they can be expanded on the same basis, see (4.21). This implies that fields \(B\) and \(B^\dagger\) are conserved in the separate classes of functions introduced above.

The term \(\nabla \Pi_2\) that appears in the equation (4.11) has the same structure as \(B_0\) or \(B^\dagger\), if

\[
\Pi_2 \in \mathcal{E}_{ass}, \quad \Pi_2 \in \mathcal{E}_{ssc}, \quad \Pi_2 \in \mathcal{E}_{scc}, \quad \Pi_2 \in \mathcal{E}_{ccc}
\]

(4.23)

These expansion automatically satisfies the boundary conditions that are needed on \(\Pi_2\) (see 4.16).

With \(u\) of the form (4.20) and \(B, B^\dagger\) of the form (4.21), both terms \(2\lambda_1 \nabla^2 u\) and \(\int_0^T B \times (\nabla \times B^\dagger) \, dt\) are within the same class of functions as (4.20). Restricting

\[
\Pi_1 \in \mathcal{E}_{ccc}
\]

(4.24)
we then have the guarantee that

\[ \left( \frac{\delta L}{\delta u} \right)_x \in \mathcal{E}_{sc}, \quad \left( \frac{\delta L}{\delta u} \right)_y \in \mathcal{E}_{cs}, \quad \left( \frac{\delta L}{\delta u} \right)_z \in \mathcal{E}_{cs} \]  

which means \( \delta L/\delta u \) will be in the same class of functions as \( u \), see (4.20). This is important since \( \delta L/\delta u \) will be used in the velocity field update, see (4.27).

4.2.4.2 Extension to the periodic box & projectors

The proposed Galerkin expansions are not periodic in the cube of size 1 but all of them are periodic on a cube of size 2. By numerically extending the fluid domain to a double sized cube, one can use a standard (dealiased) pseudo-spectral periodic box code to timestep the direct and the adjoint induction equations. Our periodic code uses a predictor corrector scheme for the flow-interaction terms and exact integration rule for the diffusive terms.

The fields \( u \) and \( B_0 \) need to be initialized within the right classes of functions \( \mathcal{E}_{css}, \mathcal{E}_{css}, \ldots \) and this is done using projectors, given in Appendix 4.6.1. Even though the equations conserve the fields within these classes, small numerical errors induce some drift. At each iteration in the optimization loop (after update), we remove these small errors by projecting the new \( u \) and \( B_0 \) on the chosen classes. Alternatively, we could have used sine and cosine transforms to make dedicated and more efficient numerical codes, but here it was not necessary to adopt this strategy.

4.2.4.3 Optimization scheme

The optimization itself is an iterative procedure. We initialize the algorithm with random solenoidal and normalized \( u \) and \( B_0 \) that satisfy the boundary conditions (step (0)). Each iteration in the optimization loop is decomposed in 4 steps. The magnetic field is time-stepped from time 0 to time \( T \), satisfying the induction equation, Gauss’ law and the boundary conditions (step (1)). Knowing \( B_T \), one initializes \( B_T^\dagger \) using the compatibility equation (4.12) (step (2)). The adjoint equation (4.13) is integrated backwards from time \( T \) to time 0, such that \( B_T^\dagger \) remains solenoidal and that boundary conditions are satisfied (step (3)). This results in knowledge of \( B_0^\dagger \), which is needed to evaluate \( \delta L/\delta B_0 \). The time integral \( \int_0^T B \times (\nabla \times B^\dagger) \, dt \) that appears in \( \delta L/\delta u \) is calculated using Simpson’s composite quadrature rule, which demands the knowledge of \( B \) and \( B^\dagger \) at all times; this can causes excessive memory demands and is avoided by using a checkpoint strategy, see Willis [2012]. We are then ready to propose better estimates for \( u \) and \( B_0 \) (step (4)). We precondition a diagonal approximation to the Hessian of the form:

\[ \frac{\delta^2 L}{\delta u \delta u}(m) \approx -2\lambda_1 \pi^2 m^2, \quad \frac{\delta^2 L}{\delta B_0 \delta B_0}(m) \approx -2\lambda_2 \]  

(4.26)
We note \( \mathbf{m} = (m_x, m_y, m_z) \) and \( m^2 = (m_x^2 + m_y^2 + m_z^2) \). This allows us to write updates as:

\[
\hat{\mathbf{u}}(\mathbf{m}) := \hat{\mathbf{u}}(\mathbf{m}) + \frac{\Delta_1}{2\lambda_1 \pi^2 m^2} \mathcal{L}_{\delta \mathbf{u}}(\mathbf{m}) \quad (4.27)
\]

\[
\hat{\mathbf{B}}_0(\mathbf{m}) := \hat{\mathbf{B}}_0(\mathbf{m}) + \frac{\Delta_2}{2\lambda_2} \mathcal{L}_{\delta \mathbf{B}_0}(\mathbf{m}) \quad (4.28)
\]

which is a preconditioned descent method. In the code, we relax \( \Delta_1 \in [0, 1] \) and \( \Delta_2 \in [0, 1] \) to prevent large steps in wrong directions, following precisely the same method as Pringle et al. [2012].

The update cannot be evaluated as long as values of \( \Pi_1, \Pi_2, \lambda_1, \lambda_2 \) are not set. Interestingly, they are exactly determined by requiring that the updated fields still satisfy the constraints. The values of \( \Pi_1 \) and \( \Pi_2 \) are set by requiring that the updated fields \( \mathbf{u}, \mathbf{B}_0 \) remain solenoidal, \( \lambda_1, \lambda_2 \) are fixed by the requirement that the updated \( \mathbf{u} \) and \( \mathbf{B}_0 \) remain normalized.

After the update, the forward branch of the loop can be relaunched and the entire process iterated as many times as necessary. We measure progress in the optimization through

\[
r_i = \sqrt{\left\langle \left( \frac{\delta \mathcal{L}}{\delta \mathbf{u}} \right)_i^2 + \left( \frac{\delta \mathcal{L}}{\delta \mathbf{B}_0} \right)_i^2 \right\rangle} \quad (4.29)
\]

where \( i = 1, 2, \ldots \) is the iteration number. In essence, we need \( \lim_{i \to +\infty} r_i = 0 \) for convergence, but in numerical simulations it is not easy to determine a threshold value for \( r_i \), beneath which we can call an optimization sufficiently converged.

Note finally, that the optimizer can get stuck in local minima if they exist and for this reason, it is important to repeat optimizations with different and independent initial random fields. We will perform a perturbation study around the identified optima.

4.2.4.4 Testing

As a first test of our code we reproduced Willis’ results. In the absence of all projectors, using periodic flows, we reproduce the minimal magnetic \( Rm \) for dynamo action under the enstrophy norm for a periodic flow in a cube as \( Rm_{c,min} = 2.48\pi^2 \). The extra factor of \( \pi^2 \) results from the use of a different length scale in the definition (4.6) of \( Rm \), (our periodic box has size 2, Willis’ box has size \( 2\pi \)). Note that for a unit box with periodic boundaries, Willis’ result becomes \( Rm_{c,min} = 9.92\pi^2 \); we shall need this reference value in our comparisons of §4.3.3.

The projectors used to restrict the fields to particular classes only appear in few places in the code: at initialization of the random fields and after each update. They have been tested in a separate manner and we are confident that these minimal modifications are correct.
4.3 Results

All results presented in this section have been obtained using a strict protocol. We initialize $u, B_0$ with normally distributed random spectral coefficients, project out the non-solenoidal part, restrict the functions to the specified classes and normalize the fields properly. We solve direct and adjoint induction equations with $32^3$ resolution for NNT and NTT type boundary conditions and $48^3$ for NNN and TTT.

The question arises of how to set the terminal time $T$. To be sure of dynamo action we want this to be several magnetic decay times, and we choose this to be 4 decay times. The decay time in a size $L$ box for the magnetic field with all four types of boundary conditions cannot be larger than

$$t_{\text{decay}} = \frac{L^2}{\eta \pi^2} \quad (4.30)$$

Our time scale is measured in units $S^{-1}$, and thus we convert this time into these units. This leads to a non-dimensional time horizon $T = 4Rm/\pi^2$ when the box is of size unity. Our computations confirm that this is long enough to get past the transient growth stage and allows for a reasonably short computational time ($\leq 5$ minutes for one iteration). We call an optimization “converged” after $i$ iterations, if the residue $r_i \lesssim 10^{-3}$.

4.3.1 Illustrating the iterative optimization in progress

We fix $Rm = 7.80\pi^2$ and implement NNT boundary conditions for the magnetic field. Figure 4.6a displays $\langle B^2 \rangle$ as a function of time $t$, as the optimization makes progress. The initial random fields cannot support a dynamo at iteration 1, and we see exponential decay at late times. As we iterate the optimization loop, the final magnetic energy gradually increases, such that at iteration 261 it is very slightly growing with time but essentially no longer changing as the iterations proceed. This converged optimal solution is a slightly supercritical dynamo, because we show in §4.3.2 that the minimal dynamo threshold $Rm = Rm_{c,min} = 7.52\pi^2$ for NNT boundary conditions.

Figure 4.6b shows the corresponding error measure $r_i$ as a function of iteration number $i$. From the start until the end, this error goes down by 5 orders of magnitude, which indicates the success of the optimization. The erratic path on the descent is the result of the way $\Delta_1$ and $\Delta_2$ are varied. This may perhaps be avoided, but we did not find better ways than Pringle et al. [2012a] to increase the speed of convergence.

4.3.2 Growth rates $\gamma$ of optimized dynamos as a function of $Rm$

In a more systematic survey, we varied $Rm$ in significant intervals. For each value of $Rm$, 5 independent optimizations are launched from different random
Figure 4.6. An illustration of the iterative optimization procedure. Magnetic fields with imposed NNT boundary conditions are considered, $Rm = 7.80\pi^2$. (a) For different values of the iteration, the magnetic energy as a function of time. (b) The non-dimensional residue $r_i$ as a function of iteration $i$.

Figure 4.7. Growth rates of optimized dynamos as a function of $Rm$ and for different magnetic boundary conditions. (a) NNT and NTT boundaries. (b) NNN and TTT boundaries.

seeds. We measure the asymptotic growth rates $\gamma$ of the optimized dynamos at late times $t$, where

$$\langle |B(x, t)|^2 \rangle \sim e^{2\gamma t}$$

In practice, we measure the growth rate in the following way: we integrate the induction equation using the optimal $u$ and the initial $B_0$ over an extended time horizon to $T = 12Rm/\pi^2$. The energy growth rate $\gamma$ is measured during the last diffusive time interval, where we are always far away from the initial transient. In Figure 4.6a, the growth rate of the magnetic energy in the final iteration is $\gamma = 0.005$ using this definition.

In figure 4.7, we group all the optimal growth rates $\gamma$ obtained from these independent optimizations as a function of $Rm$ and for the four types of boundary conditions. Figure 4.7a, shows cases NNT and NTT. We immediately recognize that both types of boundary conditions lead to very similar optimal growth rates.
We also recognize the existence of 3 distinct lines. The growth rates from 5 sets of independent runs randomly fall onto these 3 lines. The line most to the left defines the real optimal branch, but some runs did converge towards suboptimal branches. Figure 4.7b, shows cases NNN and TTT. Here both types of boundary conditions also lead to very similar optimal growth rates, but we only have one optimal line. Furthermore, the suboptimal branches of NNT (or NTT, since both give similar growth rates) case persist for a wide range of $Rm$. They do not collapse into one branch even at $Rm \ll Rm_{c,min}$.

![Graph](image)

Figure 4.8. A zoom-out picture of the optimal growth rates as a function of $Rm$ for the NNT case. For each $Rm$, there are 5 independent runs started from random initial fields. We will only see one point if the results fall on the same branch. Yellow: optimal growth rates near $Rm_{c,min}$. Green: optimal growth rates over a wide range of $Rm$.

### 4.3.3 Minimal dynamo thresholds $Rm_{c,min}$

An important quantity in this study is $Rm_{c,min}$: the minimal critical magnetic Reynolds number. Within the specified class of flows, no flow will act as a dynamo when $Rm < Rm_{c,min}$. We measure these lower bounds for dynamo action, by performing a linear regression on the optimal growth rates of figure 4.7 which allows us to identify $Rm_{c,min}$ where $\gamma = 0$. The results are given in the first row of Table 4.1. The mixed boundary conditions (NNT, NTT) allow for a lower $Rm_{c,min}$ than with perfectly conducting or pseudovacuum boundary conditions (TTT, NNN).

In the same table 4.1, we added some reference values for critical dynamo thresholds. Willis’ (2012) periodic optimal dynamo has a larger threshold than our mixed boundary optimal. We can also compare to thresholds for Roberts [1972] and ABC flows. Using the fact that for these flows the enstrophy and rms speed are equal to unity in a $2\pi$ box, we can find the values of $Rm_u$ from published values: for Roberts the value 8.79 (note [17] of Willis [2012] and Figure 4 of Alexakis [2011] for a supercritical value of 10) is adjusted by a factor of $2\pi$ to scale to a unit cube; for ABC 1:1:1 we adjust the classic value of 8.9 Arnold &
Table 4.1. Some properties of the optimal flows, together with some other flows of interest. The first four columns have given magnetic boundary conditions (NNT etc.) whereas the next three have periodic magnetic boundary conditions. The rms (root mean square) vorticity is set to unity. The periodic flow is the optimal reported in Willis (2012), rescaled to a unit box; the Roberts flow is an ABC flow with $A = B = 1$, $C = 0$. The ABC flow 1:1:1 has all coefficients equal. The critical $Rm_u$ is the minimal threshold for dynamo action with unity kinetic energy as defined in (4.35). For our optimal flows, they are calculated from rms speed and from $Rm = Rm_{c,\text{min}}$ as in (5.88).

4.3.4 Spatial profiles & kinetic energy spectra

The spatial profiles of the velocity field at the minimal thresholds $Rm_{c,\text{min}}$ are represented by streamlines in figure 4.9. Lines are colored by intensity and initialized at random locations. In all cases, we see that the flow is properly confined to the cube as dictated by our boundary conditions.

In the flows for NNT and NTT optima, we see one major vortex (figures 4.9a and 4.9b). Both velocity fields also seem quite correlated, and this will be measured more precisely subsequently. In Table 4.2 and 4.3, we give the first 5 dominant modes for the optimal flow and the final magnetic field for NNT and NTT optima. We find that 95% of the enstrophy and $>89\%$ of the final magnetic energy are contained in these 5 modes. Plus, the first 2 dominant modes in the optimal flow (NNT: 83% of the enstrophy, NTT: 86% of the enstrophy) can be written as:

\[
\begin{align*}
\text{NNT} & : \begin{bmatrix}
A_x(x, y, z) \\
A_y(x, y, z) \\
A_z(x, y, z)
\end{bmatrix} =
\begin{bmatrix}
0.16 (2\pi)^{-2}\sin(2\pi y) \sin(2\pi z) \\
0.77 \pi^{-2}\sin(\pi x) \sin(\pi z) \\
-0.18 (2\pi)^{-2}\sin(2\pi x) \sin(2\pi y)
\end{bmatrix} \\
\text{NTT} & : \begin{bmatrix}
A_x(x, y, z) \\
A_y(x, y, z) \\
A_z(x, y, z)
\end{bmatrix} =
\begin{bmatrix}
-0.17 (2\pi)^{-2}\sin(2\pi y) \sin(2\pi z) \\
0.78 \pi^{-2}\sin(\pi x) \sin(\pi z) \\
0.18 (2\pi)^{-2}\sin(2\pi x) \sin(2\pi y)
\end{bmatrix}
\end{align*}
\]

The critical magnetic Reynolds number $Rm_c$ corresponding to the reduced optimal flow with 2 dominant modes is $9.58\pi^2$ for NNT type and is $9.38\pi^2$ for NTT type.
Figure 4.9. Velocity field streamlines of the optimal flow at the minimal critical magnetic Reynolds number $Rm_{c,min}$ and for different magnetic boundary conditions. (a) NNT optimal flow. (b) NNT optimal flow. (c) NNN optimal flow. (d) TTT optimal flow.

In the flows for NNN and TTT optima, we see three vortices (figures 4.9c and 4.9d) and again a significant correlation if one rotates the profiles properly. However, this pair cannot be easily described by a few dominant modes. Both flows and final magnetic fields for NNN and TTT optima have higher percentage contributions from small scales than the NNT and NTT pair.

The spectral content of a flow-field is often characterized using the one-dimensional kinetic energy spectrum.

$$E(k) = |m|$$

and show them in figure 4.10. The energy density decreases steeply and exponentially which is an indication of spectral spatial convergence. Decreasing several orders of magnitude from $k \approx 1$ to $k \approx 12 - 16$, we clearly have a spatially resolved calculation. Numerical errors due to the finite grid spacing are consequently expected to be small.

Late time magnetic field eigenmodes are shown in figure 4.11. We see the signature of the different magnetic boundary conditions in each of the plots, but magnetic field eigenmodes are no longer correlated by pairs. We see $S$ shaped structures in the mixed boundary cases and spiralling structures in both NNN and TTT cases.
Table 4.2. NNT: First 5 dominant modes of optimal velocity field and final magnetic field, a counting for 95% of the enstrophy and 90% of the final magnetic energy. The coefficients of $\hat{B}_{x,y,z}$ have been normalized to have unit norm.

<table>
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<tr>
<th>$m_x$</th>
<th>$m_y$</th>
<th>$m_z$</th>
<th>Coefficient</th>
<th>$m_x$</th>
<th>$m_y$</th>
<th>$m_z$</th>
<th>Coefficient</th>
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<td>1</td>
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</tr>
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<td>1</td>
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<td>$0.88$</td>
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<tr>
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<td>1</td>
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<td>$-0.53$</td>
</tr>
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<td>2</td>
<td>$-0.10$</td>
</tr>
<tr>
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<td>1</td>
<td>$-0.06/\pi$</td>
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<td>1</td>
<td>2</td>
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</tr>
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<td>$-0.06$</td>
</tr>
</tbody>
</table>

Table 4.3. NNT: First 5 dominant modes of optimal velocity field and final magnetic field, a counting for 95% of the enstrophy, 89% of the final magnetic energy. The coefficients of $\hat{B}_{x,y,z}$ have been normalized to have unit norm.

<table>
<thead>
<tr>
<th>$m_x$</th>
<th>$m_y$</th>
<th>$m_z$</th>
<th>Coefficient</th>
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4.3.5 Perturbation study

Compared to the large scale nature of the optimization and the fact that we can only launch a small number of independent optimizations, one might fear that the optima are perhaps only local optima. Such local optima can indeed exist and even have an important basin of attraction in parameter space (we observed them in figure 4.7a). To ensure the robustness of our results, we perform a perturbation study on the identified optima at the minimal dynamo thresholds.

To do so, we generate a normally distributed random perturbation flow with variable amplitude. We add this perturbation flow to the optimal velocity field at $Rm_{c,min}$ and renormalize so as to have a unit enstrophy in the perturbed flow, denoted $u_p$. We then integrate the induction equation with this new flow $u_p$ while keeping $B_0$ unchanged and measure late time growth rates $\gamma_p$. We define a correlation amplitude

$$\epsilon = \frac{\langle u_p \cdot u_o \rangle}{\langle u_p^2 \rangle^{1/2} \langle u_o^2 \rangle^{1/2}}$$

Equation 4.34

to measure how far the new velocity field $u_p$ differs from the unperturbed optimal field $u_o$. This process is repeated using 400 different perturbations of various amplitude and each of these runs adds a point to the plot of figure 4.12, which shows the perturbed growth rate $\gamma_p$ as a function of correlation amplitude $\epsilon$. None of the perturbations allow us to find growth rates $\gamma_p$ larger than 0, which is an indication that our optima are correctly calculated.

4.4 Analysis and discussion

4.4.1 Helicity

Helicity $H = \mathbf{u} \cdot (\nabla \times \mathbf{u})$ is a popular quantity in dynamo theory that measure the alignment of the flow and its vorticity. Several laminar dynamos such as the Ponamorenko-flow, Robert’s flow, and the ABC-flow are helical and satisfy the
Beltrami property $\nabla \times \mathbf{u} \sim \mathbf{u}$, but also in mean field dynamo theory [Moffatt, 1978], helicity plays a prominent role. How helical are our optimal dynamos?

In figure 4.13, we show some isosurfaces of helicity of the optimal flow at $Rm_{c,min}$ for the four types of magnetic boundary conditions. In mixed boundary cases NNT and NTT, we see two symmetrical lobes of helicity. This symmetry is lost in the cases of TTT and NNN. Figure 4.14 shows probability density functions of helicity. We observe a strong pairwise correlation as before. In all set-ups NNT, NTT, NNN, TTT, the value $H = 0$ is the most probable within the cube. Cases NNT and NTT are similar and the pdfs are symmetrical, implying that helicity is zero on average. This is not the case with NNN and TTT, where these optima have a preferentially positive helicity. Mean helicities are reported in Table 4.1 and remain well below unity.
Figure 4.12. Perturbation study: the optimal dynamo flows at threshold are perturbed by random flows. We show dynamo growth rates $\gamma_p$ found with these perturbed flows as a function of correlation amplitude. None of the points is above the optimal value $\gamma = 0$ and as the correlation amplitude goes up, we see that the effect of the perturbations decreases.

Figure 4.13. Helicity isosurface of amplitude: (a) $-0.4/\pi$ (yellow) and $0.4/\pi$ (red) for NNT and NNT optimal flow. (b) $-0.1/\pi$ (blue) and $0.4/\pi$ (green) for NNN and TTT optimal flow.

4.4.2 Minimal magnetic Reynolds number based on rms speed

The magnetic Reynolds number (4.6) we used in this work is not very standard in the dynamo literature. We needed to use this definition since it is compatible with the enstrophy normalization which was necessary because optimizations with normalized kinetic energy do not yield converged optima. A more standard definition for the magnetic Reynolds number is based on rms speed $U$:

$$Rm_u = \frac{UL}{\eta}$$

We can calculate this $Rm_u$ a posteriori, since we can measure

$$\frac{U}{SL} = \langle u^2 \rangle^{1/2}$$
Figure 4.14. Probability density function of helicity in the box for the different optimal flows at criticality $Rm_{\text{min,c}}$. Figure courtesy of Dr. Herreman.

from the optima. In this way, we have

$$Rm_u = Rm\langle u^2\rangle^{1/2} \quad (4.37)$$

which yields the values reported in Table 4.1. Interestingly it seems that with this definition of $Rm_u$ we can reinterpret the results. The NNN and TTT optima have now the lowest critical thresholds, before the mixed boundary condition optima NNT and TTT.

4.4.3 Symmetry of the cube and its consequences

To study symmetries in the flows and equations, we shift the coordinate system to the centre of the cube (but do not change notation to avoid unnecessary complexity). In this frame, the cubical boundary surface is the union of coordinate surfaces $x = \pm 1/2$, $y = \pm 1/2$, $z = \pm 1/2$. This boundary is clearly mapped onto itself, by any possible permutation of $x, y, z$ combined with any possible change of sign. More explicitly, with $\mathbf{x} = (x, y, z)$, a cube is symmetrical with respect to all operations $\mathcal{R}x$:

$$\mathcal{R}x = (s_1 x, s_2 y, s_3 z) \quad , \quad \mathcal{R}x = (s_2 y, s_1 x, s_3 z)$$

$$\mathcal{R}x = (s_2 y, s_3 z, s_1 x) \quad , \quad \mathcal{R}x = (s_3 z, s_2 y, s_1 x)$$

$$\mathcal{R}x = (s_3 z, s_1 x, s_2 y) \quad , \quad \mathcal{R}x = (s_1 x, s_3 z, s_2 y) \quad (4.38)$$

with $s_1, s_2, s_3 = \pm 1$. This parametrizes the 48 member symmetry group of the cube (or octahedral) $O_h$. Next to the trivial identity, each transform can be associated with a rotation or a reflection with respect to a mirror plane. Operators $\mathcal{R}$ can be represented using orthogonal matrices $\mathcal{R}$, $(\mathcal{R}^{-1} = \mathcal{R}^T)$.

We study the presence and the consequences of these symmetries in the optimized dynamo problem. The symmetries explain why optima are degenerate and why we find exactly the same optimal growth rates in pairs (NNT and TTT, NNN and TTT).
4.4.3.1 Trivial consequence of symmetry: degeneracy of the optima

The equations of the kinematic dynamo problem are invariant under any coordinate transform \( x = R^T \tilde{x}, \tilde{x} = Rx \) that involves \( R \) an orthogonal matrix:

\[
\begin{align*}
\partial_t B &= \nabla \times (u \times B) + Rm^{-1}\nabla^2 B \\
\nabla \cdot B &= 0
\end{align*}
\]

\[
\begin{align*}
\partial_t \tilde{B} &= \tilde{\nabla} \times (\tilde{u} \times \tilde{B}) + Rm^{-1}\tilde{\nabla}^2 \tilde{B} \\
\tilde{\nabla} \cdot \tilde{B} &= 0
\end{align*}
\]

(4.39)

Here both fields are related as

\[
\begin{align*}
u(x) &= R^T \tilde{u}(Rx) \quad , \quad B(x) = R^T \tilde{B}(Rx)
\end{align*}
\]

(4.40)

An immediate consequence in the present context of optimized dynamo action is that if the boundary conditions are also invariant under \( R \) transformation, we can say that

\[
u(x) \text{ is an optimal dynamo } \iff R^T u(Rx) \text{ is an optimal dynamo}
\]

(4.41)

In the cases of NNN and TTT, we have the same type of boundary conditions everywhere, which implies that NNN and TTT optima are both 48-fold degenerate. The mixed boundaries NNT and NTT have symmetry groups that are reduced to dihedral symmetry:

\[
\begin{align*}
R_x &= (s_1x, s_2y, s_3z) \\
R_{\tilde{x}} &= (s_2y, s_1x, s_3z) \quad , \quad R_x &= (s_1x, s_2y, s_3z) \\
R_{\tilde{x}} &= (s_1x, s_3z, s_2y)
\end{align*}
\]

(4.42)

with \( s_1, s_2, s_3 = \pm 1 \) and thus only 16 members. As a result NNT and NTT optima are 16-fold degenerate. The fact that we observe \( 3 = 48/16 \) separate “optimality” branches in the mixed boundary case (see figure 4.7a) is probably also related to this reduced symmetry group of the boundaries.

In the simulations, we do see this trivial degeneracy: depending on the random initialization, the optimizer converges to optima that have the same optimal growth rates, but with rotated or mirror reflected spatial structures.

4.4.3.2 Symmetry & anti-correlation in the optimal flows

Instead of investigating the symmetry of the equations and boundary conditions, we can also measure whether the optimal solutions themselves are symmetric. Let us introduce some notations and concepts. Two vector field \( \mathbf{V}_1(x) \) and \( \mathbf{V}_2(x) \) are correlated (+) or anti-correlated (-) by an isometry \( R \) when

\[
R^T \mathbf{V}_1(Rx) = \pm \mathbf{V}_2(x)
\]

(4.43)

Choosing \( \mathbf{V}_1 = \mathbf{V}_2 = \mathbf{V} \), we can check whether the vector field \( \mathbf{V} \) is symmetrical (+) or antisymmetrical (-) with respect to some \( R \). Let us note \( \mathbf{V}_{i,R} = R^T \mathbf{V}_i(Rx) \) and

\[
s_{ij} = \frac{\langle \mathbf{V}_{i,R} \cdot \mathbf{V}_{j,R} \rangle}{\langle \mathbf{V}_{i,R}^2 \rangle^{1/2} \langle \mathbf{V}_{j,R}^2 \rangle^{1/2}}
\]

(4.44)
with \(i, j = 1, 2\). Using this quantity we can study the (anti)-correlations and (anti)-symmetries of the different optimal flows in a systematic way and with respect to all 48 isometries \(\mathcal{R}\) of the cube.

For NNT and NTT optimal flows, \(V_1 = u_{\text{NNT}}\) and \(V_2 = u_{\text{NTT}}\), we have found several high scores \(|s_{ij}| > 0.9\) listed in table 4.4. The first line in the left table, shows that these optimal flows are inversion symmetric:

\[
\begin{align*}
\mathbf{u}_{\text{NNT}}(x) &= -\mathbf{u}_{\text{NNT}}(-x) \quad , \quad \mathbf{u}_{\text{NTT}}(x) = -\mathbf{u}_{\text{NTT}}(-x) \\
\end{align*}
\]

This immediately explains why these flows have no mean helicity. The other isometries are not exact, but the scores are still high enough to say that there is a significant correlation. In the right-hand table, we see that the optimal flows \(u_{\text{NNT}}\) and \(u_{\text{NTT}}\) are almost perfectly anti-correlated by an isometry. The most negative score \(\min(s_{12}) = -0.995\) is found for the operation \(\mathcal{R}x = (z, -y, x)\) and its inverse. This corresponds to a rotation of \(\pi\) about the axis \((\hat{e}_x + \hat{e}_z)/\sqrt{2}\) and a reflection with respect to a plane with that vector as unit normal. Up to 0.5% we can say that

\[
\mathbf{u}_{\text{NTT}}(x) \simeq -\mathcal{R}^T u_{\text{NNT}}(\mathcal{R}x) 
\]

When applied to the boundary, the transform \(\mathcal{R}x = (z, -y, x)\) essentially maps the NNT boundary into a TNN boundary, which is the exact complementary of a NTT boundary, under the exchange N\(\leftrightarrow\)T. As explained below, this anti-correlation explains why NNT-optima and NTT-optima have the same growth rates.

For NNN and TTT optimal flows, \(V_1 = u_{\text{NNN}}\) and \(V_2 = u_{\text{TTT}}\), we find maximal correlations, \(\max |s_{11}| = 0.42\) for NNN, \(\max |s_{22}| = 0.61\) for TTT. This is not significant: all symmetries are broken in NNN and TTT optimal flows, in agreement with figures 4.9c and 4.9d. We do find an almost perfect anti-correlation between the different optima: \(\min(s_{12}) = -0.97\), for a single isometry \(\mathcal{R}x = (y, x, -z)\). Up to 3% we can say that

\[
\mathbf{u}_{\text{NNN}}(x) \simeq -\mathcal{R}^T u_{\text{TTT}}(\mathcal{R}x) 
\]

The transform \(\mathcal{R}x = (y, x, -z)\) corresponds to a rotation of \(\pi\) around the vector \((\hat{e}_x + \hat{e}_y)/\sqrt{2}\).  

### Table 4.4. Symmetries and anti-correlations of optimal flows \(V_1 = u_{\text{NNT}}, V_2 = u_{\text{NTT}}\) under isometries of the cube (see eq. (4.44) for the definition of \(s_{ij}\)).

<table>
<thead>
<tr>
<th>(\mathcal{R}x)</th>
<th>(s_{11})</th>
<th>(s_{22})</th>
<th>(\mathcal{R}x)</th>
<th>(s_{12})</th>
</tr>
</thead>
<tbody>
<tr>
<td>((-x, -y, -z))</td>
<td>1</td>
<td>1</td>
<td>((+z, -y, +x))</td>
<td>-0.995</td>
</tr>
<tr>
<td>((+x, -y, +z))</td>
<td>0.94</td>
<td>0.98</td>
<td>((-z, +y, -x))</td>
<td>-0.995</td>
</tr>
<tr>
<td>((-x, +y, -z))</td>
<td>0.94</td>
<td>0.98</td>
<td>((+z, +y, +x))</td>
<td>-0.96</td>
</tr>
<tr>
<td>((-z, +y, +x))</td>
<td>0.91</td>
<td>0.93</td>
<td>((-z, -y, -x))</td>
<td>-0.96</td>
</tr>
<tr>
<td>((-z, -y, +x))</td>
<td>0.91</td>
<td>0.93</td>
<td>((+x, +y, -z))</td>
<td>-0.92</td>
</tr>
<tr>
<td>((+z, +y, -x))</td>
<td>0.91</td>
<td>0.93</td>
<td>((-x, -y, +z))</td>
<td>-0.92</td>
</tr>
<tr>
<td>((+z, -y, -x))</td>
<td>0.91</td>
<td>0.93</td>
<td>((+x, -y, -z))</td>
<td>-0.92</td>
</tr>
<tr>
<td>((+z, -y, +x))</td>
<td>0.91</td>
<td>0.93</td>
<td>((-x, +y, +z))</td>
<td>-0.92</td>
</tr>
</tbody>
</table>
Considering the degeneracy of the optima, the perfect anti-correlation of the optimal flows can be simplified to

\[
\begin{align*}
\mathbf{u}_{\text{NNT}} \text{ is optimal for NNT } & \iff -\mathbf{u}_{\text{NNT}} \text{ is optimal for TTN} \\
\mathbf{u}_{\text{NNN}} \text{ is optimal for NNN } & \iff -\mathbf{u}_{\text{NNN}} \text{ is optimal for TTT} \quad (4.48)
\end{align*}
\]

which will serve as a starting point for the next section.

### 4.4.3.3 Identical growth rates for complementary boundary conditions

In recent work, Favier & Proctor [2013] have shown that for a general fluid domain \( \mathcal{V} \) with impermeable walls, a stationary dynamo \( \mathbf{u} \) which is antisymmetric with respect to an isometry \( \mathcal{R} \) of the system

\[
\mathbf{u}(\mathbf{x}) = -\mathcal{R}^{-1}\mathbf{u}(\mathcal{R}\mathbf{x}) \quad (4.49)
\]

will grow magnetic fields with the exact same growth rate \( \gamma \), for both the types of complementary pseudovacuum (N) or perfectly conducting (T) boundaries.

In the present context, none of our optimal flows are antisymmetric with respect to themselves, but we do find the same growth rates \( \gamma \) and also find pairwise anti-correlation for the optimal flows of complementary set-ups (NNT and NTT, NNN and TTT). We can explain this using the same type of argument as developed by Favier & Proctor [2013] and limit the demonstration here to the case of NNN and TTT.

Suppose an arbitrary fluid volume \( \mathcal{V} \), with perfectly conducting T-boundaries. A flow \( \mathbf{u}_T \) drives a magnetic field eigenmode \( \mathbf{b}_T(\mathbf{x}) \exp(\gamma t) \), which means that

\[
\gamma \mathbf{b}_T - \nabla \times (\mathbf{u}_T \times \mathbf{b}_T) + Rm^{-1} \nabla \times \nabla \times \mathbf{b}_T = 0 \quad (4.50)
\]

We suppose that \( \gamma \) is real. On the boundary

\[
\mathbf{u}_T \cdot \mathbf{n}|_{\Sigma} = 0 \quad , \quad \mathbf{n} \times \mathbf{e}_T|_{\Sigma} = 0 \quad (4.51)
\]

where \( \mathbf{e}_T = Rm^{-1} \nabla \times \mathbf{b}_T - \mathbf{u}_T \times \mathbf{b}_T \) is the electrical field. We now manipulate this equation by taking the scalar product of (4.50) with \( \mathbf{a}_T \) and integrating over the volume. Partial integration brings us to

\[
\left\langle (\gamma \mathbf{a}_T + \mathbf{u}_T \times (\nabla \times \mathbf{a}_T) + Rm^{-1} \nabla \times \nabla \times \mathbf{a}_T) \cdot \mathbf{b}_T \right\rangle
+ \oint_{\Sigma} (\mathbf{e}_T \times \mathbf{n}) \cdot \mathbf{a}_T \, dS + Rm^{-1} \oint_{\Sigma} ((\nabla \times \mathbf{a}_T) \times \mathbf{n}) \cdot \mathbf{b}_T \, dS = 0 \quad (4.52)
\]

The first boundary term disappears because of the boundary condition on \( \mathbf{e}_T \). A sufficient condition to get 0 on both sides is

\[
\gamma \mathbf{a}_T + \mathbf{u}_T \times (\nabla \times \mathbf{a}_T) + Rm^{-1} \nabla \times \nabla \times \mathbf{a}_T = 0 \quad (4.53)
\]

\[
+ BC : (\nabla \times \mathbf{a}_T) \times \mathbf{n}|_{\Sigma} = 0 \quad (4.54)
\]
Table 4.5. Comparison of $\beta_{\text{min}}$ and the measured $\beta$ for the final magnetic field $B_T$ at $Rm_{c,\text{min}}$.

<table>
<thead>
<tr>
<th></th>
<th>NNT</th>
<th>NTT</th>
<th>NNN</th>
<th>TTT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{\text{min}}$</td>
<td>$\pi^2$</td>
<td>$\pi^2$</td>
<td>$2\pi^2$</td>
<td>$2\pi^2$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$4.60\pi^2$</td>
<td>$4.63\pi^2$</td>
<td>$10.0\pi^2$</td>
<td>$10.0\pi^2$</td>
</tr>
</tbody>
</table>

According to the boundary condition $BC$, the field $b_N = \nabla \times a_T$ is normal to the boundaries. By taking the curl of (4.53), we find that this field $b_N$ solves

$$\gamma b_N = \nabla \times [(-u_T) \times b_N] - Rm^{-1} \nabla \times \nabla \times b_N$$  \hspace{1cm} (4.55)

$$+ BC : b_N \times n|_\Sigma = 0$$ \hspace{1cm} (4.56)

This is nothing else but the induction equation and implies what we searched for: the flow $u_N = -u_T$ is equally a dynamo for a magnetic field eigenmode that will be normal to the boundaries and it will grow at exactly the same rate $\gamma$.

4.4.4 Backus bound

Backus [1958] took a different definition for the magnetic Reynolds number $Rm_B$ in terms of the maximum strain rate of the flow. With the present scaling, we have $Rm_B = S_{\text{max}} L^2 / \eta = e Rm$ where $e = S_{\text{max}} / S$ is the maximum eigenvalue of the non-dimensional strain rate tensor with components

$$e_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i) \hspace{1cm} (4.57)$$

We calculated this maximal local strain $e$ for our optimal flows at threshold and show values in Table 4.1. We note that the NNN and TTT optimal flows display a considerably larger maximal strain than the NNT and NTT optima or the periodic box case of Willis [2012].

The Backus bound provides a minimal requirement on $Rm_B$ based on the energy equation of $B$. A necessary condition for dynamo action is (see also Proctor [1977])

$$Rm_B \geq \min \left[ \frac{\int_{\mathcal{V}_1} |\nabla \times B|^2 \, dV}{\int_{\mathcal{V}_2} |B|^2 \, dV} \right]$$ \hspace{1cm} (4.58)

In this formula $\mathcal{V}_1$ is the fluid domain and $\mathcal{V}_2$ the entire domain, but here $\mathcal{V}_1 = \mathcal{V}_2$. The largest scale magnetic fields within the fluid domain supply a lower bound on $\beta$. The measured $\beta$ for the optimal set of modes is expected to be larger, since the structure of the magnetic field is not entirely large scale.

Our best dynamo, with $e = 2.16$ and $Rm_{c,\text{min}} = 7.52\pi^2$ from Table 4.1, then has $Rm_B = 16.2\pi^2$, about 16 times larger than the Backus bound $\beta_{\text{min}}$. This indicates the maximum strain rate is significantly larger than the strain developed in most of the volume, and we know from Table 4.5 the $\beta$ realised is about $\sim 5$ times the minimal available value. This explains the observed difference.
4.5 Conclusion

By adapting the procedure of Willis [2012], we have developed a Cartesian model to find the most efficient dynamo with a flow confined within a cube. Table 4.1 shows the values of $Rm_{c,min}$ for our results and for the original results of Willis [2012] along with thresholds for some famous ABC flows. We have been careful to refer all results to the same size of box. Compared to the ABC flows, our optimal dynamos have thresholds which are about a factor 5 to 8 lower. When comparing to the optimal of Willis [2012], also using normalised enstrophy, it transpires that periodic magnetic boundary conditions are not the optimal boundary conditions to enable efficiency. One can see this heuristically by considering the smallest size magnetic structures that are allowed by the box and its boundary conditions. Periodic boundary conditions necessarily only allow a field with one full wavelength within the box, whereas our boundary conditions allow a half wavelength (see e.g. equation (4.19)). Thus it is possible to have lower dissipation and a more efficient dynamo. But this is not a sufficient condition, note the periodic box for example has a lower $Rm_{c,min}$ than the homogenous boundary cases.

The symmetries of the cube are responsible for a strong degeneracy of the optima. A more surprising consequence of symmetry is that we find that when $u$ generates an optimal dynamo for a given set of idealized boundary conditions, then $-u$ can generate an optimal dynamo too, but for a different and complementary set of boundary conditions. We explain this observation using a similar argument as the one developed by Favier & Proctor [2013]. Compared to existing results on lower bounds, we showed in §4.4.4 that our best dynamo operates about 16 times above the Backus bound.

4.6 Appendix

4.6.1 Projectors in spectral space

In our numerical method, we used a periodic box code. All fields or field components are represented on the standard Fourier basis adapted to periodic cube of size 2. A function $f(x, y, z)$ then has the expansion

$$f(x, y, z) = \sum_{m_x, m_y, m_z \in \mathbb{Z}} \tilde{f}(m_x, m_y, m_z) e^{i\pi(m_xx + m_yy + m_zz)}$$  \hspace{1cm} (4.59)

Let $\mathcal{E}$ be the space of all periodic functions on the cube with size 2. We then have

$$\mathcal{E} = \mathcal{E}_{ccc} \oplus \mathcal{E}_{ccs} \oplus \mathcal{E}_{csc} \oplus \mathcal{E}_{acc} \oplus \mathcal{E}_{asc} \oplus \mathcal{E}_{acs} \oplus \mathcal{E}_{css} \oplus \mathcal{E}_{sss}$$ \hspace{1cm} (4.60)

which is easily understood by rewriting the generic Fourier expansion using Euler’s rule. That same rule also allows to find projectors $\mathcal{P}_{ccc}, \mathcal{P}_{ccs}, \ldots, \mathcal{P}_{sss}$ that allow to restrict a function $f(x, y, z)$ to the required class. For example, for all $f \in \mathcal{E},$

$$\mathcal{P}_{ccc}f \in \mathcal{E}_{ccc} \quad , \quad \mathcal{P}_{ccs}f \in \mathcal{E}_{ccs} \quad , \quad \ldots \quad , \quad \mathcal{P}_{sss}f \in \mathcal{E}_{sss}$$ \hspace{1cm} (4.61)
These projectors are most easily defined in spectral space. Given the Fourier-space coefficients \( \tilde{f}(m_x, m_y, m_z) \) and denoting Fourier-space amplitudes \( \tilde{f}(\pm m_x, \pm m_y, \pm m_z) \) as \( \tilde{f}_{\pm\pm\pm} \), we find that:

\[
\begin{align*}
\tilde{P}_{ccc} f_{+++} &= \frac{1}{4} \Re \left( \tilde{f}_{+++} + \tilde{f}_{++-} + \tilde{f}_{+-+} + \tilde{f}_{++-} \right) \\
\tilde{P}_{ssc} f_{+++} &= \frac{1}{4} \Re \left( \tilde{f}_{+++} - \tilde{f}_{++-} + \tilde{f}_{+-+} - \tilde{f}_{++-} \right) \\
\tilde{P}_{scs} f_{+++} &= \frac{1}{4} \Re \left( \tilde{f}_{+++} + \tilde{f}_{++-} - \tilde{f}_{+-+} - \tilde{f}_{++-} \right) \\
\tilde{P}_{css} f_{+++} &= \frac{1}{4} \Re \left( \tilde{f}_{+++} - \tilde{f}_{++-} - \tilde{f}_{+-+} + \tilde{f}_{++-} \right)
\end{align*}
\]

and

\[
\begin{align*}
\tilde{P}_{ssc} f_{+++} &= \frac{i}{4} \Im \left[ \tilde{f}_{+++} + \tilde{f}_{++-} + \tilde{f}_{+-+} + \tilde{f}_{++-} \right] \\
\tilde{P}_{scs} f_{+++} &= \frac{i}{4} \Im \left[ \tilde{f}_{+++} - \tilde{f}_{++-} + \tilde{f}_{+-+} - \tilde{f}_{++-} \right] \\
\tilde{P}_{css} f_{+++} &= \frac{i}{4} \Im \left[ \tilde{f}_{+++} + \tilde{f}_{++-} - \tilde{f}_{+-+} - \tilde{f}_{++-} \right] \\
\tilde{P}_{sss} f_{+++} &= \frac{i}{4} \Im \left[ \tilde{f}_{+++} - \tilde{f}_{++-} - \tilde{f}_{+-+} + \tilde{f}_{++-} \right]
\end{align*}
\]

for all values of \( m_x, m_y, m_z \in \mathbb{Z} \). If numerical resources are not a problem, these projectors can be used to transform a periodic box code into one that sets idealized boundary conditions on the walls of a cube with half that size. Otherwise, it is strongly advised to make dedicated codes using sine and cosine transforms.

### 4.6.2 Validation of the adjoint model

We perform a perturbation study to test the validity of the adjoint model. We remove the normalization constraint on the flow field \( \mathbf{u} \), and test the integral term and the pressure term in the variational derivative \( \delta \mathcal{L}/\delta \mathbf{u} \). Let \( u_i(m_x, m_y, m_z) \) be a Fourier mode of the basis vector for a random solenoidal flow field \( \mathbf{u} \), \( i = x, y, z \), we calculate

\[
\delta \mathcal{L}_i(m_x, m_y, m_z) = \left\langle u_i(m_x, m_y, m_z) \cdot \left( \int_0^T \mathbf{B}^\dagger \times (\nabla \times \mathbf{B}) \, dt + \nabla \Pi_1 \right) \right\rangle. \tag{4.63}
\]

Then we add a small perturbation \( \epsilon \, u_i(m_x, m_y, m_z) \) to the flow field \( \mathbf{u} \), and launch a forward model for each perturbed mode with \( \tilde{\mathbf{u}} = \mathbf{u} + \epsilon \, u_i(m_x, m_y, m_z) \), the final magnetic energy after each forward time integration is \( \langle \mathbf{B}_T^2(i, m_x, m_y, m_z) \rangle \). The difference field \( \mathbf{D} \) measures the difference between the value obtained from the perturbation study and from the adjoint model, each component is given by

\[
D_i(m_x, m_y, m_z) = \frac{1}{\epsilon} \left( \ln \langle \mathbf{B}_T^2(i, m_x, m_y, m_z) \rangle - \ln \langle \mathbf{B}_T^2 \rangle \right) - \delta \mathcal{L}_i(m_x, m_y, m_z). \tag{4.64}
\]

Since all four setups use the same algorithm, we only tested the NNT case. We use a The results show good agreement, see Figure 4.15.
4.6.3 Calculation of the Lagrange multipliers

In this section we show how the value of Lagrange multiplier is calculated in order to satisfy the normalization for the update fields. Taking the velocity field update for example,

\[
u_{\text{new}} := \nu + \epsilon_u \delta \mathcal{L} \delta \nu,
\]

(4.65)

The expression of \( \epsilon_u \) then has a simple form in Fourier space in Cartesian coordinates:

\[
\epsilon_u = \frac{\Delta_1}{2 \lambda_1 \pi^2 m^2}
\]

(4.66)

where \( m \) is the total wave number. To calculate \( \lambda_1 \), we demand

\[
\langle \nu_{\text{new}}^2 \rangle = \langle \nu^2 \rangle = 1.
\]

(4.67)

This then gives

\[
(-8 + 4\Delta_1) \lambda_1^2 + 4\nu(1 - \Delta_1) \left[ \int_0^T \mathbf{B} \times (\nabla \times \mathbf{B}^\dagger) \ dt + \nabla \Pi_1 \right] \lambda_1
\]

\[
+ \frac{\Delta_1}{m^2} \left( \int_0^T \mathbf{B} \times (\nabla \times \mathbf{B}^\dagger) \ dt + \nabla \Pi_1 \right)^2 = 0
\]

(4.68)

We take the positive root since we are looking for the maximum of \( \mathcal{L} \).

The initial magnetic field is also updated using the same method:

\[
\mathbf{B}_0 := \mathbf{B}_0 + \epsilon_B \frac{\delta \mathcal{L}}{\delta \mathbf{B}_0}
\]

(4.69)

where

\[
\epsilon_B = \frac{\Delta_2}{2 \lambda_2}
\]

(4.70)

The normalization condition for the new field is:

\[
\langle \mathbf{B}_0^2 \rangle = \langle \mathbf{B}_0^2 \rangle = 1
\]

(4.71)
Substitute and simplify the equation, we now get the polynomial for $\lambda_2$,

\[
(-8 + 4\Delta_2)\lambda_2^2 + 4B_0(1 - \Delta_2) \left( B_0^\dagger + \nabla \Pi_2 \right) \lambda_2 + \Delta_2 \left( B_0^\dagger + \nabla \Pi_2 \right)^2 = 0, \quad (4.72)
\]

and we again choose a positive root.
Chapter 5

Optimal kinematic dynamos in a sphere (no-slip B.C.)

Based on manuscript: The optimal kinematic dynamo driven by steady flows in a sphere. Long Chen, Wietze Herreman, Kuan Li, Philip W. Livermore, Jiawen Luo, and Andrew Jackson.

5.1 Introduction

In Chapter 4 we tested the optimization algorithm in Cartesian coordinates. In this chapter we explore what is the optimal dynamo in a geophysically relevant spherical geometry. We perform our modelling in a full sphere so we can take advantage of a specially designed Galerkin basis. In principle the variational method can also be adapted to a spherical shell, but we do not consider it at the moment.

This model uses an electrically insulating magnetic boundary condition that is rather general and appeared in many numerical models. The fluid is confined inside the sphere. First we test the model with no-slip boundary conditions so the flow field is zero at the boundary. We later consider possible free-slip flows as a second stage project in the next chapter.

The transition from a cube to a sphere is not a simple one because the entire approach has to be adjusted. First of all, the boundary conditions pose new challenges on the Lagrangian formulation. The Lagrangian has to be modified so that the boundary terms add up to zero and we get a consistent formulation. Second, from a numerical point of view, the Galerkin method requires a different spectral representation in a spherical model. We need to change the numerical solver in order to be compatible with the new Galerkin basis. Below we just highlight some of the changes we made in spherical coordinates and show the benchmark results, a more detailed description will be in the methods section §5.2. We present our results in §5.3, followed by the conclusions in §5.4.
5.1.1 Lagrangian formalism

New challenges arise from the boundary conditions. Recall there is a boundary term that is related to the adjoint current \( J^\dagger = Rm^{-1} \nabla \times \mathbf{B}^\dagger \) in the cube model,

\[
BT = \int_0^T \oint_\Sigma (J^\dagger \times \delta \mathbf{B}) \cdot \mathbf{n} \, dS \, dt + \cdots
\]  

(5.1)

In spherical models with insulating boundary conditions, supposing \( \mathbf{B}^\dagger \) is represented by the same basis as \( \mathbf{B} \), neither \( \mathbf{B} \times \hat{r} \) nor \( J^\dagger \times \hat{r} \) at the sphere surface are necessarily zero. This apparent issue is solved by including the external insulating region as part of the domain, so the surface of the sphere now becomes an “internal” boundary. If the variations on each side of the inner boundary are equal but have opposite sign, they will cancel each other. However, there is a jump discontinuity in conducting \( \sigma \) from highly conductive to insulating across the sphere surface. Ohm’s law cannot link the current \( \mathbf{J} \) to the electric field \( \mathbf{E} \) in an insulating region. Thus the cube formulation that relies on the induction equation as a constraint breaks down. We therefore turned our attention to a primitive format where we can directly use the interface conditions of \( \mathbf{B} \) and \( \mathbf{E} \) in (1.11). The induction equation constraint in the Lagrangian is split into two parts:

\[
- \int_0^T \langle \mathbf{B}^\dagger \cdot [\partial_t \mathbf{B} + \nabla \times \mathbf{E}] \rangle \, dt - \int_0^T \langle \mathbf{E}^\dagger \cdot [\sigma \mathbf{E} + Rm \mathbf{u} \times \mathbf{B} - \nabla \times \mathbf{B}] \rangle \, dt.
\]  

(5.2)

The parameter \( \sigma_r \) is a relative conductivity and \( Rm \) is fixed as usual. More details regarding the Lagrangian formulation are given in §5.2.2.

5.1.2 A new Galerkin method

We constructed an entirely new adjoint model and update scheme for this optimization problem. Compared to another variational problem built on kinematic dynamo models by Li et al. [2011], there are several differences. In Li et al. [2011], the adjoint induction term is computed in two steps: first it is projected onto a basis without a specified boundary condition, then the undesired pressure term is removed by solving an inverse Poisson problem; the model itself does not include the external region. Here we directly project the adjoint induction term onto the all space magnetic field basis. The flow field uses a special Galerkin basis such that the Laplacian operator is represented by a diagonal matrix,

\[
\langle - \mathbf{u}_{nml} \cdot \nabla^2 \tilde{\mathbf{u}}_{n\tilde{m}\tilde{l}} \rangle = \delta_{nn}\delta_{m\tilde{m}}\delta_{l\tilde{l}}
\]  

(5.3)

for a basis vector field \( \mathbf{u}_{nml} \) with radial function level \( n \), spherical harmonic order \( m \) and spherical harmonic degree \( l \). We will see later in the optimization loop that this special norm simplifies the update step, but we have to be careful since our Galerkin basis is not orthonormal with respect to the usual kinetic norm \( \langle \mathbf{u}_{nml} \cdot \mathbf{u}_{n\tilde{m}\tilde{l}} \rangle \) (without the factor of 1/2 in the definition). Numerical code for the forward model was provided by Dr. Kuan Li.
5.1.3 Benchmark result

We benchmark the growth rate $\gamma$ of the magnetic eigenmode excited by a selected flow field for different resolutions, we also test the threshold of $Rm_t$ for non-negative transient growth. We first benchmark our forward model using an axisymmetric MDJ $t_1s_2$ flow [Livermore & Jackson, 2005]. We use three different spectral resolutions and the results are shown in Table 5.1. We see that the highest resolution $(l_{\text{max}}, n_{\text{max}}) = (32, 32)$ gives the best match with the expected growth rate, but a smaller resolution $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$ is good enough to give 3 decimal places of accuracy and has much less computational cost. For most of the optimization, we use either $(l_{\text{max}}, n_{\text{max}}) = (16, 8)$ or $(24, 12)$, then for verification purposes we add one more optimization run with $(l_{\text{max}}, n_{\text{max}}) = (24, 24)$. We also reproduced the minimal threshold for positive transient growth generated by MDJ $t_1s_2$ flow in [Livermore & Jackson, 2005]. We fix the flow field and only update the associated magnetic eigenmode in an optimization loop. The results are shown in Figure 5.1. Since the transient optimization uses a very short time window $T$, and we are not in a single mode dominated linear regime, the growth rate in Figure 5.1 a) is only an approximation.

<table>
<thead>
<tr>
<th>$(l_{\text{max}}, n_{\text{max}})$</th>
<th>16, 8</th>
<th>24, 12</th>
<th>32, 32</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$</td>
<td>-6.89873355</td>
<td>-6.92808061</td>
<td>-6.92884872</td>
</tr>
</tbody>
</table>

Table 5.1. Benchmark of the growth rate $\gamma$ for the most unstable magnetic field eigenmode ($m = 0$) generated by the axisymmetric MDJ $t_1s_2$ flow at an enstrophy cased $Rm = 545.9$ (same as $Rm_\omega$), compared with a previously reported value of $\gamma = -6.92884871$ [Livermore & Jackson, 2005]. $l_{\text{max}}$ is the maximal spherical harmonic degree, $n_{\text{max}}$ is the maximal truncation level of the radial expansion.

Figure 5.1. Benchmark result for the optimized transient growth for MDJ $t_1s_2$ flow, $(l_{\text{max}}, n_{\text{max}}) = (24, 24)$. a) Approximate growth rate $\gamma$ as a function of an enstrophy based $Rm$. We get the expected (enstrophy based) $Rm_t \sim 62$. b) Optimized magnetic norm as a function of time near $Rm_t$. 

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5.2 Methods

5.2.1 Definition of the optimization objective

Consider a sphere \( V \) of unit radius filled with an electrically conducting fluid. Outside the sphere, we suppose a current free region \( \hat{V} \) that extends to infinity. We denote by \( \Sigma_\pm \) the outer surface (+) and inner surface (−) of the sphere at the interface between \( V \) and \( \hat{V} \). In a kinematic approach, the magnetic field \( B \) needs to satisfy the non-dimensional equations

\[
\begin{align*}
\partial_t B &= Rm \nabla \times (u \times B) - \nabla \times (\nabla \times B), & x \in V, \\
\nabla \times B &= 0, & x \in \hat{V}, \\
\nabla \cdot B &= 0, & x \in V \cup \hat{V},
\end{align*}
\]

where (5.4) is the induction equation, (5.5) is the current-free condition, (5.6) is Gauss’ law for magnetism, and also the continuity condition

\[ B|_{\Sigma_+} - B|_{\Sigma_-} = 0. \]  

In this model, the flow field \( u = u(x) \) lives within the parameter space \( \mathcal{E}_u \) of steady and incompressible flows with no-slip boundary conditions such that \( \forall \ u \in \mathcal{E}_u, \)

\[ \nabla \cdot u = 0, \quad x \in V, \]  

and the boundary condition

\[ u|_{\Sigma_-} = 0. \]  

We furthermore demand a unit non-dimensional root mean enstrophy \( (\omega = 1) \), where

\[ \omega = \sqrt{\frac{1}{V} \int_V (\nabla \times u)^2 dV}. \]

If \( L, \eta \) denote dimensional values for the spherical radius and the fluid’s magnetic diffusivity, then (5.4) has been non-dimensionalized using units \( [u] = \omega^* L, [x] = L \) and \( [t] = L^2/\eta \), where \( \omega^* \) is the dimensional root mean enstrophy. The magnetic Reynolds number is then defined as

\[ Rm = \frac{\omega^* L^2}{\eta}. \]

In this model, due to no-slip boundary conditions (5.9), the dimensional root mean enstrophy \( \omega^* = S \), where \( S = \sqrt{\frac{1}{V} \int_V 2e_{ij}e_{ij} dV} \) is the global shear magnitude, and \( e_{ij}, \ i, j = r, \theta, \phi \) is the dimensional strain rate tensor. Then \( Rm \) can also be expressed using \( S \).

Since the flow is steady, the kinematic dynamo problem admits exponential solutions for the magnetic field

\[ B(x, t) \sim b(x) e^{(\gamma + \alpha_t)t} \]  

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where \( b(x) \) is an eigenvector, \( \gamma \) is the growth rate and \( \Omega \) is an oscillation frequency. As \( t \to \infty \), one can expect that the eigenvector with the largest growth rate will grow out from an arbitrary noisy initial magnetic field \( B_0 = B(x, 0) \). In this optimisation study, we want to identify which flow field \( u \in \mathcal{E}_u \) can maximize the growth rate \( \gamma \) for a given value of \( Rm \). We also calculate the lower bound on the critical magnetic Reynolds number, denoted by \( Rm_{c, \text{min}} \), below which no kinematic dynamo is possible \( \forall u \in \mathcal{E}_u \). Note here it is necessary to use the enstrophy normalization for reasons explained in the introduction.

### 5.2.2 Euler-Lagrange formalism in primitive format

Since we want to optimize the growth rate \( \gamma \), it seems most obvious to propose an optimization method that directly maximizes \( \gamma \). This can indeed be done in low-dimensional optimisation problems, see for example Holme [2003]. Considering the huge dimension of the functional space \( \mathcal{E}_u \) we have, optimizing the growth rate directly is not the easiest method to put in practice. Instead, we adapt the optimisation strategy of Willis [2012], Chen et al. [2015], and Herreman [2016] that proved successful in a cubic geometry. These methods are designed to find the best flow field \( u \) and the best seed magnetic field \( B_0 \) that maximize \( \frac{1}{V} \int_V B_T^2 \, dV \). The field \( B_T = B(x, T) \) is the magnetic field at some finite time \( T \) that needs to be long enough to overcome initial transient growth phases. Optimizing the initial \( B_0 \) then allows us to reach this exponential regime faster. The variational method we use here is built on the following Lagrangian:

\[
\mathcal{L} = \ln \langle B_T^2 \rangle - \lambda_1 \left( \langle (\nabla \times u)^2 \rangle - 1 \right) - \lambda_2 \left( \langle B_0^2 \rangle - 1 \right) - \langle \Pi \nabla \cdot u \rangle - \int_0^T \langle \psi^\dagger \nabla \cdot B \rangle \, dt - \int_0^T \langle B^\dagger \cdot [\partial_t B + \nabla \times E] \rangle \, dt
- \int_0^T \langle E^\dagger \cdot [\sigma_r E + Rm \, u \times B - \nabla \times B] \rangle \, dt. \quad (5.13)
\]

We denote

\[
\langle \ldots \rangle = \frac{3}{4\pi} \int_0^\infty \int_0^\pi \int_0^{2\pi} \cdots r^2 \sin \theta d\phi d\theta dr,
\]

and suppose that all functions and fields are regular at \( r = 0 \) and decay sufficiently quickly as \( r \to \infty \) for this measure to make sense. The first term in (5.13) is the objective functional that we want to maximize, namely the logarithm of the norm of magnetic field at time \( T \). In the following terms, \( \lambda_1, \lambda_2, \Pi(x), \psi^\dagger(x, t), B^\dagger(x, t) \) and \( E^\dagger(x, t) \) are Lagrange multipliers. The second and third terms normalize \( u \) and \( B_0 \) respectively. The fourth and fifth terms impose the solenoidal conditions on \( u \) and \( B \) respectively. The sixth term and seventh terms impose Faraday’s law and Ampère’s law separately. The number \( \sigma_r \) is a relative conductivity: \( \sigma_r = 1, x \in V \) and \( \sigma_r = 0, x \in \hat{V} \). We suppose that the physical boundary conditions (5.7), (5.9) and

\[
\hat{r} \times (E|_{\Sigma_+} - E|_{\Sigma_-}) = 0 \quad (5.15)
\]
apply to the fields \( \mathbf{B}, \mathbf{u}, \mathbf{E} \) and denote by \( \mathbf{\hat{r}} \) the radial unit vector. Unlike in Willis [2012] and Chen et al. [2015], we include Ampère’s law and Faraday’s law separately in \( \mathcal{L} \) rather than the induction equation (5.4) alone, which is why we speak of a primitive formalism. This step is needed to impose a truly current-free exterior as in (5.5). It allows us to simplify the treatment of boundary terms on \( \Sigma_{\pm} \) that arise in the derivation of the non-trivial Euler-Lagrange (EL) equations. We also impose the solenoidal condition on \( \mathbf{B} \) at all times.

At the optimum the Lagrangian \( \mathcal{L}(\mathbf{u}, \mathbf{B}, \mathbf{B}_0, \mathbf{B}_T, \mathbf{E}, \lambda_1, \lambda_2, \Pi, \psi^\dagger, \mathbf{B}^\dagger, \mathbf{E}^\dagger) \) must be stationary, meaning that \( \delta \mathcal{L} = 0 \) for arbitrary variations in each of its variables. Each variational derivative needs to disappear separately which defines eleven EL equations that define our optimization problem. The physical constraints define six equations: the solenoidal conditions as in (5.6) and (5.8), the normalization constraints on \( \mathbf{B}_0 \) and \( \mathbf{u} \), Ampère’s law and Faraday’s law. The remaining five non-trivial variational derivatives are

\[
\begin{align*}
\frac{\delta \mathcal{L}}{\delta \mathbf{B}_T} &= \frac{2\mathbf{B}_T}{\langle \mathbf{B}_T^2 \rangle} - \mathbf{B}_T^\dagger, \\
\frac{\delta \mathcal{L}}{\delta \mathbf{E}} &= -\sigma_r \mathbf{E}^\dagger - \nabla \times \mathbf{B}^\dagger, \\
\frac{\delta \mathcal{L}}{\delta \mathbf{B}} &= \partial_t \mathbf{B}^\dagger + \text{Rm} \mathbf{u} \times \mathbf{E}^\dagger + \nabla \times \mathbf{E}^\dagger + \nabla \psi^\dagger, \\
\frac{\delta \mathcal{L}}{\delta \mathbf{u}} &= \text{Rm} \int_0^T \mathbf{B} \times (-\sigma_r \mathbf{E}^\dagger) \, dt - 2\lambda_1 \nabla \times \nabla \times \mathbf{u} + \nabla \Pi, \\
\frac{\delta \mathcal{L}}{\delta \mathbf{B}_0} &= \mathbf{B}_0^\dagger - 2\lambda_2 \mathbf{B}_0,
\end{align*}
\]

where \( \mathbf{B}_T^\dagger = \mathbf{B}^\dagger(\mathbf{x}, T) \), and \( \mathbf{B}_0^\dagger = \mathbf{B}^\dagger(\mathbf{x}, 0) \). In our numerical method, we can directly set the variational derivative (5.16)-(5.18) to zero, thus gives us another three EL equations. The remaining two variational derivatives (5.19) and (5.20) are not zero unless \( \mathcal{L} \) is at its optimum, so they are used as descent directions. In brief, nine “primitive” EL equations are used as constraints in optimization and two variational derivatives are needed to update the initial conditions.

Because of (5.17) and the presence of \( \nabla \psi^\dagger \) in (5.18), the adjoint magnetic field has a gauge freedom \( \mathbf{B}^\dagger \rightarrow \mathbf{B}^\dagger + \nabla \phi \). Therefore, we can add the supplementary requirement that

\[
\nabla \cdot \mathbf{B}^\dagger = 0. \tag{5.21}
\]

Note that this choice is compatible with (5.16) and necessary for (5.20) to remain within the same parameter space as \( \mathbf{B} \). We also need to address the boundary terms that are generated in the process of deriving the non-trivial EL equations. To give an example, the partial integration

\[
- \langle \Pi \nabla \cdot \delta \mathbf{u} \rangle = \langle \nabla \Pi \cdot \delta \mathbf{u} \rangle - \int_\Sigma \Pi(\mathbf{\hat{r}} \cdot \delta \mathbf{u}) \mathbf{\hat{r}} \cdot dS, \tag{5.22}
\]

generates the contribution \( \nabla \Pi \) to \( \delta \mathcal{L}/\delta \mathbf{u} \) and also one boundary term that appears as an integral over the surface of the sphere. In this problem there are quite a few
boundary terms and their sum needs to cancel at the optimum in order to have a consistent theory. We find

\[
0 = \oint \Pi (\hat{r} \cdot \delta u)\big|_{\Sigma_-} dS - \oint 2\lambda_1 \left[ \delta u \times (\nabla \times u) \right] \cdot \hat{r}\big|_{\Sigma_-} dS \\
+ \int_0^T \oint \left[ (\hat{r} \times B^\dagger) \cdot \delta E\big|_{\Sigma_-} - (\hat{r} \times B^\dagger) \cdot \delta E\big|_{\Sigma_+} \right] dS dt \\
+ \int_0^T \oint \left[ (\hat{r} \times E^\dagger) \cdot \delta B\big|_{\Sigma_-} - (\hat{r} \times E^\dagger) \cdot \delta B\big|_{\Sigma_+} \right] dS dt \\
- \int_0^T \oint \left[ \psi^\dagger (\hat{r} \cdot \delta B)\big|_{\Sigma_-} - \psi^\dagger (\hat{r} \cdot \delta B)\big|_{\Sigma_+} \right] dS dt.
\]

(5.23)

Normally one would expect having boundary terms from variations on the surface of \( \hat{V} \) situated infinitely far away. In this model, the magnetic field \( B \) decays at least as fast as \( r^{-3} \) in the insulating region \( \hat{V} \), where \( r \) is the distance to the origin, so the boundary variations on the surface of \( \hat{V} \) as \( r \to \infty \) are negligible. If we suppose that the field variations \( \delta u \) satisfy no-slip conditions (5.9), the first two boundary terms are zero. Then, the inclusion of the \( \hat{V} \) region allows us to cancel the remaining boundary terms by matching them from \( \Sigma_- \) to \( \Sigma_+ \). Supposing continuity of the magnetic field \( \delta B \) and the tangential electrical field variations \( \delta E \) (5.7), (5.15), we combine the remaining terms into

\[
0 = \int_0^T \oint \left[ (\hat{r} \times (B^\dagger|_{\Sigma_-} - B^\dagger|_{\Sigma_+})) \cdot \delta E\big|_{\Sigma_-} \right] dS dt \\
+ \int_0^T \oint \left[ (\hat{r} \times (E^\dagger|_{\Sigma_-} - E^\dagger|_{\Sigma_+})) \cdot \delta B\big|_{\Sigma_-} \right] dS dt \\
- \int_0^T \oint \left[ \psi^\dagger (\hat{r} \cdot \delta B)\big|_{\Sigma_-} - \psi^\dagger (\hat{r} \cdot \delta B)\big|_{\Sigma_+} \right] dS dt.
\]

(5.24)

This expression cannot be further reduced using the boundary conditions of the field variations and simply informs us that the adjoint fields need to satisfy the boundary conditions

\[
\psi^\dagger|_{\Sigma_+} - \psi^\dagger|_{\Sigma_-} = 0, \quad \hat{r} \times (B^\dagger|_{\Sigma_+} - B^\dagger|_{\Sigma_-}) = 0, \\
\hat{r} \times (E^\dagger|_{\Sigma_+} - E^\dagger|_{\Sigma_-}) = 0.
\]

(5.25)

From the solenoidal condition of the adjoint magnetic field (5.21), we find a supplementary condition

\[
\hat{r} \cdot (B^\dagger|_{\Sigma_+} - B^\dagger|_{\Sigma_-}) = 0.
\]

(5.26)

In other words, by requiring the sum of all boundary terms to vanish, we just derived the continuity conditions for \( \psi^\dagger, B^\dagger \) and \( E^\dagger \). This brings us to the conclusion that, with the gauge (5.21), adjoint fields \( B^\dagger \) and \( E^\dagger \) satisfy the exact same boundary conditions as the direct fields \( B \) and \( E \). This is an eminently desirable property, since it allows us to use the same solenoidal Galerkin expansions for both direct field \( B \) and adjoint field \( B^\dagger \).
5.2.3 Reduced set of Euler-Lagrange equations

Now we have dealt with the boundary terms, we can eliminate the fields $E$ and $E^\dagger$ from the previous “primitive” set of EL equations and present the reduced set of EL equations that we will actually solve. Upon initialization and at each iteration in the optimisation loop, we must have the flow field $u$ and a seed magnetic field $B_0$ that satisfy the normalization constraints

$$
\langle (\nabla \times u)^2 \rangle = 1, \quad \langle B_0^2 \rangle = 1,
$$

the solenoidal conditions (5.6) and (5.8), and the boundary conditions (5.7) and (5.9). Note that the flow field is entirely confined to the sphere so the all-space integration (7.10) does not change the enstrophy norm defined in (7.8).

In the optimization loop itself, we have three parts on which we iterate. First we solve the forward/direct problem. By combining Ampère’s law and Faraday’s law in region $V$, we solve the induction equation (5.4) forward in time for $t: 0 \rightarrow T$ and subject to the solenoidal condition (5.6) and boundary conditions (5.7). With the direct field $B_T$ known, we can then initialize the adjoint magnetic field at time $t = T$ as

$$
B_T^\dagger = \frac{2B_T}{\langle B_T^2 \rangle}.
$$

Elimination of $E^\dagger$ in the adjoint Ampères and Faraday’s laws (5.17) and (5.18), yields the adjoint problem:

$$
\begin{align*}
\partial_t B^\dagger &= Rm \mathbf{u} \times (\nabla \times B^\dagger) + \nabla \times \nabla \times B^\dagger - \nabla \psi^\dagger, & \mathbf{x} \in V, \\
\nabla \times B^\dagger &= 0, & \mathbf{x} \in \hat{V}, \\
\nabla \cdot B^\dagger &= 0, & \mathbf{x} \in V \cup \hat{V}.
\end{align*}
$$

In the second part, we solve (5.29) backward in time for $t: T \rightarrow 0$ while respecting the solenoidal condition (5.21) and the boundary conditions (5.25)-(5.26).

In the third part we need to consider the update using variational derivatives (5.19) and (5.20) which lead to the only two EL equations that are not automatically satisfied. We iterate through the optimisation loop so that $\delta L/\delta u \rightarrow 0$ and $\delta L/\delta B_0 \rightarrow 0$. To calculate the integral in $\delta L/\delta u$, we must know $B$ and $B^\dagger$ at all times. Multipliers $\lambda_1$, $\lambda_2$, $\Pi$ are still undetermined. As in Chen et al. [2015] and Pringle et al. [2012b], we use a preconditioned descent method in which we use only part of the second variation

$$
\delta^2 L \approx 2\lambda_1 \langle \delta u \cdot \nabla^2 \delta \mathbf{u} \rangle - 2\lambda_2 \langle \delta B_0 \cdot \delta B_0 \rangle + \ldots
$$

with respect to variables $\mathbf{u}$ and $B_0$ to allow faster convergence. To be more specific, let us denote the update as

$$
\begin{align*}
\mathbf{u} : &= \mathbf{u} + \alpha_1 \Delta \mathbf{u}, \\
B_0 : &= B_0 + \alpha_2 \Delta B_0,
\end{align*}
$$

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with $\alpha_1, \alpha_2 \ll 1$ two relaxation parameters. We calculate the increments $\Delta u$ and $\Delta B$ as if (5.32) would be exact and as if $\alpha_1 = \alpha_2 = 1$ would correspond to a Newton step, which sets

$$\frac{\delta L}{\delta u} + 2\lambda_1 \nabla^2 u = 0, \quad (5.34)$$

$$\frac{\delta L}{\delta B_0} - 2\lambda_2 \Delta B = 0. \quad (5.35)$$

The magnetic field update is always rather trivial, since we can explicitly evaluate $\Delta B_0$, to arrive at

$$B_0 := B_0 + \frac{\alpha_2}{2\lambda_2} \frac{\delta L}{\delta B_0}. \quad (5.36)$$

The value of $\lambda_2$ is finally set by requiring that the updated $B_0$ remains normalized as (5.27). Note that the magnetic field will automatically satisfy the right boundary conditions after this update. The velocity field update is much less trivial. Due to the presence of the Laplacian operator $\nabla^2$ in front of $\Delta u$, we cannot write at this point an explicit update formula for the flow. There is also a second difficulty: owing to formula (5.19) for $\delta L/\delta u$, there is no guarantee that the updated velocity field will automatically satisfy the no-slip boundary conditions. We tackle both issues, by projecting the flow $u$ on a very particular vector field basis that is defined below and so we postpone the explicit equation for the velocity field update to §2.5.

### 5.2.4 Galerkin expansions for $u$, $B$ and $B^\dagger$

We solve this optimization problem using a Galerkin method. This method builds the solenoidal condition and boundary conditions into the field expansions of $u$, $B$ and $B^\dagger$. We denote

$$\begin{bmatrix} u \\ B \\ B^\dagger \end{bmatrix} = \sum_{n=1}^{n_{\text{max}}} \sum_{l=-l_{\text{max}}}^{l_{\text{max}}} \sum_{m=-l}^{l} \begin{bmatrix} v_{nml} \ u_{nml}^t + w_{nml} \ u_{nml}^p \\ c_{nml} \ B_{nml}^t + d_{nml} \ B_{nml}^p \\ c_{nml}^\dagger \ B_{nml}^{t\dagger} + d_{nml}^\dagger \ B_{nml}^{p\dagger} \end{bmatrix}. \quad (5.37)$$

Here $v_{nml}, w_{nml}, c_{nml(t)}, d_{nml(t)}, c_{nml}^\dagger, d_{nml}^\dagger$ are the spectral coefficients. We can use the same basis vector fields of $B$ to represent $B^\dagger$ since the adjoint magnetic field is solenoidal in the present gauge and because it satisfies the same boundary conditions as $B$. We use

$$u_{nml}^t(r, \theta, \phi) = \begin{cases} \nabla \times (l_{n}^{\ell}(r) \ Y_{l}^{m}(\theta, \phi) \hat{r}), & r \in V, \\ 0, & r \in \hat{V}, \end{cases} \quad (5.38)$$

$$u_{nml}^p(r, \theta, \phi) = \begin{cases} \nabla \times \nabla \times (s_{n}^{\ell}(r) \ Y_{l}^{m}(\theta, \phi) \hat{r}), & r \in V, \\ 0, & r \in \hat{V}, \end{cases}$$
\[
\mathbf{B}_{\text{nnl}}^\parallel (r, \theta, \phi) = \begin{cases} 
\nabla \times (q_n^l(r) Y_l^m(\theta, \phi)\hat{r}) , & r \in V, \\
0, & r \in \hat{V}, 
\end{cases}
\]
\[
\mathbf{B}_{\text{nnl}}^\perp (r, \theta, \phi) = \begin{cases} 
\nabla \times \nabla \times (p_n^l(r) Y_l^m(\theta, \phi)\hat{r}) , & r \in V, \\
-lp_n^l(1) \nabla (r^{-l-1} Y_l^m(\theta, \phi)) , & r \in \hat{V}, 
\end{cases}
\] (5.39)

as the toroidal (with a superscript \(t\)) and poloidal (with a superscript \(p\)) basis vector fields for \(\mathbf{u}\) and \(\mathbf{B}\). In this notation, \(Y_l^m(\theta, \phi)\) are the spherical harmonics.

For the flow field \(\mathbf{u}\) we use the polynomials
\[
t_n^l(r) = T_{nl} r^{l+1} \left( P_{n-1}^{(0,l+1/2)} (2r^2 - 1) - P_{n-1}^{(0,l+1/2)} (2r^2 - 1) \right),
\] (5.40)
\[
s_n^l(r) = S_{nl} r^{l+1} \sum_{i=1}^{3} c_i P_{n+2-i}^{(0,l+1/2)} (2r^2 - 1),
\]
\[
c_1 = 2l + 4n + 1,
\]
\[
c_2 = -2(2l + 4n + 3),
\]
\[
c_3 = 2l + 4n + 5,
\] (5.41)

and for the magnetic field \(\mathbf{B}\) we use
\[
q_n^l(r) = Q_{nl} r^{l+1} (1 - r^2) P_{n-1}^{(2,l+1/2)} (2r^2 - 1),
\] (5.42)
\[
p_n^l(r) = P_{nl} r^{l+1} \left( c_1 P_{n}^{(0,l+1/2)} (2r^2 - 1) + c_2 P_{n-1}^{(0,l+1/2)} (2r^2 - 1) \right),
\]
\[
c_1 = n(2l + 2n - 1),
\]
\[
c_2 = -(n + 1)(2n + 2l + 1).
\] (5.43)

Here \(n = 1, \ldots, n_{\text{max}}\) and \(l = 1, \ldots, l_{\text{max}}\) and \(P_{\lambda}^{(\alpha, \beta)}\) are Jacobi polynomials. The numbers \(T_{nl}, S_{nl}, Q_{nl}\) and \(P_{nl}\) are normalization factors. The procedure of constructing this polynomial basis is described by Livermore & Ierley [2010], Livermore [2009], and Livermore [2010]. In Appendix 5.5.1 we provide more technical details on how to use this basis. Here we only present the essential properties:

1. All basis fields are infinitely differentiable at the origin \(r = 0\). This gives the form of the polynomials as \(r^{l+1}(a_0 + a_1 r^2 + a_2 r^4 + \cdots)\) for each \(l\).

2. All basis fields satisfy boundary conditions at \(r = 1\). These are no-slip boundary conditions for the flow field and continuity conditions for the magnetic field. This requires
\[
t_n^l(1) = 0, \quad s_n^l(1) = \frac{\partial s_n^l}{\partial r}(1) = 0, \quad q_n^l(1) = 0, \quad \frac{\partial p_n^l(1)}{\partial r} + l p_n^l(1) = 0,
\] (5.44)

for the radial functions.
3. The vector field basis is orthonormal with respect to a predefined inner product. Here we have chosen to use
\[
\langle (\nabla \times u^l_{nml}) \cdot (\nabla \times u^l_{n'm'l'}) \rangle = \delta_{nn'}\delta_{mm'}\delta_{ll'},
\]
and
\[
\langle (\nabla \times u^p_{nml}) \cdot (\nabla \times u^p_{n'm'l'}) \rangle = \delta_{nn'}\delta_{mm'}\delta_{ll'},
\]
(5.45)
These scalar products are positive definite and symmetric and they have particular benefits when it comes to calculating norms both full and partial:
\[
\langle (\nabla \times u)^2 \rangle = \langle (\nabla \times u^l)^2 \rangle + \langle (\nabla \times u^p)^2 \rangle = \sum_{l,m,n} v_{nml}^2 + w_{nml}^2,
\]
(5.47)
\[
\langle B^2 \rangle = \langle (B^l)^2 \rangle + \langle (B^p)^2 \rangle = \sum_{l,m,n} c_{nml}^2 + d_{nml}^2,
\]
(5.48)
\[
\langle (\nabla \times u_{m,n})^2 \rangle = \sum_{m,n} v_{nml}^2 + w_{nml}^2,
\]
(5.49)
\[
\langle (\nabla \times u^l_{m,n})^2 \rangle = \sum_{m,n} v_{nml}^2 + w_{nml}^2,
\]
(5.50)
\[
\langle (\nabla \times u^p_{m,n})^2 \rangle = \sum_{m,n} v_{nml}^2 + w_{nml}^2,
\]
(5.51)
where superscript \(p\) and \(t\) refer to the poloidal and toroidal components, and partial sums of \(B\) follow the same convention as in (5.49)–(5.51). Using partial integration, the no-slip boundary conditions, and the solenoidal property of the basis functions, we also have
\[
\langle -u^l_{nml} \cdot \nabla^2 u^l_{n'm'l'} \rangle = \delta_{nn'}\delta_{mm'}\delta_{ll'},
\]
\[
\langle -u^p_{nml} \cdot \nabla^2 u^p_{n'm'l'} \rangle = \delta_{nn'}\delta_{mm'}\delta_{ll'},
\]
(5.52)
which simplifies the update step for the flow.

5.2.5 The optimization algorithm
We initialize the algorithm with randomly distributed spectral coefficients or we restart from previously stored fields. In all cases the initial coefficients are normalized such that
\[
\sum_{l,m,n} v_{nml}^2 + w_{nml}^2 = 1, \quad \sum_{l,m,n} c_{nml}^2 + d_{nml}^2 = 1.
\]
(5.53)
We then enter the optimization loop. Each iteration consists of an initialization (possibly combined with an update), a forward integration, a backward integration and an update, similar to that of Kerswell et al. [2014].
We inject the field expansion into the forward problem (5.4) and project it onto the magnetic field basis using the orthonormality condition. This gives a system of ordinary differential equations

\[ \partial_t c_{nml} = R_m a_{nml} + \sum_{n'} T_{nn'} c_{n'ml}, \]
\[ \partial_t d_{nml} = R_m b_{nml} + \sum_{n'} P_{nn'} d_{n'ml}, \]

(5.54)
to be integrated for \( t : 0 \to T \). On the right hand side, the matrix elements

\[ T_{nn'} = \langle B^t_{nml}, \nabla^2 B^t_{n'ml} \rangle, \]
\[ P_{nn'} = \langle B^p_{nml}, \nabla^2 B^p_{n'ml} \rangle, \]

(5.55)
capture the effect of magnetic diffusion; they are precomputed in Mathematica. More explicit expressions are given in the Appendix 5.5.1.2. The spectral coefficients of the induction term projected onto the basis vector fields are

\[ a_{nml} = \langle B^t_{nml}, [\nabla \times (u \times B)] \rangle, \]
\[ b_{nml} = \langle B^p_{nml}, [\nabla \times (u \times B)] \rangle. \]

(5.56)

(5.57)

To calculate these terms in practice, we choose to introduce a physical space grid that is composed of Fourier grid points along \( \phi \) and Gaussian quadrature points along \( r \) and \( \theta \), see Appendix 5.5.1.5. The numerical scheme for time-integration is Crank-Nicolson for the diffusive terms and second order Adams-Bashforth for the induction terms.

The initialization condition for the adjoint magnetic field is given by the direct magnetic field at time \( T \) as in (5.16). In terms of spectral coefficients, we have

\[ c_{nml}^+(T) = \frac{2 c_{nml}(T)}{\sum_{l,m,n} c_{nml}(T)^2 + d_{nml}(T)^2}, \]
\[ d_{nml}^+(T) = \frac{2 d_{nml}(T)}{\sum_{l,m,n} c_{nml}(T)^2 + d_{nml}(T)^2}. \]

(5.58)

(5.59)

A similar projection of the adjoint induction equation (5.29) onto the basis of \( B \) yields

\[ \partial_t c_{nml}^+ = R_m a_{nml}^+ - \sum_{n'} T_{nn'} c_{n'ml}^+, \]
\[ \partial_t d_{nml}^+ = R_m b_{nml}^+ - \sum_{n'} P_{nn'} d_{n'ml}^+, \]

(5.60)

(5.61)

which we integrate backwards in time for \( t : T \to 0 \). The diffusion matrices \( T \) and \( P \) are unchanged from (5.55). The adjoint induction terms are

\[ a_{nml}^+ = \langle B^t_{nml}, [u \times (\nabla \times B^t)] \rangle, \]
\[ b_{nml}^+ = \langle B^p_{nml}, [u \times (\nabla \times B^t)] \rangle. \]

(5.62)

(5.63)
Also here, we calculate these terms by a transformation to physical space, see Appendix 5.5.1.3. We use a similar time-discretisation scheme as in the forward model. The field $\psi^\dagger$ really is never of concern. When we use this Galerkin basis, the projection of $\psi^\dagger$ onto the basis of $B$ gives: $\langle B_{i,nml} \cdot \nabla \psi^\dagger \rangle = \langle B_{i,nml}^{\dagger} \cdot \nabla \psi^\dagger \rangle = 0$.

The initial magnetic field update is easy to understand, since we can directly project the update formula (5.36) onto the vector field basis. In terms of spectral coefficients, we have

$$c_{nml}(0) := c_{nml}(0) + \frac{\alpha_2}{2\lambda_2} \left( c_{nml}^{\dagger}(0) - 2\lambda_2 c_{nml}(0) \right)$$

$$d_{nml}(0) := d_{nml}(0) + \frac{\alpha_2}{2\lambda_2} \left( d_{nml}^{\dagger}(0) - 2\lambda_2 d_{nml}(0) \right)$$

(5.64) (5.65)

where $\delta c_{nml}$ and $\delta d_{nml}$ denote the incremental change of spectral coefficient between consecutive iterations. By requiring that the updated seed magnetic field remains normalized, we find a quadratic polynomial that sets $\lambda_2$:

$$\sum_{l,m,n} 4\lambda_2^2 (\alpha_2 - 2) + 4\lambda_2 (1 - \alpha_2)(c_{nml}(0) c_{nml}^{\dagger}(0) + d_{nml}(0) d_{nml}^{\dagger}(0))$$

$$+ \alpha_2 \left( c_{nml}^{\dagger}(0)^2 + d_{nml}^{\dagger}(0)^2 \right) = 0.$$  

(5.66)

We choose the largest positive root of $\lambda_2$, since we want to maximize $\mathcal{L}$.

To update $u$, we must first calculate the integral term that appears in $\delta \mathcal{L}/\delta u$. We store the spectral coefficients $c_{nml}(t_i)$ and $d_{nml}(t_i)$ of $B$ at all discrete times. Since the code is parallelized for a distributed memory architecture, a checkpointing strategy is not required. During the backward time integration, we then calculate the integral, projected on the basis, using the trapezoidal rule:

$$V_{nml} = \sum_{i=0}^{N} \beta_i \Delta t \left( u_{nml}^{t_i} \cdot \left[ B_{i} \times (\nabla \times B_{i}^{\dagger}) \right] \right),$$

$$W_{nml} = \sum_{i=0}^{N} \beta_i \Delta t \left( u_{nml}^{p} \cdot \left[ B_{i} \times (\nabla \times B_{i}^{\dagger}) \right] \right).$$

(5.67)

Here we denote $B_{i} = B(\mathbf{x}, t_i)$, $\Delta t$ is the timestep size, $N$ is the total number of timesteps and $\beta_0 = \beta_N = 0.5$, $\beta_i = 1$, $\forall i \in 1, \ldots, N - 1$ integration weights. In a similar vein to the calculation of the induction terms, we need a transformation to physical space to calculate the volume integrals that appear in (5.67) because of the non-linear terms, see Appendix 5.5.1.3. We expand the field $\Delta u$ onto the vector field basis of $u$ and project (5.34) onto the vector field basis. Using the property (5.52), we then find an explicit formula for the spectral coefficients of $\Delta u$ that finally sets the update formula for the spectral coefficients of $u$:

$$v_{nml} := v_{nml} + \frac{\alpha_1}{2\lambda_1} (V_{nml} - 2\lambda_1 v_{nml})$$

$$= v_{nml} + \delta v_{nml},$$

(5.68)
\[ w_{nml} := w_{nml} + \frac{\alpha_1}{2\lambda_1} (W_{nml} - 2\lambda_1 w_{nml}) \]
\[ = w_{nml} + \delta w_{nml}, \quad (5.69) \]

where \( \delta v_{nml} \) and \( \delta w_{nml} \) denote the change in the spectral coefficients of \( u \). The value of \( \lambda_1 \) is calculated by demanding that the normalization constraints (5.27) remain satisfied for the updated field. This leads to a quadratic polynomial for \( \lambda_1 \),
\[ \sum_{l,m,n} 4\lambda_1^2 (\alpha_1 - 2) + 4\lambda_1 (1 - \alpha_1) (V_{nml} v_{nml} + W_{nml} w_{nml}) + \alpha_1 (V_{nml}^2 + W_{nml}^2) = 0, \quad (5.70) \]
and we take again the largest positive root. With this update performed, we return to the forward integration and iterate through the whole loop until convergence. At each iteration in the optimization loop, we measure progress through the incremental change in the fields
\[ r_{B_0}^2 = \sum_{l,m,n} \delta c_{nml}(0)^2 + \delta d_{nml}(0)^2, \]
\[ r_U^2 = \sum_{l,m,n} \delta v_{nml}^2 + \delta w_{nml}^2, \quad (5.71) \]
and the total residue is
\[ r_t = \sqrt{r_U^2 + r_{B_0}^2}. \quad (5.72) \]
Besides tracking the residue, we also follow how \( \langle B_0^2 \rangle \) evolves. We terminate the optimization when \( r_t \) is smaller than a fixed value and when \( \langle B_0^2 \rangle \) no longer changes significantly. The relaxation parameters \( \alpha_1, \alpha_2 \) are prescribed and adjusted depending on the value of \( r_t \) during the optimization. We typically choose \( 0.1 < \alpha_j < 0.5, \ j = 1, 2 \) for the first 5 iterations if starting from random initial conditions, then sharply reduce \( \alpha_1 \) to 0.01. This reduction in \( \alpha_1 \) is to prevent the optimizer from oscillating around a fixed point in the parameter space of \( u \). If the residue \( r_t < 0.005 \), which indicates we are closer to the optimum than at the beginning, we increase the relaxation parameters again to \( 0.04 < \alpha_j < 0.1 \) to speed up convergence. We directly use step size \( 0.04 < \alpha_j < 0.1 \) if restarting from previously stored fields, which in general are moderately converged with a relatively small \( r_t \). The optima we found do not depend on specific values of \( \alpha_j \) within the given range: we repeated the optimizations with different choices of \( \alpha_j \) but nevertheless reached the same optimum.

5.2.6 Degeneracy of the optimum

This optimization problem does not have a unique solution, since symmetry implies an infinite but trivial degeneracy. The symmetry group of the sphere is the orthogonal group \( O(3) \), that includes rotational symmetries and reflection symmetries. Any particular transform in the group can be represented using an
orthogonal matrix $\mathcal{R}$. For any given flow $\mathbf{u}$ or magnetic field $\mathbf{B}$, we can define transformed fields as

$$
\tilde{\mathbf{u}}(\mathbf{x}) = \mathcal{R}^T \mathbf{u}(\mathcal{R}\mathbf{x}), \quad \tilde{\mathbf{B}}(\mathbf{x}, t) = \mathcal{R}^T \mathbf{B}(\mathcal{R}\mathbf{x}, t).
$$

(5.73)

Under the proper transformation rules for the adjoint variables and multipliers, it is not difficult to show that our Lagrangian is invariant under rotations and reflections, meaning that

$$
\mathcal{L}({\mathbf{u}, \mathbf{B}, \cdots}) = \mathcal{L}(\tilde{\mathbf{u}}, \tilde{\mathbf{B}}, \cdots)
$$

(5.74)

This means that optimal solutions that maximize $\mathcal{L}$ will always be infinitely degenerate. If $\mathbf{u}$ is an optimal dynamo that drives the field $\mathbf{B}$, then any transformed field $\tilde{\mathbf{u}}$ is also an optimal dynamo that drives the field $\tilde{\mathbf{B}}$.

### 5.3 Results

#### 5.3.1 Preliminary tests

Before running the optimization, we also verify the projection of variational derivative (5.19) onto the basis of $\mathbf{u}$. This quantity contains information about the adjoint model at all time steps and is important for the update. We set $\lambda_1 = 0$ in (5.19) for this test due to the convenient choice of orthonormal properties of the vector bases in (5.52), also to remove the constraint on unity enstrophy in (5.27). We want to compare how the Lagrangian varies with respect to a small perturbation on the flow field $\mathbf{u}$ using two methods. First, we compute the variations using a forward model. Since we have all other constraints satisfied, each component of the variation $\delta \mathcal{L}$ is given by

$$
\delta \mathcal{L}^\rho_{nm\ell} = \frac{\ln \langle \tilde{\mathbf{B}}_T^2 \rangle - \ln \langle \mathbf{B}_T^2 \rangle}{\epsilon},
$$

(5.75)

where $\tilde{\mathbf{B}}_T$ is the final magnetic field at time $T$ amplified by a given random flow field plus a small perturbation: $\mathbf{u} + \epsilon \mathbf{u}_\rho_{nm\ell}$, $\rho = p, t$, and $\mathbf{B}_T$ is computed without adding perturbations. Each component with a different index in $n, m, \ell$ needs to be calculated separately using a forward model. Second, we calculate the variational derivative $\frac{\delta \mathcal{L}}{\delta \mathbf{u}}$ projected onto the vector space of $\mathbf{u}$. In contrast, the projection of $\frac{\delta \mathcal{L}}{\delta \mathbf{u}}$ is calculated once using an adjoint model as in (5.67). The two variations are related by taking the limit of the perturbation amplitude $\epsilon$ to zero:

$$
\lim_{\epsilon \to 0} \delta \mathcal{L}^\rho_{nm\ell} = \left\langle \frac{\delta \mathcal{L}}{\delta \mathbf{u}} \cdot \mathbf{u}_\rho_{nm\ell} \right\rangle.
$$

(5.76)

We then compare the right-hand side of (5.75) and (5.76) in spectral space by setting $\epsilon$ to a very small value. All realisations used here have the same initial $\mathbf{B}_0$ and $\mathbf{u}$. The test result shows good agreement, see Figure 5.2.

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Figure 5.2. Verification of the adjoint model. Parameters used in the test: $Rm = 60$, $T = 0.1$, $\Delta t = 10^{-4}$, $\varepsilon = 10^{-4}$, and $(l_{max}, n_{max}) = (24, 12)$. a) Poloidal flow coefficients. b) Toroidal flow coefficients. There is almost exact overlay of the curves depicting the variations in $L$ obtained through two methods.

5.3.2 An example of an optimization run

An optimization run generally needs a few thousand iterations to converge from random initial conditions. It takes about 2 minutes per iteration on 24 cores for $(l_{max}, n_{max}) = (24, 12)$ resolution, $\Delta t = 10^{-4}, T = 2$. In Figure 5.3 we show an example at $Rm = 64.45$. The flow field and seed magnetic field start from random values. The convergence towards the optimal as a function of iterations is shown, and clearly most of the improvement happens in the first thousand iterations.
5.3.3 Systematic survey

In a systematic survey, we launch optimizations for various values of the control parameters. Detailed information on all optimization runs is given in Table 5.2 and Table 5.3. We use time step $\Delta t \leq 10^{-4}$ and $\alpha_1, \alpha_2 \in [0.04, 0.1]$ in the final phase of the relaxation scheme, close to the value of 0.05 used in Duguet et al. [2013]. The total integration time is mainly $T = 1.5$ or $T = 2$ except $T = 2.5$ in one optimization for verification. The tolerance on $r_t$ also varies. $\gamma$ is the asymptotic growth rate of magnetic field, $l_{\text{max}}$ is the maximum spherical harmonic degree, $n_{\text{max}}$ is the maximum degree in radial basis functions, $r_t$ is the residue and “u restart ?” indicates either a start from previously stored fields or not (no, meaning it starts from random initial data).

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Table 5.2. The optimisation results, listed in four groups with gradually refining ranges of \( Rm \). The growth rates listed here are also plotted in Figure 2 in the main text. We use time step \( \Delta t \leq 10^{-4} \) and \( \alpha_1, \alpha_2 \in [0.04, 0.1] \) in the final phase of the relaxation scheme. \( \gamma \) is the asymptotic growth rate of magnetic field, \( l_{max} \) is the maximum spherical harmonic degree, \( n_{max} \) is the maximum degree in radial basis functions, \( r_t \) is the residue and \( \text{"u restart ?"} \) indicates either a restart from previously stored fields (yes) or not (no, meaning a random start). Without specification the total time window \( T = 2 \). The initial starting points for models R1 and R2 are independent of each other.

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Table 5.3. Additional optimisation runs, all start from random initial fields. We do not see local optimal states other than the optimum we have identified before. The scatter in the growth rates are due to less stringent numerical schemes. Here we have used a lower resolution \((l_{\text{max}}, n_{\text{max}}) = (16, 8)\), higher tolerance \(r_t \geq 10^{-3}\) and a shorter time window \(T = 1.5\) in exchange of more independent runs. The time step \(\Delta t = 10^{-4}\) and the relaxation parameters \(\alpha_1, \alpha_2 \in [0.04, 0.15]\).

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Figure 5.4. Main figure: the growth rate as a function of \(Rm\) for all optimization runs from Table 5.2. Inset figure: the near-zero growth rate as a function of \(Rm\) coloured by different resolutions. Orange: \((l_{\text{max}}, n_{\text{max}}) = (16, 8)\). Green: \((l_{\text{max}}, n_{\text{max}}) = (24, 12)\). Purple: \((l_{\text{max}}, n_{\text{max}}) = (24, 24)\).

All growth rates \(\gamma\) from Table 5.2 are shown in Figure 5.4. In the first series
of runs, we varied $Rm \in [10,75]$ using a low resolution $(l_{\text{max}}, n_{\text{max}}) = (16,8)$ and a relatively high tolerance on $r_t = \mathcal{O}(10^{-5}) \sim \mathcal{O}(10^{-4})$. This located the minimal dynamo threshold approximately in between $Rm_{c,\text{min}} \in [60, 70]$. Keeping the same resolution, we explored a smaller interval $Rm \in [64.1, 65]$ with lower tolerances $r_t = \mathcal{O}(10^{-5})$, marked by orange stars in the inset of Figure 5.4. This suggested a $Rm_{c,\text{min}} \approx 64.6$ for this resolution. An increase of resolution to $(l_{\text{max}}, n_{\text{max}}) = (24,12)$ around the threshold is marked by green crosses in Figure 5.4. An additional optimization with $(l_{\text{max}}, n_{\text{max}}) = (24,24)$, is marked by a purple diamond in Figure 5.4. We see that the optimization results do not improve significantly compared to those with resolution $(l_{\text{max}}, n_{\text{max}}) = (24,12)$ and $r_t < 10^{-5}$. In Figure 5.5, we show the logarithm of the magnetic energy as a function of time for optimized solutions from Table 5.2 near the minimal onset of dynamos. We clearly see that the exponential regime is well-established and that the optimal dynamos are non-oscillatory ($\Omega = 0$). This indicates $T = 2$ is long enough to overcome the initial transient. The red curve highlights the run at the optimal dynamo threshold. Finally we have located the optimal dynamo threshold at

$$Rm_{c,\text{min}} \approx 64.45.$$  \hspace{1cm} (5.77)

To ensure that we did not get stuck at a local optimum, we ran an independent optimization at $Rm_{c,\text{min}}$ called the model R2, without restarting from a previous optimum. This second independent optimization confirms the location of the threshold. We also launched another $\sim \mathcal{O}(10^3)$ numbers of independent optimizations for verification. The obtained growth rates $\gamma$ from Table 5.2 and Table 5.3 with a random start are plotted in Figure 5.6 a)-b). No consistent sub-optimal branches were seen. We found the growth rate in this model eventually
improves with more iterations, as opposed to the cases with suboptimal branches where the growth rates for some models stay at a lower value no matter how small the residue becomes. The scatter we see here in Figure 5.6 a)-b) is mostly likely due to different tolerance level for the total residue $r_t$.

![Figure 5.6](image_url)

Figure 5.6. The optimized growth rates as a function of $R_m$ using models with a random start. The total residue $r_t$ varies between $6 \times 10^{-3}$ to $8 \times 10^{-6}$. In all cases the growth rate improves towards approximately the same ‘true’ value at a fixed $R_m$. a) A wide range of $R_m$ is covered in the systematic survey. b) A zoom-in picture of the optimized growth rates as a function of $R_m$ near $R_{m,c,min}$.

### 5.3.4 The spatial structure of the optimal solution at $R_{m,c,min}$

We analyse the spatial structure of the optimal fields $\mathbf{u}$ and $\mathbf{B}_T$ at $R_{m,c,min}$ in both physical and spectral space. In physical space, the 3D structure of the streamlines of $\mathbf{u}$ and $\mathbf{B}_T$ are shown in Figure 5.7 a) and b), field lines are coloured by the local field intensity, small scale structures are not shown in the plots for clarity. More visualizations regarding the optimal flow field $\mathbf{u}$ can be found in Appendix 5.5.2. In Figure 5.7 a), the field lines appear to be twisting in a twofold manner. In the intersection where they meet, which is near the center, we see a drastic increase in the flow speed.
Figure 5.7. Spatial structures of the optimal fields: a) streamlines of $u$, b) streamlines of $B_T$. Field lines are coloured by local field intensity (red = intense, blue = weak) and indicate a localized structure near the center. Structures with very small field intensity are not shown here. The plotted domain is $r \in [0, 1]$.

Figure 5.8. The relative helicity probability distribution function sampled on $> 10^6$ uniformly distributed random grids.

We also observe that the velocity and vorticity fields are nearly parallel in the centre, which means the flow is helical there. Due to this strong helical motion in the centre and weak motion near the boundary, we get a two-peak distribution for the PDF of the relative helicity $H/\sqrt{\langle u^2 \rangle}/\sqrt{\langle (\nabla \times u)^2 \rangle}$, shown in Figure 5.8. We use a uniformly distributed random grids as the sampling points:

$$\phi = 2\pi a_1, \quad \theta = \arccos(1 - 2a_2), \quad r = (a_3)^{1/3}$$

(5.78)

where $a_i \in [0, 1], i = 1, 2, 3$ are randomly generated numbers. The velocity and vorticity fields in the centre are shown Figure 5.9 a). The magnetic field seems to be enhanced strongly next to the spiral. This is evident when we combine Figures 5.7 a)-b) and Figure 5.9 b)-c), where we show the interaction of the flow field $u$ and the magnetic field $B_T$, together with the structure of the vorticity field $\nabla \times u$. The Mollweide map of the radial magnetic field at the sphere’s surface confirms the dominant component is mostly dipolar, see Figure 5.9 d). All plots mentioned in this paragraph are based on model R1; model R2 has the same spatial structures.
Figure 5.9. a) Streamlines of the velocity field (red) and the vorticity field (black) within $r \leq 1$. b) The velocity field direction (red) and vorticity field direction (black) are nearly parallel within $r \leq 0.1$. c) Streamlines of the velocity field (orange), the vorticity field (black) and the magnetic field $B_T$ (blue) within $r \leq 1$. The magnetic field is strongest next to the helical fluid motion. d) The Mollweide projection of the radial component $B_r$ of $B_T$ at the surface of the sphere. The vector field $B_T$ has been rotated such that the dominant dipole axis is vertical.

up to a rotation.

In Figure 5.10 a), we plot the field $B_T$ extended to two radii. We see the field lines get wound up as soon as they enter the sphere; outside they are mostly dipolar. In Figure 5.10 b) we show streamlines of $B_T$ obtained from a second independent run for comparison. They are identical to each other up to a rotation.

Overall we get a quite complex structure in both $u$ and $B_T$, that apparently lacks reflection symmetry. Note that this lack of reflection symmetry was also observed in the optimal dynamos in cubes with perfectly conducting or pseudo-vacuum boundaries (homogeneous cases NNN and TTT in Chen et al. [2015]). However, we have a rotational symmetry of $\pi$ around a fixed axis that the cubic model does not have. If converted to spectral space, this is equivalent to a symmetry with only even $m$ modes when the rotational axis is aligned with the $\hat{z}$ direction.
Besides looking directly at the optimal fields, we also want to understand what are the averaged spatial distributions. We introduce a radial distribution of kinetic energy

\[ U(r)^2 = U^t(r)^2 + U^p(r)^2, \quad U^p(r)^2 = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (u^p)^2 \sin \theta \, d\theta d\phi, \quad \rho = t, p, \]

for the optimal flow \( u \), toroidal part \( u^t \) and poloidal part \( u^p \). Similarly we define \( B_T(r)^2, B_T^t(r)^2, B_T^p(r)^2 \) for the magnetic eigenvector. We also show the radial distribution of two important quantities: helicity and shear (measured by the absolute maximal strain rate). The toroidal part of the radially varying helicity is given by

\[ H^t(r) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} u^t \cdot \nabla \times u^p \sin \theta \, d\theta d\phi. \]

Similarly \( H^p(r) \) measures the poloidal part. In total the radial distribution of helicity is \( H(r) = H^t(r) + H^p(r) \). The radial profile of shear is given by

\[ S_{\text{max}}(r) = \max_{\phi \in [0,2\pi], \theta \in [0,\pi]} |\text{eig} (\nabla u + \nabla u^\top)/2|. \]

The results are shown in Figure 5.11 a)-d). It is clear from Figure 5.11 a) that the flow is concentrated in the centre; near the boundary the fluid is almost stagnant. Bullard & Gubbins [1977] have shown a stagnant conducting layer can reduce the magnetic energy loss by diffusion, thereby promoting dynamo action. Perhaps it is not a surprise to see this behaviour again in our model. The helicity distribution in Figure 5.11 c) is no longer approximately proportional to the kinetic energy distribution in Figure 5.11 a) for \( r > 0.1 \), again showing the alignment of \( u \) and \( \nabla \times u \) breaks down within a certain range of \( r \). We also observe that the magnetic
energy in Figure 5.11 b) almost follows the shear distribution in Figure 5.11 d). This may at first seem to point to the Omega effect [Moffatt, 1983], although in our model the relation between shear and flow is more complex so there is no easy way to relate $u$ and $B_T$ through $S_{max}$. For this reason, we cannot give a definite answer regarding the physics involved in the optimal dynamo. What we can say is that shear (as measured by the absolute maximal strain rate) plays an important role in amplifying the magnetic field.

In comparison, the spatial profiles for the NNT/NTT models in a cube clearly have a reflectional symmetry with respect to the mid-plane. Figure 5.12 a)-c) show the spatial profiles of the NTT optimal flow. The NNT case gives the same optimal flow up to a symmetry transformation, so we omit it here.

Figure 5.12. Averaged 1D distributions of the optimal flow. a) NTT kinetic energy. b) NTT enstrophy. c) NTT helicity.
The optimal magnetic field for the NNT case and the NTT case have very different structures due to different boundary conditions, but the averaged 1D profile is similar up to a transformation. In Figure 5.13 a)-b) we show their magnetic energy profiles.

![Figure 5.13. Averaged 1D distributions of the optimal magnetic eigenvectors. a) NTT magnetic energy. b) NNT magnetic energy.](image)

5.3.5 Analysis in spectral space

The spatial structure of the fields can also be specified in spectral space. In Figure 5.14, we show power spectra of $\langle (\nabla \times u)^2 \rangle$ and $\langle B_{T_l}^2 \rangle$ as a function of the spherical harmonic degree $l$ for the optimal solutions.

![Figure 5.14. Power spectra of $\langle (\nabla \times u)^2 \rangle$ and $\langle B_{T_l}^2 \rangle$ as a function of the spherical harmonic degree $l$ for the optimal solutions.](image)

we show power spectra of $\langle (\nabla \times u)^2 \rangle$ and $\langle B_{T_l}^2 \rangle$ as a function of $l$. They are rapidly decaying, which confirms that the spatial resolution we have used is sufficient. In Table 5.4, we report global measures for $u$ and $B_T$ as a function of $l$. We notice the $l = 1$ and $l = 3$ modes dominate the enstrophy. We also notice that the fields have low rms speed compared to the root mean enstrophy. This indicates that we have strong shear in our optimal flow.

We notice that 94% of the enstrophy (squared value) comes from the first three spherical harmonic degrees. The dominant flow field with only these three degrees with $l_{\text{max}} = 3$ has a critical magnetic Reynolds number $Rm_c = 66.29$ when the non-dimensional enstrophy is rescaled to 1. This slight increase in the critical
point indicates very little influence from higher spherical harmonic degrees in the optimal $u$.

As discussed in section 5.2.6, the optimal solution is infinitely degenerate. Here we compare spatial structures of two independently obtained optimal solutions at $Rm_{c,\text{min}}$ in Table 5.2. Both optima have different orientations, but if we look at the rotationally invariant measures $\langle (\nabla \times u_{l,n})^2 \rangle$ of the dominant modes, in Table 5.5, we find the same values up to 4 decimal places. In total 20 modes of $u_{l,n}$ are needed to capture 80% of the enstrophy (squared value).

Alternatively, we can also sum up all index $n$ and compare each spherical harmonic mode with index $l, m$. Since the amplitude of each $m$ mode changes with rotation, we must fix an orientation for the optimal $u$. We rotate the first two Euler angles in spectral space using Wigner D-matrices such that the coefficient $u_{nml}^p = u_{401}^p$ is maximized, and then rotate the third Euler angle such that $u_{nml}^p = u_{123}^p$ is maximized. In this way, the rotational symmetry axis is along $\hat{z}$ direction and the sum of non-negative $m$ modes are maximized. We impose a cut-off of absolute value 0.01 for all spectral coefficients after rotation. This gives us only 86 nonzero spectral coefficients out of 14976 in total for the optimal $u$ in model R1.

The leading spherical harmonic modes are given in Table 5.6 and all nonzero modes with $l \leq 3$ are shown in Table 5.7. We see an even $m$ symmetry in Table 5.7 which matches with the spatial structures in Figure 5.7 a). Due to selection rules [Bullard & Gellman, 1954], the magnetic field at time $T$ can only have either all even or all odd $m$ modes if $u$ has only even $m$ modes. In this model, only the odd $m$ modes of $B_T$ are present, as shown in Table 5.7. After rotation and reduction, the critical magnetic Reynolds number ($Rm_c$) increases slightly to 64.73 from $Rm_{c,\text{min}} = 64.45$; the dominant flow with $l \leq 3$ has $Rm_c = 66.34$ increased slightly from 66.29 before rotation and reduction. Both numbers reported here have root mean enstrophy rescaled to 1. The change in $Rm_c$ is small, which then shows the reduced model is a good approximation to the full optimum. We will further investigate the reduced model in §5.3.10.

At the level of individual spherical harmonic modes, we notice from Table 5.6 that the first spherical harmonic mode $(l, m) = (1, 0)$ after rotation and reduction has approximately the same enstrophy for both poloidal and toroidal components. It turns out this mode has a normalized helicity $\tilde{H}_1^0 = 0.95$ where

$$
\tilde{H}_l^m = \frac{\langle u_l^m \cdot \nabla \times u_l^m \rangle}{\sqrt{\langle u_l^m \rangle^2 \langle (\nabla \times u_l^m)^2 \rangle}}.
$$

(5.82)

This corresponds to the strong central flow we have shown in Figures 5.7 a). Other secondary structures are weaker, so the overall normalized helicity for the optimal flow $u$ is only $\sim 0.65$. Helicity is an important measure in fluid dynamics and its significance for dynamo action has been discussed in many places, e.g. review by Gubbins [2008]; Moffatt [1983], as well as specific examples given by ?. While our optimal dynamo does have large helicity for some dominant components, helicity alone cannot explain all the optimal structures we have.

98
\[
\langle (\nabla \times \mathbf{u})^2 \rangle \quad l = 1 \quad l = 2 \quad l = 3 \quad l = 4 \quad l = 5
\]
\[
\langle \mathbf{u}_l^2 \rangle \quad 4.40 \times 10^{-3} \quad 2.12 \times 10^{-3} \quad 4.77 \times 10^{-3} \quad 0.42 \times 10^{-3} \quad 0.04 \times 10^{-3}
\]
\[
\langle (\mathbf{B}_l)^2 \rangle \quad 1.27 \quad 0.62 \quad 0.16 \quad 0.04 \quad 0.02
\]

Table 5.4. The enstrophy, kinetic energy and magnetic energy for the first five \(l\) modes in models \(R_{m_{c,\text{min}}}\) and \(R_{m_{c,1}}\), both give the same value up to three digits.

\[
\langle (\nabla \times \mathbf{u}_{l,n})^2 \rangle \quad \mathbf{u}_{3,1}^p \quad \mathbf{u}_{3,2}^p \quad \mathbf{u}_{4,1}^\ell \quad \mathbf{u}_{4,1}^r \quad \mathbf{u}_{5,3}^p
\]
model R1 : 0.11549423 0.08946892 0.05917234 0.05808290 0.05398641
model R2: 0.11545455 0.08946926 0.05917836 0.05807418 0.05399249

\[
\langle (\mathbf{B}_{T,l,n})^2 \rangle \quad \mathbf{B}_{1,1}^t \quad \mathbf{B}_{1,1}^p \quad \mathbf{B}_{1,2}^t \quad \mathbf{B}_{1,2}^p \quad \mathbf{B}_{2,1}^t \quad \mathbf{B}_{2,1}^p \quad \mathbf{B}_{1,2}^t \quad \mathbf{B}_{1,2}^p
\]
model R1: 0.452304 0.269096 0.231813 0.168114 0.127885 0.05398641 0.05399249
model R2: 0.451951 0.269058 0.231987 0.168547 0.127885 0.05398641 0.05399249

Table 5.5. Leading components of enstrophy norm for \(\mathbf{u}_{l,n}\) and magnetic energy norm for \(\mathbf{B}_{T,l,n}\) in models R1 and R2. A summation over \(m\) has been performed for the comparison.

\[
\langle (\nabla \times \mathbf{u}_{l,m})^2 \rangle \quad \mathbf{u}_{3,1}^p \quad \mathbf{u}_{3,2}^p \quad \mathbf{u}_{4,1}^\ell \quad \mathbf{u}_{4,1}^r \quad \mathbf{u}_{5,3}^p
\]
\[
\langle (\mathbf{B}_{T,l,m})^2 \rangle \quad \mathbf{B}_{1,1}^t \quad \mathbf{B}_{1,1}^p \quad \mathbf{B}_{1,2}^t \quad \mathbf{B}_{1,2}^p \quad \mathbf{B}_{2,1}^t \quad \mathbf{B}_{2,1}^p \quad \mathbf{B}_{1,2}^t \quad \mathbf{B}_{1,2}^p
\]
model R1: 0.452304 0.269096 0.231813 0.168114 0.127885 0.05398641 0.05399249
model R2: 0.451951 0.269058 0.231987 0.168547 0.127885 0.05398641 0.05399249

Table 5.6. Leading components of enstrophy norm for \(\mathbf{u}_{l,m}\) and magnetic energy norm for \(\mathbf{B}_{T,l,m}\) in model R2 after rotation and reduction. A summation over \(n\) has been performed for the comparison.

\[
\langle (\nabla \times \mathbf{u}_{l,m})^2 \rangle \quad \mathbf{u}_{1}^0 \quad \mathbf{u}_{2}^0 \quad \mathbf{u}_{2}^2 \quad \mathbf{u}_{3}^2 \quad \mathbf{u}_{3}^0 \quad \mathbf{u}_{3}^2
\]
\[
\langle (\mathbf{B}_{T,l,m})^2 \rangle \quad \mathbf{B}_{1,1}^t \quad \mathbf{B}_{1,1}^{-1} \quad \mathbf{B}_{1,2}^t \quad \mathbf{B}_{1,2}^{-1} \quad \mathbf{B}_{3,1}^t \quad \mathbf{B}_{3,1}^{-1} \quad \mathbf{B}_{3,3}^t \quad \mathbf{B}_{3,3}^{-3}
\]
model R1: 0.11549423 0.08946892 0.05917234 0.05808290 0.05398641 0.05399249
model R2: 0.11545455 0.08946926 0.05917836 0.05807418 0.05399249
model R3: 0.11545455 0.08946926 0.05917836 0.05807418 0.05399249

Table 5.7. The enstrophy and magnetic energy norm summed over index \(n\) for all nonzero modes with \(l \leq 3\) and \(|m| \leq 3\) in model \(R_{m_{c,1}}\) after rotation and reduction.
5.3.6 Perturbation study

In this section, we perform a perturbation study to verify the optimality of the growth rate at $R_{m_{c,\text{min}}}$. A perturbed field $U_{\text{per}}$ is the optimal field $u$ plus a small portion of a randomly generated flow field, subsequently rescaled to have a unit enstrophy. We define a correlation amplitude,

$$C_p = \frac{\langle u_{\text{per}} \cdot U \rangle}{\sqrt{\langle (u_{\text{per}})^2 \rangle \langle U^2 \rangle}}$$

(5.83)

similar to that in Chen et al. [2015] but only for the dominant modes $l \leq 3$, then launch a forward run with $u_{\text{per}}$ and measure the perturbed growth rate $\gamma_p$. The result of multiple random perturbations is shown in Figure 5.15. The growth rate rapidly decreases as more perturbations are added to $u$, which indicates that random perturbations quickly reduce the flow’s optimality.

5.3.7 Transient growth

In dynamo models, a seed magnetic field can be transiently amplified by a conductive flow field for a short period even when it decays later [Livermore & Jackson, 2004, 2006]. This can clearly be seen in Figure 5.5 for $t < 0.15$. Using our optimization method with very short optimizing time windows $T$, we can maximize the transient growth and then measure the magnetic Reynolds number $R_{m_{t,\text{min}}}$ at which this maximum transient growth is zero. Numerically, using $T = 0.001$ and $\Delta t = 10^{-5}$, we find the minimal transient magnetic Reynolds number

$$R_{m_{t,\text{min}}} = 30.21,$$

(5.84)

see Figure 5.16 a). The optimal flow field at $R_{m_{t,\text{min}}}$ has equatorial symmetry ($E^S$). Compared with the optimal flow $u$ found with long $T = 2$ in Figure 5.16 b), we see this magnetic field with maximized transient growth decays faster at later times as expected. The value of $R_{m_{t,\text{min}}}$ provides an important physical measure,
since it marks the ultimate lower bound where no increase in magnetic energy can be observed for any given time window. Any dynamo action needs to maintain the magnetic energy at least for some time, which then requires $Rm > Rm_{t,\text{min}}$; this also includes dynamos generated by time-dependent flows with a typical time scale $\partial u/\partial t \ll T$ where $T \ll 1$ is a short transient time window. This $Rm_{t,\text{min}}$ is 53% below the optimal threshold $Rm_{c,\text{min}}$ for sustained dynamo action which is quite different than what was observed by Willis [2012] in the periodic cube.

5.3.8 Comparison with theoretical bounds

Our magnetic Reynolds number $Rm$ is not the most conventional in dynamo theory, but is the one that relates to the class of enstrophy normalized fields $\mathcal{E}_u$. We can define two other magnetic Reynolds numbers using different scales for the flow field:

$$Rm_u = \frac{UL}{\eta}, \quad Rm_s = \frac{S_{\text{max}}L^2}{\eta}$$

(5.85)

where $U$ is the dimensional rms flow velocity, and $S_{\text{max}}$ is the dimensional absolute maximum strain rate. This allows us to convert the results from root mean enstrophy or shear based $Rm$ to kinetic-energy based ($Rm_u$) and strain rate based ($Rm_s$) magnetic Reynolds numbers:

$$Rm_u = \langle u^2 \rangle^{\frac{1}{2}} Rm, \quad Rm_s = \left( \max_{V} \left| \text{eig} \left( \frac{1}{2} (\partial_i U_j + \partial_j U_i) \right) \right| \right) Rm,$$

(5.86)

using the non-dimensional optimal flow field $u$ and its components $u_r, u_\theta, u_\phi$ in models R1 and R2. This yields $Rm_u = 7$ and $Rm_s = 215$. The value of $Rm_u = 7$ really is very low and close to the values we have measured in the cube with unit sizes [Chen et al., 2015]. According to Proctor [2015], such a low value should be no real surprise since a theoretical lower bound on $Rm_u$ just simply does not exist.
We can further check how far we are above theoretical lower bounds using definitions other than $Rm_u$. In particular, we choose three bounds to compare with, they are

- (Backus, 1958): $Rm_s > \pi^2$,
- (Proctor, 1977): $Rm_s > 12.29$,
- (Childress, 1969): $Rm u_{\text{max}} > \pi$.

The Backus/Proctor bound use strain rate based magnetic Reynolds number, and the Childress bound uses the maximum speed of the flow as a typical scale. Using our conventions, we find $Rm_s/12.29 \approx 17$ and $Rm u_{\text{max}}/\pi \approx 14$, which are clearly above the theoretical limit. This can be attributed to the fact that theoretical bound calculations systematically overestimate the spatial extent of the magnetic fields [Herreman, 2016].

Besides the bounds listed above, Proctor [1979] derived a bound for dynamo action that is immediately applicable to our present results. He derived that

$$D > \frac{\pi \eta^2}{4L}$$

for a sphere of radius $L$, where $D = \int_V e_{ij} e_{ij} \, dV$ is proportional to viscous dissipation and $e_{ij}$ is the dimensional strain rate tensor. Translating this to our notation, we note that

$$2D = \frac{4}{3} \pi L^3 S^2.$$  

By dint of no-slip conditions, $S = \omega^*$, and we find immediately that

$$Rm = \frac{\omega^* L^2}{\eta} > \frac{\sqrt{6}}{2} \approx 0.61.$$  

Clearly our dynamo operates well above this bound. Proctor speculated that the best lower bound might be ten times larger than the one given here, and indeed we find that the best dynamo is operating at a value of $Rm$ over one hundred times larger.

### 5.3.9 Comparison with other flows

In this section we compare several properties of our optimal flow to some selected models in the literature. We do not include self-consistent dynamos in a spherical shell here due to the complexity of these models. Note that in Christensen & Aubert [2006], they found the limit for dynamo action is $Rm_u \sim 60$ when converted to our units (radius as the length scale), which is about 8 times higher than our optimal dynamo. Instead, we focus on kinematic dynamos driven by two families of flows, called KR type [Kumar & Roberts, 1975] and DJ type [Dudley & James, 1989]. The KR flow consists of three parts: differential rotation, meridional circulation and a simplified model for convection columns. The DJ flow has large scale axisymmetric structures. The boundary conditions are not limited to no-slip for these models unlike our model. Specifically, we compare with the
study of Kumar & Roberts [1975], Love & Gubbins [1996a], Dudley & James [1989], Sarson [2003], Livermore & Jackson [2004], Holme [2003] and the precise definition of the flows abbreviated as KR, GKR, STW, DJ, MDJ. 

The explicit field representation of the optimized DJ flow by Holme [2003] is unknown, so we could not include it in the comparison table.

We first compare the critical magnetic Reynolds numbers for the onset of dynamo action. All the studies we compare with have used

\[ Rm^* = \frac{\bar{u}L}{\eta} \]  

as magnetic Reynolds number. \( L \) is always the dimensional radius but there is little homogeneity in what \( \bar{u} \) should be (e.g., maximal dimensional speed, rms dimensional speed). In order to compare critical magnetic Reynolds numbers of different dynamo studies, we need to rescale all results to a more clear definition. Denoting by \( \bar{u} \) the dimensional flow scales, \( S_{\text{max}} \) the dimensional absolute maximum strain rate, and \( u^* \) the non-dimensional flow field, we systematically compute the non-dimensional measures for rms speed, root mean enstrophy and absolute maximal strain rate for all models. We can then calculate the magnetic Reynolds numbers as a function of the previously published values. We use

\[
Rm_u = \langle (\text{u}^*)^2 \rangle^{\frac{3}{2}} Rm^*, \quad Rm = \langle (\nabla \times \text{u}^*)^2 \rangle^{\frac{3}{2}} Rm^*, \\
Rm_s = \left( \max_v |\text{eig} \frac{1}{2}(\partial_i u_j^* + \partial_j u_i^*)| \right) Rm^*
\]

in which we have used rescaling factors \( \text{rms u}^*, \omega^* = \sqrt{\langle (\nabla \times \text{u}^*)^2 \rangle} \), and \( S_{\text{max}}/\bar{u} \) to convert \( Rm^* \) to \( Rm_u \), \( Rm \) and \( Rm_s \) respectively. The comparison of critical magnetic Reynolds number is shown in Table 5.8. We see our optimal flow field has improved the existing lower bound on the critical \( Rm \) of DJ by at least a factor of 3. As for the transient growth, other known values of the critical transient magnetic Reynolds number \( Rm_t \), below which no magnetic energy growth is possible in a sphere [Livermore & Jackson, 2004] are

KR: \( Rm_t = 80 \), STW: \( Rm_t = 83 \), MDJ \( t_1 s_2 \): \( Rm_t = 62 \). (5.90)

These values have been converted using rms \( \nabla \times \text{u}^* \) as the rescaling factor. The \( Rm_t \) of these flows are at least 2 times larger than our \( Rm_{t,\text{min}} \).

In Table 5.9, we show some other properties of the flow related to helicity, energy ratio and maximum speed. We use the poloidal/toroidal kinetic norm given by

\[
E_P = \langle (\text{u}^p)^2 \rangle, \quad E_T = \langle (\text{u}^t)^2 \rangle,
\]

where the superscript \( p \) and \( t \) denote the poloidal and toroidal component of flow field respectively. The enstrophy norm for toroidal/poloidal flow field are given by

\[
\omega_P^2 = \langle (\nabla \times \text{u}^p)^2 \rangle, \quad \omega_T^2 = \langle (\nabla \times \text{u}^t)^2 \rangle.
\]
Table 5.8. A comparison of critical magnetic Reynolds numbers between our optimised flow (top row) and those reported in the literature (bottom section), see (5.89) and §2.2.1 for definitions. $\bar{Rm}$: the originally reported magnetic Reynolds number in the articles.

<table>
<thead>
<tr>
<th></th>
<th>$Rm_u$</th>
<th>$Rm$</th>
<th>$Rm_s$</th>
<th>rms $u$</th>
<th>$S_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$</td>
<td>7</td>
<td>64.45</td>
<td>215</td>
<td>0.108</td>
<td>3.33</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$\bar{Rm}$</th>
<th>$Rm_u$</th>
<th>$Rm$</th>
<th>$Rm_s$</th>
<th>rms $\hat{u}$</th>
<th>$\bar{S}_{\text{max}}$</th>
<th>$\hat{\omega}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KR</td>
<td>890</td>
<td>890</td>
<td>4486</td>
<td>5002</td>
<td>1</td>
<td>5.62</td>
<td>5.04</td>
</tr>
<tr>
<td>GKR</td>
<td>131</td>
<td>131</td>
<td>1327</td>
<td>1451</td>
<td>1</td>
<td>11.08</td>
<td>10.13</td>
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<td>STW</td>
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<td>479</td>
<td>2936</td>
<td>3741</td>
<td>1</td>
<td>7.81</td>
<td>6.13</td>
</tr>
<tr>
<td>DJ $t_1s_1$</td>
<td>155</td>
<td>104</td>
<td>476</td>
<td>274</td>
<td>0.671</td>
<td>1.77</td>
<td>3.07</td>
</tr>
<tr>
<td>DJ $t_1s_2$</td>
<td>95</td>
<td>60</td>
<td>310</td>
<td>233</td>
<td>0.635</td>
<td>2.45</td>
<td>3.26</td>
</tr>
<tr>
<td>DJ $t_2s_2$</td>
<td>54</td>
<td>32</td>
<td>193</td>
<td>153</td>
<td>0.587</td>
<td>2.84</td>
<td>3.57</td>
</tr>
<tr>
<td>MDJ $t_1s_2$</td>
<td>55</td>
<td>55</td>
<td>300</td>
<td>296</td>
<td>1</td>
<td>5.38</td>
<td>5.46</td>
</tr>
</tbody>
</table>

Table 5.9. Properties of the flow fields that can generate a dynamo (see §2.2.1 for the definition of flows). †: We choose the hemisphere with the larger value of helicity when the symmetry axis is aligned with the $\hat{z}$ axis.

|       | $\langle H \rangle$ | $\langle H \rangle_V^\varphi$ | max $|u|$ | $\omega_p^2/\omega_T^2$ | $E_P/E_T$ |
|-------|---------------------|-----------------------------|--------|----------------|----------|
| $u$   | 0.07                | 0.08†                       | 0.69   | 1.885          | 1.824    |

|       | $\langle \hat{H} \rangle$ | $\langle \hat{H} \rangle_V^\varphi$ | max $|\hat{u}|$ | $\omega_p^2/\omega_T^2$ | $E_P/E_T$ |
|-------|---------------------------|-----------------------------|--------|----------------|----------|
| KR    | 0                         | 0.210                      | 1.96   | 0.149          | 0.017    |
| GKR   | 0                         | 2.078                      | 2.58   | 8.117          | 1        |
| STW   | 0                         | 0.362                      | 2.38   | 0.088          | 0.015    |
| DJ $t_1s_1$ | 1.969               | 1.969                      | 1.12   | 0.630          | 0.592    |
| DJ $t_1s_2$ | 0        | 1.380                      | 1.07   | 0.838          | 0.425    |
| DJ $t_2s_2$ | 1.992               | 1.992                      | 0.94   | 0.791          | 0.679    |
| MDJ $t_1s_2$ | 0        | 2.906                      | 1.64   | 0.662          | 0.254    |

The values of poloidal and toroidal kinetic norm and enstrophy norm for various flows are shown in Table 5.10. We include the MDJ $s_2$ flow which has a $Rm_t = 61.2$, but gives no dynamo solution. The total helicity in the sphere and the helicity in the Northern hemisphere are given by

$$\langle \hat{H} \rangle = \langle \hat{u} \cdot \nabla \times \hat{u} \rangle, \quad \langle \hat{H} \rangle_V^\varphi = \frac{3}{2\pi} \int_0^1 \int_0^\pi \int_0^{2\pi} \hat{u} \cdot \nabla \times \hat{u} \ r^2 \sin \theta d\phi d\theta dr. \quad \text{(5.93)}$$

From Table 5.9 it seems that there is no clear pattern on these measured values across different dynamo models. We observe that the poloidal enstrophy to toroidal enstrophy ratio is roughly the same as poloidal kinetic energy to toroidal kinetic energy ratio for our optimal flow.
It is of interest to compare our present results to our previous results in a cube [Chen et al., 2015]. When mixed boundary conditions were used, the best dynamo had $R_{c,min} = 7.5\pi^2$ where the length scale was based on the length of the side of the cube. For the sphere the equivalent choice of a length scale is clear (it is the diameter), but for the cube this choice is not the most defensible. If we just consider all chords passing through the centre of a unit cube, it is clear that the lengths $l$ vary as one moves from a chord perpendicular to two faces to one joining opposite corners, such that $l$ is bounded by $1 \leq l \leq \sqrt{3}$. There is probably no fully satisfactory way of defining the relevant length scale in a cube, but we can derive an objective choice. We let $E\{x\}$ denote the expected value of $x$ and consider all chords present in both the sphere and the cube. For the sphere of radius $L$ it is clear that $E\{l^2\} = 4L^2 = (E\{l\})^2$, whereas in the cube, we find

$$E\{L^2\} = \frac{5}{3}\quad (5.94)$$

with the ancillary result (not needed) of $E\{L\} \approx 1.28$. Using the value (5.94) for the length scale gives $R_{c,min} = 123$ in the cube with mixed boundary conditions, whereas $R_{c,min} = 197$ with homogeneous (either pseudo-vacuum or superconducting) boundary conditions. These compare to the values in the sphere we report here when converted using $E\{l^2\} = 4L^2$ of $R_{c,min} = 258$ for insulating boundary conditions.

A complementary way of comparing is to imagine that we are given a unit volume of electrically conducting fluid and consider the two possible geometrical arrangements at our disposal: a cube and a sphere. Obviously the size of the sphere (using radius $R$) is $4\pi/3R^3 = 1$, thus $R = (3/(4\pi))^{1/3} \approx 0.62$. We choose a common length scale, which is unity for the cube and for the sphere must be measured in these units. We previously referred our $Rm$ to the radius, but the present lengthscale inflates the length units by $(0.62)^{-1}$. When we reinterpret our present value for $Rm$ on this length scale we have a new value for $Rm$ of $64.45/0.62^2 \approx 168$, now above all the cubic results. Probably we have taken this analysis as far as is sensible, but we speculate that the extra roughness of the boundaries present in the cube might be responsible for extra shearing in the optimal flow that then appears to be a better dynamo.

<table>
<thead>
<tr>
<th></th>
<th>$\omega_P^2$</th>
<th>$\omega_T^2$</th>
<th>$E_P$</th>
<th>$E_T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KR</td>
<td>3.30</td>
<td>22.13</td>
<td>0.02</td>
<td>0.98</td>
</tr>
<tr>
<td>GKR</td>
<td>91.32</td>
<td>11.25</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>STW</td>
<td>3.05</td>
<td>34.55</td>
<td>0.02</td>
<td>0.98</td>
</tr>
<tr>
<td>DJ $t_1s_1$</td>
<td>3.65</td>
<td>5.79</td>
<td>0.17</td>
<td>0.28</td>
</tr>
<tr>
<td>DJ $t_1s_2$</td>
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<td>5.79</td>
<td>0.12</td>
<td>0.28</td>
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<tr>
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<td>MDJ $t_1s_2$</td>
<td>11.87</td>
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<td>0.80</td>
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<tr>
<td>MDJ $s_2$</td>
<td>58.5</td>
<td>0</td>
<td>1</td>
<td>0</td>
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</tbody>
</table>

Table 5.10. Comparison of enstrophy norm $\omega^2$ and kinetic energy norm $E$ for various flows, $P,T$ stand for poloidal and toroidal components.
5.3.10 Reduced models

The final optimal flow we obtained has dominantly \( l \leq 3 \) structures, as well as even symmetry for the spherical harmonic order \( m \). Capturing 83% of the enstrophy, the optimal flow in this model can be approximated by five spherical harmonic modes, (either as the toroidal part \( u_{lm}^{t} \) or as the poloidal part \( u_{lm}^{p} \)):

\[
\mathbf{u} \approx u_{10}^{0} + u_{11}^{0} + u_{2}^{l-2} + u_{2}^{p-2} + u_{3}^{p2}.
\] (5.95)

Positive \( m \) corresponds to cosine modes and negative \( m \) corresponds to sine modes; the index \( n \) is summed up in this expression. We see here an even \( m \) symmetry for the optimal flow that matches with the spatial structures in Figure 5.7 a). Owing to the selection rules of Bullard & Gellman [1954], the magnetic field can only have either all even or all odd \( m \) modes when \( \mathbf{u} \) has only even \( m \) modes. In this model, only the odd \( m \) modes of \( \mathbf{B}_{T} \) are present.

If we just look at these modes and ignore the radial distribution for a moment, we see \( u_{10}^{0} \) and \( u_{11}^{0} \) are just two modes that make up the DJ \( t_{1}s_{1} \) flow, \( u_{2}^{l-2} \), \( u_{2}^{p-2} \) are part of the KR flow, and STW flow has the toroidal mode \( u_{3}^{2} \) if not the same poloidal mode \( u_{3}^{p2} \) as what we have here. These large scale modes have been studied in the past and some combinations of them are capable of producing dynamos. What is different in our model is that we have a new combination of these modes with optimal radial distributions. This particular configuration would be difficult to identify without using the variational method.

To verify the dominant structures of the optimal flow, we launched several independent optimizations from random initial fields using reduced models. The results give a good approximation to the full optimum, shown in Table 5.11.

<table>
<thead>
<tr>
<th>( Rm )</th>
<th>( \gamma )</th>
<th>( r_{t} )</th>
<th>note</th>
</tr>
</thead>
<tbody>
<tr>
<td>67.0</td>
<td>0.521</td>
<td>( 10^{-4} )</td>
<td>( \mathbf{u}: l \leq 3. \mathbf{B}: ) unrestricted.</td>
</tr>
<tr>
<td>67.0</td>
<td>0.520</td>
<td>( 10^{-4} )</td>
<td>( \mathbf{u}: l \leq 3. \mathbf{B}: ) unrestricted.</td>
</tr>
<tr>
<td>64.9</td>
<td>0.056</td>
<td>( 6.5 \times 10^{-4} )</td>
<td>( \mathbf{u}: m ) even. ( \mathbf{B}: m ) odd.</td>
</tr>
<tr>
<td>64.45</td>
<td>0.001</td>
<td>( 8 \times 10^{-6} )</td>
<td>( \mathbf{u}, \mathbf{B}: ) unrestricted</td>
</tr>
</tbody>
</table>

Table 5.11. Reduced models with random start compared with the optimum at \( Rm_{c,min} = 64.45 \). Here \( T = 2 \), resolution \( (l_{max}, n_{max}) = (24, 12) \).

5.4 Conclusions

In this study, we have found the optimal kinematic dynamo in a sphere with no-slip and insulating boundary conditions. The enstrophy based minimal critical \( Rm_{c,min} \) for the onset of a dynamo is 64.45. Compared to other known dynamo models, our optimal dynamo has lowered the critical \( Rm \) at least by a factor of 3. The rms speed is much lower compared to the global shear magnitude or root mean enstrophy in the system. The optimal flow field at \( Rm_{c,min} \) has a rotational symmetry of order 2 and a very concentrated helical structure near the centre. This indicates that a localised helix plus secondary twofold spirals are favourable for the onset of a kinematic dynamo in a sphere. The dominant spherical harmonic
modes are \((l, |m|) = (1, 0), (2, 2), (3, 2)\), when the the rotational symmetry axis is aligned with \(\hat{z}\) axis. The optimal flow structures near the boundary do not play a significant role. Therefore, we expect that the use of other boundary conditions for the flow, such as free-slip boundary conditions, will not lower \(Rm_{c,\text{min}}\) by much. In the supplementary material to this article, we have provided both the spectral coefficients and field values on grids for the optimal flow field and the associated magnetic eigenvector.

The magnetic field at the dynamo onset has mainly dipolar structures. With respect to the rotational symmetry axis of \(u\), the fastest growing magnetic field eigenmode has only odd \(m\) modes. We also find the minimal critical magnetic Reynolds number for transient growth \(Rm_{t,\text{min}} = 30.21\), indicating any time-dependent flows cannot lower the critical magnetic Reynolds number further than 30.21. We plan to extend this study in two parallel directions. One is to study how different boundary conditions on \(u\) and \(B\) affect the optimum, the other is to study the optimum with a restricted subclass of symmetry group \(O(3)\), e.g., the optimal kinematic dynamo generated by axisymmetric flows. It is also feasible to study the optimum within geophysically interesting classes of flows, such as Rossby waves or inertial waves.

5.5 Appendix

5.5.1 Orthonormal Toroidal/poloidal vector field bases

In this section we give the definitions of our Galerkin basis and other related definitions.

5.5.1.1 The Poloidal-toroidal expansions

The poloidal-toroidal decomposition for the flow field is

\[
\mathbf{u}^t(r, \theta, \phi) = \sum_{l,m,n} v_{nml} \left[ \frac{1}{r \sin \theta} t_n^l(r) \frac{\partial Y_m^l}{\partial \phi} \hat{\theta} - \frac{1}{r} t_n^l(r) \frac{\partial Y_m^l}{\partial \theta} \hat{\phi} \right],
\]

(5.96)

\[
\mathbf{u}^p(r, \theta, \phi) = \sum_{l,m,n} w_{nml} \left[ \frac{l(l+1)}{r^2} s_n^l(r) Y_m^l \hat{r} + \frac{1}{r} \frac{\partial s_n^l(r)}{\partial r} Y_m^l \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial s_n^l(r)}{\partial \theta} Y_m^l \hat{\phi} \right],
\]

(5.97)

where \(t_n^l, s_n^l\) are the radial functions and \(Y_m^l\) are the real orthonormal spherical harmonics. The field decomposition for \(B\) follows similar definitions given by

\[
\mathbf{B}^t(r, \theta, \phi) = \sum_{l,m,n} c_{nml} \left[ \frac{1}{r \sin \theta} q_n^l(r) \frac{\partial Y_m^l}{\partial \phi} \hat{\theta} - \frac{1}{r} q_n^l(r) \frac{\partial Y_m^l}{\partial \theta} \hat{\phi} \right],
\]

(5.98)

\[
\mathbf{B}^p(r, \theta, \phi) = \sum_{l,m,n} d_{nml} \left[ \frac{l(l+1)}{r^2} p_n^l(r) Y_m^l \hat{r} + \frac{1}{r} \frac{\partial p_n^l(r)}{\partial r} Y_m^l \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial p_n^l(r)}{\partial \theta} Y_m^l \hat{\phi} \right].
\]

(5.99)
There are in total $2 n_{\text{max}} l_{\text{max}} (l_{\text{max}} + 2)$ spectral coefficients for each vector field. For input and output, these coefficients are stored in memory as a one dimensional array in the order of $n = 1, \cdots, n_{\text{max}}, m = 0, m = 1, m = -1, \cdots$, then from index $l = 1, \cdots, l_{\text{max}}$. In the optimization process, the memory is often distributed to at least $l_{\text{max}}$ number of cores.

5.5.1.2 Orthogonal Galerkin polynomials

The optimization scheme relies on a convenient choice of orthogonal polynomials. These polynomials are constructed by combining Jacobi polynomials into a Galerkin basis that satisfies the required boundary conditions using the techniques pioneered by Livermore & Ierley [2010] and Livermore [2010]. The key idea is that by using a Gram-Schmidt procedure a family of orthogonal Galerkin polynomials can be iteratively constructed. However, as these authors showed, it is possible to explicitly write down the structure of Galerkin polynomial of arbitrary index as the terse sum of Jacobi polynomials. This allows us to deduce that asymptotically the recombined Jacobi polynomials are well-behaved. Using field expansions (5.96)-(7.14), the orthonormality conditions (5.45) and (5.46) in this model then requires

\begin{align}
\langle -\nabla_i^2 t_n, t_{n'} \rangle_t &= \delta_{nn'}, \\
\langle -\nabla_i^2 s_n, s_{n'} \rangle_s &= \delta_{nn'}, \\
\langle q_n, q_{n'} \rangle_t &= \delta_{nn'}, \\
\langle p_n, p_{n'} \rangle_p &= \delta_{nn'},
\end{align}

(5.100)

for radial functions, where the radial inner products are defined as

\begin{align}
\langle \alpha^l, \beta^l \rangle_t &= \frac{3}{4\pi} l(l+1) \int_0^1 \alpha^l \beta^l \, dr, \\
\langle \alpha^l, \beta^l \rangle_s &= \frac{3}{4\pi} l(l+1) \int_0^1 \left( \frac{l(l+1)}{r^2} \alpha^l \beta^l + \frac{\partial \alpha^l}{\partial r} \frac{\partial \beta^l}{\partial r} \right) \, dr, \\
\langle \alpha^l, \beta^l \rangle_p &= \frac{3}{4\pi} l(l+1) \left[ \int_0^1 \left( \frac{l(l+1)}{r^2} \alpha^l \beta^l + \frac{\partial \alpha^l}{\partial r} \frac{\partial \beta^l}{\partial r} \right) \, dr + l \alpha^l(1) \beta^l(1) \right],
\end{align}

(5.103)

and $\nabla_i^2 = \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2}$ and the last term in (5.104) augments from the fact that the inner product is defined over all space; it handles the vacuum contribution from the poloidal field.
5.5.1.3 Projection of direct/adjoint induction term

To solve the induction equation forward in time, we need to project the induction term onto the basis of \( B \). To do so, we use

\[
a_{nml} = \langle \mathbf{B}^t_{nml} \cdot (\nabla \times (\mathbf{u} \times \mathbf{B})) \rangle
= \langle (\nabla \times \mathbf{B}^t_{nml}) \cdot (\mathbf{u} \times \mathbf{B}) \rangle + \langle \nabla \cdot (\mathbf{B}^t_{nml} \times (\mathbf{u} \times \mathbf{B})) \rangle,
\]

\[
= \frac{3}{4\pi} l(l+1) \int_0^1 \int [\mathbf{u} \times \mathbf{B}]_\theta Y_l^m \sin \theta d\theta d\phi \ dr,
+ \frac{3}{4\pi} \int_0^1 \int \left\{ \int \sin \theta \left( \frac{\sin \theta}{\sin \theta} \frac{dY_l^m}{d\theta} \right) + \frac{r[\mathbf{u} \times \mathbf{B}]_\phi}{\sin \theta} \frac{dY_l^m}{d\phi} \right\} \sin \theta d\theta d\phi \ dr,
\]

(5.105)

\[
b_{nml} = \langle \mathbf{B}^p_{nml} \cdot (\nabla \times (\mathbf{u} \times \mathbf{B})) \rangle
= \langle (\nabla \times \mathbf{B}^p_{nml}) \cdot (\mathbf{u} \times \mathbf{B}) \rangle + \langle \nabla \cdot (\mathbf{B}^p_{nml} \times (\mathbf{u} \times \mathbf{B})) \rangle,
\]

\[
= \frac{3}{4\pi} \int_0^1 -\nabla_l^2 \int \left\{ \int \sin \theta \left( \frac{\sin \theta}{\sin \theta} \frac{dY_l^m}{d\theta} \right) + \frac{r[\mathbf{u} \times \mathbf{B}]_\phi}{\sin \theta} \frac{dY_l^m}{d\phi} \right\} \sin \theta d\theta d\phi \ dr.
\]

(5.106)

In practice, we calculate these integrals as follows by an exact Gaussian quadrature rule. We evaluate \( \mathbf{u} \) and \( \mathbf{B} \) on the grids (quadrature points along \( r, \theta, \phi \)), using an inverse Fourier transform along \( \phi \) and a matrix multiplication transform (MMT) along \( r \) and \( \theta \). This MMT requires us to store grid values of each radial expansion function and each associated Legendre functions in memory.

We then evaluate

\[
F_r = [\mathbf{U} \times \mathbf{B}]_r, \quad F_\theta = \frac{r}{\sin \theta} [\mathbf{U} \times \mathbf{B}]_\theta, \quad F_\phi = \frac{r}{\sin \theta} [\mathbf{U} \times \mathbf{B}]_\phi
\]

(5.107)

on the grid points and calculate their projection on the spherical harmonic basis:

\[
[F_\mu]_m^l(r, l, m) = \int \int F_\mu(r, \theta, \phi) Y_l^m(\theta, \phi) \sin \theta d\theta d\phi, \quad \mu = r, \theta, \phi
\]

(5.108)

This projection uses a Fourier transform along \( \phi \) and again MMT for the associated Legendre polynomials of \( \cos \theta \). Using the recurrence relation of spherical harmonics, we can then simplify the integrals for which we evaluate using the Gaussian quadrature rule. This is the same formula as the one used in Li et al. [2011] and \( \hat{a}^m_l \) was defined below (3.75)., which gives

\[
a_{nml} = \left\langle \left[ F_r^t \right]_l^m \right\rangle + \left( \frac{\partial q^l_n}{\partial r} - \frac{\hat{a}^m_l}{l} [F_\theta^t]_l^m \right) + \frac{\hat{a}^{m+1}_l}{l+1} [F_\theta^t]_{l+1}^m - \frac{m}{l(l+1)} [F_\phi^t]_l^m
\]

\[
= \left\langle \left[ F_r^t \right]_l^m + \frac{d}{dr} \left( \frac{\hat{a}^m_l}{l} [F_\theta^t]_l^m \right) - \frac{\hat{a}^{m+1}_l}{l+1} [F_\theta^t]_{l+1}^m + \frac{m}{l(l+1)} [F_\phi^t]_l^m \right) \right\rangle,
\]

(5.109)
on the gridpoints and project onto (r, l, m)

\[ b_{nml} = \left\langle -\nabla_i^2 p_n, \frac{\hat{a}_l^m}{l} [F_{\phi}]^m_{l+1} - \frac{m}{l(l+1)} [F_{\theta}]^m_{l} \right\rangle_t \]

\[ = \left\langle p_n, \frac{\hat{a}_l^m}{l} [F_{\phi}]^m_{l+1} - \frac{m}{l(l+1)} [F_{\theta}]^m_{l} \right\rangle_p. \]  

(5.110)

On the other hand, the diffusion does not involve non-linear terms and can be directly calculated in spectral space. This operation is represented by diffusion matrices given by

\[ T_{nn'}^l = \left\langle B_{nml}^l, \nabla^2 B_{n'ml}^l \right\rangle = \left\langle q_n^l, \nabla^2 q_{n'}^l \right\rangle_t, \]

\[ P_{nn'}^l = \left\langle B_{nml}^p, \nabla^2 B_{n'ml}^p \right\rangle = \left\langle p_n^l, \nabla^2 p_{n'}^l \right\rangle_s. \]  

(5.111)

For the backward time integration of the adjoint problem, the adjoint induction term needs to be projected onto the basis of B. We have

\[ a_{nml}^l = \left\langle B_{nml}^l, [u \times (\nabla \times B^l)] \right\rangle \]

\[ = \frac{3}{4\pi} \int_0^1 q_n^l \left\{ \int \int [r[u \times (\nabla \times B^l)]_0 dY_l^m \sin \theta \sin \phi \right. \]

\[ - \frac{r[u \times (\nabla \times B^l)]_0}{sin \theta} \left( \frac{\sin \theta dY_l^m}{d\phi} \right) \sin \theta d\theta d\phi \right\} d \Omega, \]  

(5.112)

\[ b_{nml}^l = \left\langle B_{nml}^p, [u \times (\nabla \times B^l)] \right\rangle \]

\[ = \frac{3}{4\pi} l(l+1) \int_0^1 p_n^l \left( \int \int [u \times (\nabla \times B^l)]_r Y_l^m \sin \theta d\theta d\phi \right) d \Omega \]

\[ + \frac{3}{4\pi} \int_0^1 \frac{d p_n^l}{d \Omega} \left\{ \int \int [r[u \times (\nabla \times B^l)]_0 \sin \theta \right. \]

\[ + \frac{r[u \times (\nabla \times B^l)]_0}{\sin \phi} \frac{dY_l^m}{d\phi} \sin \theta d\theta d\phi \right\} d \Omega. \]  

(5.113)

In practice, we evaluate \( \nabla \times B^l \) directly on the physical grids using an inverse Fourier transform along \( \phi \) and MMT along \( r \) and \( \theta \). We then calculate the terms

\[ H_r = [u \times (\nabla \times B^l)]_r, \quad H_\theta = \frac{r}{\sin \theta} [u \times (\nabla \times B^l)]_\theta, \quad H_\phi = \frac{r}{\sin \theta} [u \times (\nabla \times B^l)]_\phi \]  

(5.114)

on the gridpoints and project onto (r, l, m) space:

\[ [H_{\mu}]^m_{l}(r, l, m) = \int \int H_{\mu} Y_l^m d \Omega, \quad \mu = r, \theta, \phi \]  

(5.115)

using a Fourier transform and MMT. Using the recurrence rules of the spherical harmonics, we get

\[ a_{nml}^l = \left\langle q_n^l, \frac{\hat{a}_l^m}{l} [\hat{H}_\phi]^m_{l+1} + \frac{m}{l(l+1)} [\hat{H}_\theta]^m_{l} \right\rangle_t \]

\[ = \left\langle p_n^l, \frac{\hat{a}_l^m}{l} [\hat{H}_\phi]^m_{l+1} + \frac{m}{l(l+1)} [\hat{H}_\theta]^m_{l} \right\rangle_t. \]  

(5.116)

\[ b_{nml}^l = \left\langle p_n^l, [H_r]^m_{l} + \frac{d}{dr} \left( \frac{\hat{a}_l^m}{l} [\hat{H}_\phi]^m_{l+1} + \frac{m}{l(l+1)} [\hat{H}_\theta]^m_{l} \right) \right\rangle_t. \]  

(5.117)
which we can evaluate using the Gaussian quadrature rule.

5.5.1.4 Projection of nonlinear integrand in velocity update

In the velocity field update, we need to calculate

\[ V_{inml}^i = \left\langle u_{inml}^i \cdot \left[ B_{ti} \times (\nabla \times B_{t_i}^l) \right] \right\rangle, \quad (5.118) \]

\[ W_{inml}^i = \left\langle u_{inml}^p \cdot \left[ B_{ti} \times (\nabla \times B_{t_i}^l) \right] \right\rangle. \quad (5.119) \]

This projection is structurally similar to the ones we have in the adjoint induction term, so we follow almost the same method. We calculate

\[ G_r^i = [B_{ti} \times (\nabla \times B_{t_i}^l)]_r, \quad G_\theta^i = \frac{r}{\sin \theta} [B_{ti} \times (\nabla \times B_{t_i}^l)]_\theta, \quad G_\phi^i = \frac{r}{\sin \theta} [B_{ti} \times (\nabla \times B_{t_i}^l)]_\phi \]

(5.120)

on gridpoints, project onto \((r, l, m)\) space:

\[ [G_{\mu}]^m_l (r, l, m) = \int \int G_{\mu} Y^m_l d\Omega, \quad \mu = r, \theta, \phi \]

(5.121)

and then calculate

\[ V_{inml}^i = \left\langle t_n^l, \frac{\partial}{\partial l} [G_{\phi}^i]_{l-1}^m - \frac{\partial}{\partial l} [G_{\theta}^i]_{l+1}^m + \frac{m}{l(l + 1)} [G_{\phi}^i]_{l-1}^{-m} \right\rangle, \quad (5.122) \]

\[ W_{inml}^i = \left\langle s_n^l, [G_{\phi}^i]_{l}^m + \frac{d}{dr} \left( \frac{\partial}{\partial l} [G_{\theta}^i]_{l-1}^m - \frac{\partial}{\partial l} [G_{\theta}^i]_{l+1}^m + \frac{m}{l(l + 1)} [G_{\phi}^i]_{l}^{-m} \right) \right\rangle, \quad (5.123) \]

using the Gaussian quadrature rule.

5.5.1.5 Gaussian quadrature

The Gaussian quadrature rule is a numerical method to evaluate an integral in discretized space. The integration becomes a weighted sum \( \int_{-1}^{1} f(x) dx = \sum_i w_i f(x_i) \) at Gaussian quadrature points \( x_i \in [-1, 1] \) with weights defined as

\[ w_i = \frac{2}{(1 - x_i^2) \left[ \frac{d}{dx} P_d(x_i) \right]^2}. \quad (5.124) \]

Here \( P_d(x) \) is the Legendre polynomial of degree \( d \) with \( x_i \) as its roots. In this model, the function \( f \) is usually a product of the basis functions with a target function \( f_t \). Only half of the quadrature points, namely \( x_i \in [0, 1] \), are need to be stored in memory for the integration in the radial direction. The number of points is chosen to be slightly higher than the minimum degree of \( P_d(x) \) required to resolve the target function. To integrate, we use for example,

\[ \int_0^1 q^l_n(r) f_t(r) dr = \sum_i w_i q^l_n(x_i) f_t(x_i). \quad (5.125) \]
Figure 5.17. 3D structures of the optimal flow field $u$ in model R1: a) $u^2$, b) $|\nabla \times u|$, c) Helicity $u \cdot \nabla \times u$, d) Maximum positive eigenvalue of the strain rate tensor.

For the integration along $\theta$ direction, we first need to change the domain from $\theta \in [0, \pi]$ to $\cos \theta \in [-1, 1]$:

$$\int_0^{\pi} \hat{P}^m_l(\cos \theta) f_l(\cos \theta) \sin \theta d\theta = \int_{-1}^{1} \hat{P}^m_l(-\cos \theta) f_l(-\cos \theta) d\cos \theta$$  \hspace{1cm} (5.126)

for associated Legendre functions. Using even/odd symmetries of $\hat{P}^m_l(\cos \theta)$ with respect to $\theta = \pi/2$, we can reduce the number of Gaussian quadrature points to half. Along $r$ and $\theta$, we use $N_r$ and $N_\theta$ Gaussian quadrature points and along $\phi$ we use $N_\phi$ Fourier grid points. The number of spatial grid points for resolution $(l_{\text{max}}, n_{\text{max}})$ are

$$N_r = \left\lceil \frac{3(2n_{\text{max}} + l_{\text{max}} + 6) + 1}{4} \right\rceil,$$

$$N_\theta = \frac{3(l_{\text{max}} + 2)}{2} + \text{mod} \left( \frac{3(l_{\text{max}} + 2)}{2}, 2 \right),$$

$$N_\phi = 4(l_{\text{max}} + 2) + \text{mod} \left( 4(l_{\text{max}} + 2), 4 \right).$$  \hspace{1cm} (5.127)

where $\lceil \rceil$ is the ceiling function.

### 5.5.2 Visualization of the optimal flow field

We show in this section the visualizations regarding the spatial structures of the optimal flow field $u$. In Figure 5.17 we show density plots of $u^2$, $|\nabla \times u|$, helicity $u \cdot \nabla \times u$ and maximum local strain rate (defined as the maximal eigenvalue of the non-dimensional strain rate tensor). These plots confirm the tendency of the field to localize near the center and also the lack of reflection symmetry. The optimal flow has a net nonzero helicity, this is discussed in §5.3.9. As the 3D structure is quite complex, we also show some corresponding 2D slices. We choose a plane that is either parallel (shown in Figure 5.18) or perpendicular (shown in Figure 5.19) to the axis with rotational symmetry. In these plots the localization is apparent. This localisation was also observed in minimal perturbations that trigger the transition to turbulence [Duguet et al., 2013; Kerswell et al., 2014; Pringle & Kerswell, 2010; Pringle et al., 2012].

We also plot here the individual spherical harmonic degree $l$ mode of the optimal flow field after an rotation. The symmetry axis is now aligned with the $z$ axis. We see clearly that $(l, |m|) = (1, 0), (2, 2), (3, 2)$ spectral modes are dominant, as shown in Figure 5.20.
Figure 5.18. 2D slices in $yz$ plane after changing coordinates so that $z$ axis is the rotational symmetry axis, also removing components with enstrophy less than 0.01%: a) $u^2$, b) $|\nabla \times u|$, c) helicity $u \cdot \nabla \times u$, d) maximum positive eigenvalue of the strain rate tensor.

Figure 5.19. 2D slices perpendicular to the rotational symmetry axis, which is now the $z$ axis (after changing coordinates and removing components with enstrophy less than 0.01%): a) $u^2$, b) $|\nabla \times u|$, c) helicity $u \cdot \nabla \times u$, d) maximum positive eigenvalue of the strain rate tensor.

Figure 5.20. Stream lines of $u_l$ for separate spherical harmonic degree $l$ modes in model R1 with $m, n$ indices summed up. a) Spatial structures of $u_1$. a) Spatial structures of $u_2$. a) Spatial structures of $u_3$. 
Chapter 6

Optimal kinematic dynamos in a sphere (free-slip B.C.)

6.1 Modifications

We have developed the optimization scheme for a kinematic dynamo model with no-slip boundary conditions. Now we want to test it on free-slip boundaries. Most parts of the Galerkin method stay the same, the difference is in the Galerkin basis and the treatment of boundary terms. We skip the repeated part in methodology and only show the modifications. For the flow field we have the incompressible condition:

\[ \nabla \cdot \mathbf{u} = 0, \quad x \in V. \quad (6.1) \]

and the free-slip boundary conditions:

\[ \mathbf{u} \cdot \hat{r}|_{\Sigma_-} = 0, \quad (6.2) \]

where \( \hat{r} \) denotes the radial unit vector. With this new set-up, the first thing we do is to re-examine the Lagrangian formulation. Since the boundary conditions do not show up explicitly in our Lagrangian, the Lagrangian for this set-up remains the same as in (5.13). The variational derivatives also remain the same. However, the boundary terms needs to be treated differently. We have the same formula for the boundary terms,

\[
0 = - \oint \Pi(\hat{r} \cdot \delta \mathbf{u})|_{\Sigma_-} dS - \oint 2\lambda_1 \left[ \delta \mathbf{u} \times (\nabla \times \mathbf{u}) \right] \cdot \hat{r}|_{\Sigma_-} dS \\
+ \int_0^T \oint \left[ (\hat{r} \times \mathbf{B}) \cdot \delta \mathbf{E}|_{\Sigma_-} - (\hat{r} \times \mathbf{B}^\dagger) \cdot \delta \mathbf{E}|_{\Sigma_+} \right] dS dt \\
+ \int_0^T \oint \left[ (\hat{r} \times \mathbf{E}) \cdot \delta \mathbf{B}|_{\Sigma_-} - (\hat{r} \times \mathbf{E}^\dagger) \cdot \delta \mathbf{B}|_{\Sigma_+} \right] dS dt \\
- \int_0^T \oint \left[ \psi^\dagger(\hat{r} \cdot \delta \mathbf{B})|_{\Sigma_-} - \psi^\dagger(\hat{r} \cdot \delta \mathbf{B})|_{\Sigma_+} \right] dS. \quad (6.3)
\]

The boundary terms involving \( \delta \mathbf{u} \) need to cancel, which implies

\[
- \oint \Pi(\hat{r} \cdot \delta \mathbf{u})|_{\Sigma_-} dS - \oint 2\lambda_1 \left[ \delta \mathbf{u} \times (\nabla \times \mathbf{u}) \right] \cdot \hat{r}|_{\Sigma_-} dS = 0. \quad (6.4)
\]
The cross product can be rewritten as

$$ \left[ \delta \mathbf{u} \times (\nabla \times \mathbf{u}) \right] \cdot \hat{r} = \left[ (\nabla \times \mathbf{u}) \times \hat{r} \right] \cdot \delta \mathbf{u}, \quad (6.5) $$

then we get an additional constraint,

$$ \hat{r} \times (\nabla \times \mathbf{u}) |_{\Sigma_{-}} = 0. \quad (6.6) $$

This condition has to be added to the flow field on top of the free-slip boundary conditions (6.2).

We use

$$ u^t_{nml}(r, \theta, \phi) = \begin{cases} \nabla \times \left( t^i_n(r) Y^m_l(\theta, \phi) \hat{r} \right), & r \in V, \\ 0, & r \in \hat{V}, \end{cases} $$

$$ u^p_{nml}(r, \theta, \phi) = \begin{cases} \nabla \times \nabla \times \left( s^i_n(r) Y^m_l(\theta, \phi) \hat{r} \right), & r \in V, \\ 0, & r \in \hat{V}, \end{cases} $$

$$ B^t_{nml}(r, \theta, \phi) = \begin{cases} \nabla \times \left( q^i_n(r) Y^m_l(\theta, \phi) \hat{r} \right), & r \in V, \\ 0, & r \in \hat{V}, \end{cases} $$

$$ B^p_{nml}(r, \theta, \phi) = \begin{cases} \nabla \times \nabla \times \left( p^i_n(r) Y^m_l(\theta, \phi) \hat{r} \right), & r \in V, \\ -l p^i_n(1) \nabla \left( r^{-(l+1)} Y^m_l(\theta, \phi) \right), & r \in \hat{V}, \end{cases} \quad (6.7) $$

as the toroidal (with a superscript $t$) and poloidal (with a superscript $p$) basis vector fields for $\mathbf{u}$ and $\mathbf{B}$. In this notation, $Y^m_l(\theta, \phi)$ are the orthonormal real spherical harmonics. The two boundary constraints on the flow field demand that:

$$ \frac{\partial t^i_n(1)}{\partial r} = 0, \quad \nabla^2 s^i_n(1) = 0 \quad (6.8) $$

For the flow field $\mathbf{u}$ the radial functions are

$$ t^i_n(r) = T_{nl} r^{l+1} (2n-1)(n+l) P^{(0,l+1/2)}_{n-1} [2r^2 - 1] - (2n + 1)(n + l + 1) P^{(0,l+1/2)}_{n} [2r^2 - 1], \quad (6.9) $$

$$ s^i_n(r) = S_{nl} r^{l+1} (1-r^2) (2n+2l+1) P^{(1,l+1/2)}_{n-1} [2r^2 - 1] - (n+1)^2 (2n+2l+3) P^{(1,l+1/2)}_{n-1} [2r^2 - 1], \quad (6.10) $$

The square bracket means $P^{(a,l+1/2)}_{n} [2r^2 - 1]$ is a function of $2r^2 - 1$. For the magnetic field $\mathbf{B}$ we use the same polynomials as in Chapter 5 that satisfy the insulating boundary conditions,

$$ q^i_n(r) = Q_{nl} r^{l+1} (1-r^2) P^{(2,l+1/2)}_{n-1} [2r^2 - 1], \quad (6.11) $$

$$ p^i_n(r) = P_{nl} r^{l+1} \left( c_1 P^{(0,l+1/2)}_{n-1} [2r^2 - 1] + c_2 P^{(0,l+1/2)}_{n} [2r^2 - 1] \right), $$

$$ c_1 = n(2l + 2n - 1), $$

$$ c_2 = -(n+1)(2n+2l+1). \quad (6.12) $$

Here $n = 1, \ldots, n_{\text{max}}$ and $l = 1, \ldots, l_{\text{max}}$ and $P^{(\alpha,\beta)}_{\lambda}$ are Jacobi polynomials. The numbers $T_{nl}, S_{nl}, Q_{nl}$ and $P_{nl}$ are normalization factors.
<table>
<thead>
<tr>
<th>$Rm$</th>
<th>$\gamma$</th>
<th>$r_t$</th>
<th>random start</th>
</tr>
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</tr>
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<td>0.129</td>
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<td>no</td>
</tr>
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<td>no</td>
</tr>
<tr>
<td>61.63</td>
<td>0.001</td>
<td>$9.2 \times 10^{-6}$</td>
<td>no</td>
</tr>
<tr>
<td>61.64</td>
<td>0.004</td>
<td>$8.7 \times 10^{-6}$</td>
<td>no</td>
</tr>
</tbody>
</table>

Table 6.1. Optimization data set for dynamos with free-slip boundary conditions, shown in two stages. The first stage at the top is a broad range survey, the second stage at the bottom is refined search to locate $Rm_{c,min}$. All data set use resolution: $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$.

6.2 Results

In this section we show the optimization results. Based on previous optimizations with no-slip boundary conditions, we use an improved line search method to adjust the step size $\Delta$. The step size $\Delta_2$ of $B_0$ is fixed, and we set it to be larger than the step size $\Delta_1$ for the velocity field. If the total residue is larger than that in the previous step, $\Delta_1 := 0.8\Delta_1$ and we restart the simulation from the previous iteration. This saves several iterations if the update goes in the wrong direction. If the step size $\Delta_1 < 0.01$, then the new step size is reset to $\Delta_1 := 0.1 + \Delta_1$. We add this condition to avoid premature convergence to a local maximum.

6.2.1 Optimal dynamo solutions

Again we use a refinement procedure similar to the no-slip case to locate $Rm_{c,min}$. Initial test runs start from random conditions, and have non-stringent convergence level $r_t$ in order to save computational time. Once we located the approximate range of $Rm_{c,min}$, we restart from previously converged results at nearby $Rm$ and demand better convergence to ensure the accuracy of the optimum. The simulation results are presented in Table 6.1. In the first series of runs, we varied $Rm \in [40, 70]$ using resolution $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$ and a relatively high toler-
Figure 6.1. Growth rate as a function of $Rm$ for optimized flows satisfying impermeable boundary conditions. Resolutions: $l_{\max} = 24$, $n_{\max} = 12$. 

ance on $r_t = \mathcal{O}(10^{-3}) \sim \mathcal{O}(10^{-4})$. This located the minimal dynamo threshold approximately in between $Rm_{c,\min} \in [61, 62]$. Then we gradually reduce the range of $Rm$, and finally we locate the optimal dynamo threshold at

$$Rm_{c,\min} \approx 61.62$$  \hspace{1cm} (6.13)

with a lower tolerance of $r_t \approx 10^{-5}$. In Figure 6.1, we plot the growth rate $\gamma$ as a function of $Rm$. We can fit the growth rate $\gamma$ with a parabolic curve, given by

$$\gamma = 0.0033Rm^2 - 0.0749Rm - 7.8598.$$ \hspace{1cm} (6.14)

This curve gives an estimate of the critical magnetic Reynolds number based on measurements at $Rm \ll Rm_{c,\min}$. It is not clear however if this parabolic fitting is generally valid.

We check our optimal solution at $Rm_{c,\min}$ by plotting the power spectrum of obtained $u$ and $B_T$ in Figure 6.2. The magnitude drops very quickly with increasing spherical harmonic degree $l$, which shows our resolution is sufficient and the result is converged. We then analyse the structures for the optimal flow field and its associated magnetic eigenmode in both physical space and spectral space. In physical space, we plot the streamlines of both $u$ and $B_T$. The streamline plots can help us create a qualitative picture of the field in 3D. The color indicates the magnitude of the field. We show the streamline plots in Figure 6.3. The flow field and magnetic field look almost identical to that in the no-slip case up to a rotation and reflection.

In spectral space, we analyse the distribution of enstrophy norm and magnetic norm in terms of spherical harmonic degree $l$, spherical harmonic mode $m$ and radial expansion degree $n$. We repeat the same analysis as for the no-slip case. In total 20 modes of $u_{l,n}$ are needed to capture 83% of the enstrophy (squared value), which is a spectral indication of a complex spatial structure. Alternatively, we can also sum up all index $n$ and compare each spherical harmonic mode with index $l, m$. We rotate the first two Euler angles in spectral space using Wigner D-matrices.
Figure 6.2. Power spectrum for the optimal flow field $u$ and the associated magnetic eigenmode $B_T$. 

Figure 6.3. a) The optimal flow field. b) The associated optimal magnetic eigenmode.

such that the coefficient $u^p_{nm} = u^p_{401}$ is maximized, and then rotate the third Euler angle such that $u^p_{nm} = u^p_{123}$ is maximized. In this way, the rotational symmetry axis is along $\hat{z}$ direction and the sum of non-negative $m$ modes are maximized. We impose a cut-off of absolute squared value 0.0112 for all spectral coefficients so that the dominant modes are in one symmetry class. In this case, we see an even $m$ symmetry for the flow field $u$. There are 73 nonzero spectral coefficients out of 14976 in total for the dominant optimal $u$. The leading spherical harmonic modes are given in Table 6.2-6.5. We see an odd $m$ symmetry for magnetic eigenvector $B_T$ when it is rotated by the same angle as $u$.

We also show the main properties of the flow field in Table 6.6, $\langle H \rangle$, poloidal to toroidal enstrophy and kinetic energy ratios are calculated in spectral space, while the values of $|u_{max}|$ and $S_{max}$ are measured in physical space using a grid search method. All amplitudes are comparable to the no-slip case. We notice that the helicity is negative now, this is due to the property of a pseudovector. The sign flips with respect to a reflection transformation. There is nothing more than a symmetry transformation to map the negative value to the positive value.
\( \langle (\nabla \times \mathbf{u})^2 \rangle \) & \( l = 1 \) & \( l = 2 \) & \( l = 3 \) & \( l = 4 \) & \( l = 5 \) \\
\( \langle \mathbf{u}^2 \rangle \) & \( 0.435 \) & \( 0.166 \) & \( 0.360 \) & \( 0.032 \) & \( 0.005 \) \\
\( \langle (B_T)^2 \rangle \) & \( 5.33 \times 10^{-3} \) & \( 4.25 \times 10^{-3} \) & \( 6.01 \times 10^{-3} \) & \( 0.37 \times 10^{-3} \) & \( 0.04 \times 10^{-3} \) \\
\( \langle \mathbf{B}^2 \rangle \) & \( 1.18 \) & \( 0.57 \) & \( 0.14 \) & \( 0.03 \) & \( 0.02 \)

Table 6.2. The enstrophy, kinetic energy and magnetic energy for the first five \( l \) modes at \( \text{Rm}_{c,\text{min}} \).

\( \langle (\nabla \times \mathbf{u}_{l,n})^2 \rangle \) 12848 0.08791 0.06220 0.05985 0.05980

Table 6.3. Leading components of enstrophy norm for \( \mathbf{u}_{l,n} \) and magnetic energy norm for \( \mathbf{B}_{Tl,n} \) in models \( \text{Rm}_{c,\text{min}} \).

\( \langle (\nabla \times \mathbf{u}_{m}^2) \rangle \) 0.273 0.226 0.208 0.057 0.045

Table 6.4. Leading components of enstrophy norm for \( \mathbf{u}_{m}^2 \) and magnetic energy norm for \( \mathbf{B}_{Tm}^2 \) after rotation and reduction.

\( \langle (\nabla \times \mathbf{u}_{m}^2) \rangle \) 0.4345 0.0309 0.0324 0.1018 0.0402 0.3132 0.0044

Table 6.5. The enstrophy and magnetic energy norm with \( l \leq 3 \) and \( |m| \leq 3 \) in model \( \text{Rm}_{c,\text{min}} \) after rotation and reduction.

\[ \langle H \rangle \quad \langle \mathbf{u} \rangle^{1/2} \quad \max |\mathbf{u}| \quad \omega P/\omega T^2 \quad E_P/E_T \quad S_{\text{max}} \]

\[ \mathbf{u} \quad -0.08 \quad 0.13 \quad 0.65 \quad 1.83 \quad 1.53 \quad 2.97 \]

Table 6.6. Properties of the optimal flow field.

### 6.2.2 Optimal transient solution

In addition, we also optimized the transient growth for this free-slip case. We keep other parameters the same, and just reduce the total time window \( T \). Since a shorter time window requires fewer time steps, we can run thousands of iterations...
until a very low tolerance \( r_t \approx 10^{-5} \) is reached. The minimal critical magnetic Reynolds number for any positive transient magnetic energy growth is \( Rm_{t,\text{min}} = 28.85 \). The flow field has \( E^S \) symmetry just as in the no-slip case. We plot the streamlines here in Figure 6.4. The field structures are very simple. The leading components in spectral space are shown in Table 6.7-6.9. We see the dominant flow component is a poloidal dipole field.

![Figure 6.4. a) Transient optimal flow field. b) Optimal transient magnetic eigen-mode.](image)

<table>
<thead>
<tr>
<th>( l = 1 )</th>
<th>( l = 2 )</th>
<th>( l = 3 )</th>
<th>( l = 4 )</th>
<th>( l = 5 )</th>
</tr>
</thead>
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<td>( \langle (\nabla \times \mathbf{u})^2 \rangle )</td>
<td>0.512</td>
<td>0.422</td>
<td>0.055</td>
<td>0.093</td>
</tr>
<tr>
<td>( \langle (\mathbf{B}_T)^2 \rangle )</td>
<td>0.949</td>
<td>0.039</td>
<td>0.011</td>
<td>0.001</td>
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</tbody>
</table>

Table 6.7. The enstrophy, kinetic energy and magnetic energy for the first five \( l \) modes at \( Rm_{t,\text{min}} \)

<table>
<thead>
<tr>
<th>( \mathbf{u}_m )</th>
<th>( \mathbf{u}_m^{p-1} )</th>
<th>( \mathbf{u}_m^{p0} )</th>
<th>( \mathbf{u}_m^{i1} )</th>
<th>( \mathbf{u}_m^{p1} )</th>
<th>( \mathbf{u}_m^{p2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \langle (\nabla \times \mathbf{u}_m)^2 \rangle )</td>
<td>0.465</td>
<td>0.202</td>
<td>0.172</td>
<td>0.046</td>
<td>0.022</td>
</tr>
<tr>
<td>( \mathbf{B}_T )</td>
<td>( \mathbf{B}_T^{p-1} )</td>
<td>( \mathbf{B}_T^{p0} )</td>
<td>( \mathbf{B}_T^{i1} )</td>
<td>( \mathbf{B}_T^{p1} )</td>
<td>( \mathbf{B}_T^{p2} )</td>
</tr>
<tr>
<td>( \langle (\mathbf{B}_T)^2 \rangle )</td>
<td>0.465</td>
<td>0.227</td>
<td>0.203</td>
<td>0.046</td>
<td>0.026</td>
</tr>
</tbody>
</table>

Table 6.8. Leading components of enstrophy norm for \( \mathbf{u}_m \) and magnetic energy norm for \( \mathbf{B}_T \) after rotation and reduction.

<table>
<thead>
<tr>
<th>( \langle H \rangle )</th>
<th>( \langle \mathbf{u} \rangle^{1/2} )</th>
<th>( \omega_p^2/\omega_T^2 )</th>
<th>( E_p/E_T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{u} )</td>
<td>( \sim 0 )</td>
<td>0.16</td>
<td>3.76</td>
</tr>
</tbody>
</table>

Table 6.9. Properties of the optimal transient field.
6.3 Conclusions

In this study, we optimized the kinematic dynamo in a sphere with free-slip boundary conditions. We use electrically insulating boundary conditions for the magnetic field, a commonly used boundary condition inspired by planetary dynamos. We cannot give a general rule that ultimately predicts optimal solution in any setting. We can, however, identify the optimal solution for a given system. The minimal critical magnetic Reynolds number for the dynamo onset here is $Rm_{c,min} = 61.62$. For the flow field, we have a low rms speed compared to the global shear magnitude or root mean enstrophy, again there is a rotational symmetry of order 2 and a very concentrated structure near the centre. The helicity is highly local, the overall helicity is rather small. We see the optimal flow field at $Rm_{c,min}$ has a weak presence near the boundary. As expected, this leads to similar results in almost all aspects as previously discussed optimal dynamo with no-slip boundary conditions. For example, the poloidal flow is stronger than the toroidal flow. The dominant spherical harmonic modes are $(l, |m|) = (1,0), (2,2), (3,2)$, when the rotational symmetry axis is aligned with $\hat{z}$ axis. The structures of the dominant optimal flow field are more complex than previously known KR or DJ dynamos. The magnetic field at the dynamo onset has mainly dipolar structures. With respect to the rotational symmetry axis of $\mathbf{u}$, the fastest growing magnetic field eigenmode has only odd $m$ modes.

In addition, we also optimized the transient growth for the magnetic field. The minimal critical magnetic Reynolds number for any positive magnetic energy growth is $Rm_{t,min} = 28.85$. The transient flow field is very simple and has $E^S$ symmetry. It shows a simple one convection roll is able to briefly increase the strength of a magnetic field. The distribution is likely to be local as the further away from the high speed zone, the weaker the field strength.
Chapter 7

Optimal kinematic dynamos in a sphere (with symmetries)

7.1 Introduction

In Chapter 5 and 6, we optimized kinematic dynamos with no-slip and free-slip boundary conditions in a sphere. We do not impose other restrictions other than boundary conditions, so the optima we get represent the best general solutions. In this chapter, we apply the same optimization scheme to study dynamos within a fixed symmetry class. We hope to identify which broad category of spatial structures are superior for dynamo action, and if so, by how much. Of course we are still using a kinematic model so we cannot generalize the results to a more complex model, but we can set the lower bound on $R_m$ for any extended models within the same symmetry class. We choose five topics to study as listed below; all settings have electrically insulating boundary conditions for the magnetic field and no-slip boundary condition for the flow field.

7.1.1 Five different symmetry classes

The five different symmetry classes in this chapter roughly speaking can be divided into three groups according to the symmetry we are interested in for either $\mathbf{u}$ or $\mathbf{B}$: the first one focuses on axisymmetric solutions, the next two deal with reflection symmetries and the last two combine the axisymmetry and the reflection symmetry.

1. The first task is to identify the optimal axisymmetric $\mathbf{u}$ field (spherical harmonic order $m = 0$) for dynamo action. We want to find out how low the $Rm_c$ of a dynamo can be with such a simple structure for the flow field. In a kinematic model, the magnetic field splits into separate solutions with different index $m$ due to the selection rule in §3.4.2. This is informally referred to as a “two and a half dimensional” problem. Computationally this is simpler than the fully 3D problems, but we encountered a new problem when we allowed all $m$ modes of $\mathbf{B}$ to be present. The optimization process produced a very strong axisymmetric magnetic field in our finite time window and masked the asymptotic magnetic energy growth. After many
iterations, the initial magnetic field is almost purely axisymmetric, then it becomes very difficult to show the growth of other magnetic eigenmodes. We then set the axisymmetric part of $B$ to zero so that the computer program can select other growing eigenmodes at a later time $T$. The optimal magnetic eigenmode has $m = 1$, just as expected.

2. The next two sets use an equatorially symmetric ($E^S$) flow field. Due to symmetry separation in the induction equation, with this symmetry for the flow field, the magnetic eigenmodes can be anti-symmetric with respect to reflection about the equatorial plane ($E^A$), this group of solutions is also called the dipole family. The first poloidal dipole mode is in this family.

3. Magnetic eigenmodes can also be symmetric with respect to reflection about the equatorial plane ($E^S$), this group of solutions is also called the quadrupole family. The next poloidal dipole mode is in this family. As mentioned in a comprehensive study of symmetry properties in dynamo models [Gubbins & Zhang, 1993], the terminology of “quadrupole family” is not entirely satisfactory since it includes the equatorial dipole solution. The meaning of “quadrupole” used here should be distinguished from the one used in the multipole expansion.

There are some very interesting results in the literature with this symmetry. The KR optimization explored the four subsets, and mapped out the phase space with this symmetry selection. They conclude that the axial dipole solutions are preferred with westward surface drift, axial quadrupole solutions are preferred for eastward surface drift, and equatorial dipoles solutions are preferred for convection with little differential rotation or meridional circulation [Gubbins et al., 2000b].

4. The last group sets two symmetries for the flow field, in addition to being axisymmetric, the flow field can be symmetric with respect to reflection about the equatorial plane ($E^S$). The magnetic field not only separates with different $m$ but also splits with either $E^A$ or $E^S$. We do not enforce the symmetry separation, but the optimal solution should naturally choose a symmetry with the lower $Rm_e$.

5. The flow field can also be anti-symmetric with respect to reflection about the equatorial plane ($E^A$). This one has only separation in spherical harmonic mode $m$ for the magnetic field. The magnetic field cannot be separated based on either $E^A$ or $E^S$ symmetry.

We also study the optimal transient growth for the last four set-ups in this chapter. Now there is no restriction on $m = 0$ for the magnetic field, we allow axisymmetric magnetic field to dominate for a short period. The restriction on symmetry classes reduces the vector space for dynamo solutions of the flow field $u$. In consequence, we expect the critical magnetic Reynolds number to be higher compared to set-ups without restrictions.
7.1.2 General setting of the model

The general setting for all six setups are listed below, then we will show model-specific settings and present the optimization results in the following sections. The magnetic field \( B = B(x, t) \) satisfies the induction equation, the current-free condition outside the sphere, Gauss’ law for magnetism and the continuity condition at the surface of the sphere,

\[
\partial_t B = Rm \nabla \times (u \times B) - \nabla \times (\nabla \times B), \quad x \in V, \tag{7.1}
\]

\[
\nabla \times B = 0, \quad x \in \hat{V}, \tag{7.2}
\]

\[
\nabla \cdot B = 0, \quad x \in V \cup \hat{V}, \tag{7.3}
\]

\[
B|_{\Sigma^+} - B|_{\Sigma^-} = 0, \tag{7.4}
\]

\( V \) is the fluid domain inside the sphere, \( \hat{V} \) is the external insulating region, \( \Sigma^\pm \) denote the two sides of the boundary at the surface of the sphere. The flow field \( u = u(x) \) satisfies the incompressible condition and the no-slip boundary conditions,

\[
\nabla \cdot u = 0, \quad x \in V, \tag{7.5}
\]

\[
u|_{\Sigma^-} = 0. \tag{7.6}
\]

The magnetic Reynolds number is

\[
Rm = \frac{\omega^* L^2}{\eta}, \tag{7.7}
\]

where \( \omega^* \) is the dimensional root mean enstrophy, \( L \) is the radius of the sphere. As a result of this non-dimensionalization scheme, the non-dimensional root mean enstrophy \( \omega = 1 \), where

\[
\omega = \sqrt{\frac{1}{V} \int_V (\nabla \times u)^2 dV}. \tag{7.8}
\]

Let us start with the Lagrangian for a general dynamo optimization,

\[
\mathcal{L} = \ln \left( \langle B^2 \rangle \right) - \lambda_1 \left( \langle (\nabla \times u)^2 \rangle - 1 \right) - \lambda_2 \left( \langle B_0^2 \rangle - 1 \right) - \langle \Pi \nabla \cdot u \rangle - \int_0^T \langle \psi \nabla \cdot B \rangle \ dt - \int_0^T \langle B^\dagger \cdot [\partial_t B + \nabla \times E] \rangle \ dt \]

\[
- \int_0^T \langle E^\dagger \cdot [\sigma r E + Rm u \times B - \nabla \times B] \rangle \ dt. \tag{7.9}
\]

We denote

\[
\langle \ldots \rangle = \frac{3}{4\pi} \int_0^\infty \int_0^\pi \int_0^{2\pi} \cdots r^2 \sin \theta dr d\theta d\phi. \tag{7.10}
\]

The derivation of variational derivatives is the same as in Chapter 5. For each of the six setups, we impose the symmetry constraint directly on the Galerkin basis.
The modifications on the Lagrangian are reflected on the spectral representations of $u$ and $B$. The poloidal-toroidal decomposition of the flow field is given by

$$u^t(r, \theta, \phi) = \sum_{l,m,n} v_{nml} \left[ \frac{1}{r \sin \theta} t_n^l(r) \frac{\partial Y_i^m}{\partial \phi} \theta - \frac{1}{r} t_n^l(r) \frac{\partial Y_i^m}{\partial \theta} \phi \right], \quad (7.11)$$

$$u^p(r, \theta, \phi) = \sum_{l,m,n} w_{nml} \left[ \frac{l(l+1)}{r^2} s_n^l(r) Y_i^m \hat{r} + \frac{1}{r} \frac{\partial s_n^l(r)}{\partial r} \frac{\partial Y_i^m}{\partial \theta} \theta + \frac{1}{r \sin \theta} \frac{\partial s_n^l(r)}{\partial r} \frac{\partial Y_i^m}{\partial \phi} \phi \right], \quad (7.12)$$

where $t_n^l$, $s_n^l$ are the radial functions and $Y_i^m$ are the real orthonormal spherical harmonics. The magnetic field $B$ is given by

$$B^t(r, \theta, \phi) = \sum_{l,m,n} c_{nml} \left[ \frac{1}{r \sin \theta} q_n^l(r) \frac{\partial Y_i^m}{\partial \phi} \theta - \frac{1}{r} q_n^l(r) \frac{\partial Y_i^m}{\partial \theta} \phi \right], \quad (7.13)$$

$$B^p(r, \theta, \phi) = \sum_{l,m,n} d_{nml} \left[ \frac{l(l+1)}{r^2} p_n^l(r) Y_i^m \hat{r} + \frac{1}{r} \frac{\partial p_n^l(r)}{\partial r} \frac{\partial Y_i^m}{\partial \theta} \theta + \frac{1}{r \sin \theta} \frac{\partial p_n^l(r)}{\partial r} \frac{\partial Y_i^m}{\partial \phi} \phi \right]. \quad (7.14)$$

The adjoint magnetic field $B^\dagger$ is not physical so it does not have restrictions on symmetry classes. We only reinforce the symmetry constraint at the update step, when the variational derivatives are projected onto the space of the corresponding fields $u$ and $B_0$.

### 7.2 Axisymmetric flows

The additional requirement for this part is to keep only the axisymmetric flow field, which corresponds to all spherical harmonic modes with $m = 0$. The vector field representation for $u$ is

$$u^t(r, \theta, \phi) = \sum_{l,m,n} v_{nml} \left[ -\frac{1}{r} t_n^l(r) \frac{\partial Y_i^m}{\partial \theta} \right], \quad (7.15)$$

$$u^p(r, \theta, \phi) = \sum_{l,m,n} w_{nml} \left[ \frac{l(l+1)}{r^2} s_n^l(r) Y_i^m \hat{r} + \frac{1}{r} \frac{\partial s_n^l(r)}{\partial r} \frac{\partial Y_i^m}{\partial \theta} \theta \right] \quad (7.16)$$

In spectral space, this means the flow field satisfies:

$$v_{nml} = w_{nml} = 0, \quad \text{if } m \neq 0. \quad (7.17)$$

For the update as in (5.68), we need

$$\delta v_{nml} = \delta w_{nml} = 0, \quad \text{if } m \neq 0 \quad (7.18)$$

The rest follows the same procedure as in Chapter 5.

We show the simulation results in three refinement stages in Table 7.1.
<table>
<thead>
<tr>
<th>$Rm$</th>
<th>$\gamma$</th>
<th>$l_{\text{max}}$</th>
<th>$n_{\text{max}}$</th>
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<td>$10^{-5}$</td>
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</table>

Table 7.1. Optimization data set for the axisymmetric flow problem.

The first stage gives a rough estimate, we use random initial points; the second stage focuses at a smaller range of $Rm$, we still start from random; the third and last stage restarted from previous results with lower value of allowed residue $r_t$. We did not start with a very low $Rm$ because the $Rmc$ for axisymmetric flows has to be greater than $Rmc_{\text{min}} \sim 65$ in the unrestricted case. In the first stage, we varied $Rm \in [90, 110]$ using resolution $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$ and a relatively high tolerance on $r_t = \mathcal{O}(10^{-3})$. This located the minimal dynamo threshold approximately at $Rmc \in [96, 97]$. As seen from previous simulations, the resolution $l_{\text{max}} = 24$ is sufficient since the spectral amplitudes are very small after $l > 3$, but more modes in $n$ may need to be included. Just to be on the safe
side, we increase the spectral resolution to \((l_{\text{max}}, n_{\text{max}}) = (24, 24)\) after stage one. Finally we located the optimal dynamo threshold at \(Rm_c = 96.38\) in stage three. In Figure 7.1, we also plot the growth rate from \(Rm \in [90, 105]\), there seems to be only one maximum. The power spectrum shows good convergence, as seen in Figure 7.2.

![Figure 7.1](image1.png)

Figure 7.1. The optimized growth rate \(\gamma\) as a function of \(Rm\) for axisymmetric flows.

![Figure 7.2](image2.png)

Figure 7.2. Power spectrum of enstrophy for the optimal axisymmetric \(u\) and magnetic field energy at \(Rm_c\).

In physical space, we plot the streamlines of the optimal fields in Figure 7.3. The flow field clearly has a toroidal differential rotation component. We notice there is also a lack of reflection symmetry. One side of the sphere is stronger than the other. The asymmetry between two hemispheres is perhaps not so rare. One roll dynamo action was found at least by one author [Moss, 2008].
Figure 7.3. The optimal axisymmetric flow and the associated magnetic eigenmode. a) Streamlines of the optimal flow field. b) Streamlines of the magnetic field.

7.3 Dipole families

This setting requires the flow field $\mathbf{u}$ to satisfy $E^S$ symmetry and the magnetic field to satisfy $E^A$ symmetry. In spectral space, this means the toroidal flow field satisfies:

$$v_{nml} = 0, \quad \text{if } l - m \text{ is even},$$

and the poloidal flow field satisfies:

$$w_{nml} = 0, \quad \text{if } l - m \text{ is odd}.$$  \hfill (7.19)

For the toroidal magnetic field the spectral coefficients need to satisfy

$$c_{nml}(t) = 0, \quad \text{if } l - m \text{ is odd},$$

and for the poloidal flow field,

$$d_{nml}(t) = 0, \quad \text{if } l - m \text{ is even}.$$  \hfill (7.20)

For the update we need the incremental changes $\delta v_{nml}, \delta w_{nml}, \delta c_{nml}(t), \delta d_{nml}(t)$ to satisfy the same symmetry requirement as the corresponding fields.

The optimization results are presented in Table 7.2. In the first series of runs, we vary $Rm \in [70, 90]$ and choose a relatively high tolerance $r_t = 10^{-3}$. In second stage we search for $Rm_c \in [79, 80]$ with $r_t = 10^{-4}$, and finally we locate the optimal dynamo threshold at $Rm_c \approx 79.16$ with $r_t = 10^{-5}$.

<table>
<thead>
<tr>
<th>$Rm$</th>
<th>$\gamma$</th>
<th>$r_t$</th>
<th>random start</th>
</tr>
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<tbody>
<tr>
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</tr>
<tr>
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<td>$10^{-3}$</td>
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</tr>
<tr>
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<td>$10^{-3}$</td>
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<td>-1.050</td>
<td>$10^{-3}$</td>
<td>yes</td>
</tr>
<tr>
<td>77.0</td>
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<td>yes</td>
</tr>
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<td>78.0</td>
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<td>$10^{-3}$</td>
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<tr>
<td>79.0</td>
<td>-0.093</td>
<td>$10^{-3}$</td>
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</tbody>
</table>
Table 7.2. Optimization data for the dipole family solution. Resolutions: \((l_{\text{max}}, n_{\text{max}}) = (24, 12)\).

<table>
<thead>
<tr>
<th>(Rm)</th>
<th>(\gamma)</th>
<th>(r_t)</th>
<th>random start</th>
</tr>
</thead>
<tbody>
<tr>
<td>79.1</td>
<td>-0.019</td>
<td>(10^{-4})</td>
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</tr>
<tr>
<td>79.2</td>
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<td>(10^{-4})</td>
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</tr>
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</tr>
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<tr>
<td>79.19</td>
<td>0.007</td>
<td>(10^{-5})</td>
<td>no</td>
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</table>

In Figure 7.4, we plot the growth rate \(\gamma\) as a function of \(Rm\) from all simulations. There is only one optimal branch. The power spectrum for the optimal solution at \(Rm_c\) is shown in Figure 7.5, we see that it is well converged. The streamlines of the flow field \(\mathbf{u}\) and its magnetic eigenvector \(\mathbf{B}_T\) are shown in Figure 7.6 a)-b). Compared to the unrestricted case, the flow is still concentrated at the centre. We see an axial dipole magnetic field plus some toroidal field components here.
Figure 7.5. Power spectrum of the optimal dipole family solution: contribution to enstrophy and magnetic energy.

Figure 7.6. The optimal dipole family solution. a) The optimal flow field. b) The associated optimal magnetic eigenmode $B_T$.

### 7.4 Quadrupole families

The flow field in this setting has $E^S$ symmetry, and the magnetic field has $E^S$ symmetry, which implies the toroidal flow field satisfies

$$v_{nml} = 0, \quad \text{if } l - m \text{ is even}, \quad (7.23)$$

and the poloidal flow field satisfies:

$$w_{nml} = 0, \quad \text{if } l - m \text{ is odd}. \quad (7.24)$$

For the toroidal magnetic field the spectral coefficients need to satisfy

$$c_{nml}(t) = 0, \quad \text{if } l - m \text{ is even}, \quad (7.25)$$
and for the poloidal flow field,
\[ d_{\text{nl}}(t) = 0, \quad \text{if } l - m \text{ is odd.} \quad (7.26) \]

Same conditions apply for the incremental changes \( \delta v_{\text{nl}}, \delta w_{\text{nl}}, \delta c_{\text{nl}}(t), \delta d_{\text{nl}}(t) \).

In the first series of runs, we varied \( Rm \in [70, 86] \). It is noticeable that sometimes the growth rate is lower when we increase \( Rm \). To check if this is caused by poor convergence, we then lower the tolerance to \( r_t \sim O(10^{-4}) \) until a very small improvement in \( \gamma \) is observed. But the growth rate does not increase much with a better convergence. Then it is very likely there is another suboptimal branch. We then repeat the same simulation with random start twice for \( Rm \in [75, 84] \). When we plot the growth rate, there is clearly a suboptimal branch, see Figure 7.7. This located the minimal dynamo threshold approximately in between \( Rm_c \in [81, 83] \) for the branch with higher growth rate, we restarted from solution from this branch and located the optimal dynamo threshold at \( Rm_c \approx 82.68 \). All simulation results are presented in Table 7.3 using resolution \( (l_{\text{max}}, n_{\text{max}}) = (24, 12) \).

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Table 7.3. Optimization data set for the quadrupole family solution. Resolutions: $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$.

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<tr>
<td>82.69</td>
<td>0.001</td>
<td>$2 \times 10^{-6}$</td>
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</tbody>
</table>

Figure 7.7. Growth rate as a function of $Rm$ for the quadrupole family of $B$. Resolutions: $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$.

Figure 7.8. Power spectrum of the optimal quadrupole family solution: contribution to enstrophy and magnetic energy.

The power spectrum of the optimal solution is shown in Figure 7.8. We plot the streamlines of the optimal fields in Figure 7.9. The flow field clearly has a
different structure compared to the dipole family solution. This shows the sym-
metry selection of the magnetic field does influence the structures of the optimal 
flow field.

![Figure 7.9](image)

Figure 7.9. The optimal quadrupole family solution. a) The optimal flow field. b) The optimal magnetic field $B_T$.

### 7.5 Axisymmetric $E^S$ flows

In this part, we combine two symmetry classes for the flow field $u$. We set the 
flow field to be axisymmetric

$$v_{nml} = w_{nml} = 0, \quad \text{if } m \neq 0. \quad (7.27)$$

In addition, the flow field needs to have $E^S$ symmetry. This means the toroidal 
flow field also satisfies:

$$v_{nml} = 0, \quad \text{if } l - m \text{ is even}, \quad (7.28)$$

and the poloidal flow field also satisfies:

$$w_{nml} = 0, \quad \text{if } l - m \text{ is odd}. \quad (7.29)$$

The same rule applies for the update.

We show the simulation results in three refinement stages in Table 7.4. The 
first is a survey over a range of $Rm$, we repeat simulations from random start but 
do not see suboptimal branches. In the second stage we locate the approximate 
range of $Rm_c \in [114.4, 114.8]$. The last stage of refinement gives $Rm_c = 114.51$. In 
Figure 7.10, we plot the growth rate $\gamma$ as a function of magnetic Reynolds number. 
No suboptimal branches are found.

For all optimizations in this section, we choose resolution $(l_{max}, n_{max}) = (24, 24)$ 
instead of $(l_{max}, n_{max}) = (24, 12)$ to give more freedom for structures along the ra-
dial direction. We did not use higher degree $l$ for two reasons, the first is that the 
numerical cost is much higher yet it does not improve significantly the results as 
judged by the power spectrum of the optimal solution. Even though the power 
spectrum does not decay as fast as in previous simulations, it still has a sufficient 
drop of $O(10^{-10})$ in magnitude as shown in Figure 7.11. The second reason is that
higher number \( n \) in radial direction contains rapid oscillations. These structures do not represent the dominant large structures.

<table>
<thead>
<tr>
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<th>( \gamma )</th>
<th>( r_t )</th>
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<td>( 10^{-3} )</td>
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<td>0.005</td>
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<td>114.57</td>
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</table>

Table 7.4. Optimization data set. Resolutions: \((l_{max}, n_{max}) = (24, 24)\).

The power spectrum of the optimal solution is shown in Figure 7.11. The optimal solutions in this case are well converged. We plot the streamlines of the optimal fields in Figure 7.12. The magnetic field again has a dominant equatorial dipole. The addition of \( E^S \) symmetry causes the flow to split from one spiral in §7.2 to two spirals—one copy of spiral patterns in each hemisphere.
Figure 7.10. Growth rate as a function of \( Rm \) for non-axisymmetric \( \mathbf{B} \) amplified by axisymmetric \( E^S \) flow \( \mathbf{u} \). Resolutions: \( (l_{\max}, n_{\max}) = (24, 24) \).

Figure 7.11. Power spectrum of the optimal axisymmetric \( E^S \) flow \( \mathbf{u} \) and the magnetic field at a later time \( T \).

Figure 7.12. The optimal axisymmetric \( E^S \) flow and its associated magnetic eigenvector. a) Streamlines of the optimal flow \( \mathbf{u} \). b) Streamlines of magnetic field \( \mathbf{B}_T \).
7.6 Axisymmetric $E^A$ flows

In this part, the flow field $\mathbf{u}$ needs to be axisymmetric

$$v_{nml} = w_{nml} = 0, \quad \text{if } m \neq 0,$$

and has $E^A$ symmetry. On top of the constrain (7.30), the toroidal flow field satisfies:

$$v_{nml} = 0, \quad \text{if } l - m \text{ is odd},$$

and the poloidal flow field satisfies:

$$w_{nml} = 0, \quad \text{if } l - m \text{ is even}.$$

As usual, the same symmetry constraints apply for the update.

We show the simulation results in three refinement stages in Table 7.5. First stage is a survey over a potential range of $Rm_c$. Since we already know the threshold of axisymmetric flows, the $Rm_c$ of axisymmetric $E^A$ flows must be higher, so we directly survey $Rm \in [100, 150]$ with a relatively high tolerance on $r_t = O(10^{-3})$. We notice there is a splitting in the growth rate, and repeat the simulation twice from random start for $Rm \in [135, 140]$. The second stage is restarted from the higher branch and shows $Rm_c < 138.5$. The last refinement stage gives the $Rm_c = 138.37$. We use $(l_{\max}, n_{\max}) = (24, 24)$ to give more freedom for structures along the radial direction.

The growth rate of all simulations are plotted in Figure 7.13. There are two branches. For the optimal branch at $Rm_c$, the power spectrum does not decay as fast as in the no-slip case, but still there is a $O(10^{-10})$ amplitude drop for the last spherical harmonic degree, shown in Figure 7.14.

<table>
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Table 7.5. Optimization data set. Resolutions: \((l_{\text{max}}, n_{\text{max}}) = (24, 24)\).

<table>
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<tr>
<td>138.39</td>
<td>0.002</td>
<td>(10^{-5})</td>
<td>no</td>
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Figure 7.13. Growth rate \(\gamma\) as a function of \(Rm\) for non-axisymmetric \(\mathbf{B}\) amplified by axisymmetric \(E^A\) flow \(\mathbf{u}\). Resolutions: \((l_{\text{max}}, n_{\text{max}}) = (24, 24)\).

The streamlines of the optimal solution are shown in Figure 7.15. We see the dominant magnetic field component is an axial dipole.
Figure 7.14. Power spectrum of the optimal axisymmetric $E^A$ flow $u$ and the magnetic energy at later time $T$.

Figure 7.15. The optimal axisymmetric $E^A$ flow and its associated magnetic eigenvector. a) Streamlines of the optimal flow field. b) Streamlines of the magnetic field.

7.7 The properties of the optimal fields

In this section we discuss collectively the optimal dynamos in different symmetry classes. We first identify what are the dominant modes, then compare their flow properties.

In Table 7.6, we show the amplitude of enstrophy, kinetic energy, and magnetic energy for the first five spherical harmonic degrees. In all models the kinetic energy is much lower than the enstrophy. For the three cases of axisymmetric $u$, the dominant spherical harmonic degree is either $l = 2$ or $l = 3$, and the dominant magnetic field has $l = 1$. This shows that we need at least two to three convection rolls to support a large scale dynamo efficiently. For the dipole/quadruple family, first four spherical harmonic degrees ($l \leq 4$) of $u$ are dominant, and $l = 1$ or $l = 2$ is dominant for the magnetic field. Although the $Rm_c$ for the dipole/quadruple family is lower compared to axisymmetric $u$ models, it is more difficult to realize their optimal flows in the lab. We need the controlling of all four spherical harmonic
degrees in dynamo experiments.

We also show the leading \((l,m)\) components of \(\mathbf{u}\) and \(\mathbf{B}_T\) fields in Table 7.7. For models with axisymmetric flows, the magnetic eigenmodes separate into groups with different \(m\). The least decaying mode is \(m = 1\), so we always get \(m = 1\) mode. For the dipole/quadruple family, the dominant \(m\) varies between \(0 \leq |m| \leq 3\).

<table>
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<th>(l = 2)</th>
<th>(l = 3)</th>
<th>(l = 4)</th>
<th>(l = 5)</th>
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<td>0.361</td>
<td>0.220</td>
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<td>0.093</td>
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<table>
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<tr>
<td>3)</td>
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<td>4.23 \times 10^{-3}</td>
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<td>4)</td>
<td>5.88 \times 10^{-3}</td>
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<td>0.02 \times 10^{-3}</td>
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<td>5)</td>
<td>2.43 \times 10^{-3}</td>
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<table>
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<th>(l = 4)</th>
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<td>0.095</td>
<td>0.208</td>
<td>0.144</td>
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<tr>
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<td>0.272</td>
<td>0.074</td>
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<tr>
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<td>0.906</td>
<td>0.494</td>
<td>0.101</td>
<td>0.043</td>
<td>0.010</td>
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<td>0.781</td>
<td>0.529</td>
<td>0.307</td>
<td>0.110</td>
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Table 7.6. The enstrophy, kinetic energy and magnetic energy for the first five \(l\) modes at \(Rm_{c,min}\) for various symmetry classes. From top row to bottom row in each section of the table: 1) axisymmetric flow, 2) the flow \(\mathbf{u}\) has \(E^5\) symmetry and \(\mathbf{B}\) has \(E^A\) symmetry, 3) the flow \(\mathbf{u}\) has \(E^S\) symmetry and \(\mathbf{B}\) has \(E^S\) symmetry, 4) axisymmetric \(E^S\) flow, 5) axisymmetric \(E^A\) flow.
Table 7.7. Leading components of enstrophy norm for $u^m$ and magnetic energy norm for $B_T^m$. From top row to bottom row in each section of the table: 1) axisymmetric flow, 2) the flow $u$ has $E^S$ symmetry and $B$ has $E^A$ symmetry, 3) the flow $u$ has $E^S$ symmetry and $B$ has $E^S$ symmetry, 4) axisymmetric $E^S$ flow, 5) axisymmetric $E^A$ flow.

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<th>$B_T^{t_1}$</th>
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<td>0.126</td>
<td>0.110</td>
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<tr>
<td>3)</td>
<td>1.063</td>
<td>0.415</td>
<td>0.181</td>
<td>0.143</td>
<td>0.106</td>
<td>0.415</td>
<td>0.181</td>
<td>0.143</td>
<td>0.106</td>
<td>0.415</td>
<td>0.181</td>
<td>0.143</td>
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<tr>
<td>4)</td>
<td>0.654</td>
<td>0.349</td>
<td>0.251</td>
<td>0.144</td>
<td>0.088</td>
<td>0.349</td>
<td>0.251</td>
<td>0.144</td>
<td>0.088</td>
<td>0.349</td>
<td>0.251</td>
<td>0.144</td>
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<td>0.837</td>
<td>0.429</td>
<td>0.349</td>
<td>0.322</td>
<td>0.273</td>
<td>0.429</td>
<td>0.349</td>
<td>0.322</td>
<td>0.273</td>
<td>0.429</td>
<td>0.349</td>
<td>0.322</td>
</tr>
</tbody>
</table>


|       | $\langle H \rangle$ | $\sqrt{\langle u^2 \rangle}$ | $\max V |u|$ | $\omega_P^2/\omega_T^2$ | $E_P/E_T$ | $S_{\max}$ | $\langle (B_{T\text{dipole}})^2 \rangle/\langle (B_T)^2 \rangle$ |
|-------|---------------------|-------------------------------|-----------|-----------------------|-----------|-----------|------------------------------------------|
| all   | 0.07                | 0.11                          | 0.69      | 1.885                 | 1.824     | 3.33      | 0.31                                     |
| Axi   | -0.12               | 0.14                          | 0.78      | 1.17                  | 1.05      | 2.02      | 0.45                                     |
| $E^A$ | 0                   | 0.11                          | 0.43      | 1.32                  | 1.24      | 3.28      | 0.36                                     |
| $E^S$ | 0                   | 0.10                          | 0.67      | 2.37                  | 3.39      | 4.20      | 0.50                                     |
| Axi-$E^S$ | 0               | 0.13                          | 0.54      | 1.23                  | 0.90      | 6.78      | 0.58                                     |
| Axi-$E^A$ | 0                | 0.13                          | 0.54      | 1.09                  | 0.97      | 1.58      | 0.36                                     |

All optimal models in this chapter have a weak boundary layer. Since the total shear is normalized, the majority of the shear is then concentrated in the bulk, although not all models have a concentrated region in the centre like the unrestricted case. This helps to reduce the overall kinetic energy. There is also evidence that a stagnant layer may help dynamo action [Bullard & Gubbins, 1977]. In Table 7.8 we list common properties of the optimal flow fields. We notice the following points: 1) the $E^A/E^S$ symmetry selection always gives zero net helicity in our model, because of the exact hemispherical symmetry. 2) The rms speed is about 0.1 for all models. So the values of $Rm_u$ in these models are one order of magnitude lower than enstrophy based $Rm$. 3) The poloidal to toroidal kinetic energy ratio is between approximately 1 to 2, which shows the poloidal flow needs to be sufficiently strong to drive a dynamo efficiently. The enstrophy ratio is similar to the kinetic energy ratio. 4) The amount of the poloidal dipole (both axial and equatorial) component varies with models. It generally makes up about 30% to 60% of the total magnetic energy. Also note that the maximum strain rate for the axisymmetric $u$ model is lower, so the maximum strain rate based
\( Rm_s = Rm S_{\text{max}} \) is actually lower than the unrestricted no-slip and free-slip case. The axisymmetric DJ flows have comparable values of \( Rm_s \).

### 7.8 The optimal transient solutions

In this section, we discuss collectively about the optimal transient solutions with symmetries. We find that both dipole and quadrupole family have the same threshold as the no-slip case: \( Rm_t = 30.21 \). Are the optimized transient fields actually the same? We check this by rotating the spectral components of the optimal transient flow fields and found they can be matched exactly. This means the classification of dipole or quadrupole family has limitations. One type can, although not always, be transferred to another type. For axisymmetric \( E^S \) flows, the critical value is \( Rm_t = 31.74 \); for axisymmetric \( E^A \) flows, the critical value is \( Rm_t = 36.08 \). The enstrophy and magnetic energy for the first five spherical harmonic modes for these four models mentioned above is shown in Table 7.9. Most energy is concentrated in just one or two spherical harmonic degrees.

<table>
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<tr>
<th>( \langle (\nabla \times \mathbf{u}_l)^2 \rangle )</th>
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<th>( l = 2 )</th>
<th>( l = 3 )</th>
<th>( l = 4 )</th>
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<td>1)</td>
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<td>( \sim 10^{-4} )</td>
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<tr>
<td>2)</td>
<td>0.53</td>
<td>0.41</td>
<td>0.05</td>
<td>0.01</td>
<td>( \sim 10^{-4} )</td>
</tr>
<tr>
<td>3)</td>
<td>0</td>
<td>0.972</td>
<td>0</td>
<td>0.027</td>
<td>0</td>
</tr>
<tr>
<td>4)</td>
<td>0.942</td>
<td>0</td>
<td>0.056</td>
<td>0</td>
<td>0.002</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \langle (B_l)^2 \rangle )</th>
<th>( l = 1 )</th>
<th>( l = 2 )</th>
<th>( l = 3 )</th>
<th>( l = 4 )</th>
<th>( l = 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1)</td>
<td>0.95</td>
<td>0.04</td>
<td>0.01</td>
<td>( \sim 10^{-4} )</td>
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<tr>
<td>2)</td>
<td>0.95</td>
<td>0.04</td>
<td>0.01</td>
<td>( \sim 10^{-4} )</td>
<td>0</td>
</tr>
<tr>
<td>3)</td>
<td>0.974</td>
<td>0</td>
<td>0.026</td>
<td>0</td>
<td>( \sim 10^{-4} )</td>
</tr>
<tr>
<td>4)</td>
<td>0.873</td>
<td>0.120</td>
<td>0.006</td>
<td>0.001</td>
<td>( \sim 10^{-4} )</td>
</tr>
</tbody>
</table>

Table 7.9. The enstrophy and magnetic energy for the first five \( l \) modes at \( Rm_t \). 1) dipole family: the flow \( \mathbf{u} \) has \( E^S \) symmetry and \( \mathbf{B} \) has \( E^A \) symmetry, 2) quadrupole family: the flow \( \mathbf{u} \) has \( E^S \) symmetry and \( \mathbf{B} \) has \( E^S \) symmetry, 3) axisymmetric \( E^S \) flow, 4) axisymmetric \( E^A \) flow.

A list of leading spherical harmonic modes for axisymmetric \( E^S/E^A \) models is given in Table 7.10. For axisymmetric \( E^S \) flows, the optimal transient flow field is a poloidal field; the associated optimal transient magnetic eigenmode is also poloidal and the leading component is an axial dipole. The dominant mode of the optimal transient flow is \( s_0^0 \). Interestingly, this is the same mode as the best transient flow identified by Livermore & Jackson [2004] among a selected group of prescribed flows (the radial function differs); the associated magnetic eigenmode also matches. For axisymmetric \( E^A \) flows, the optimal transient flow field has only poloidal components, but the magnetic field now has both poloidal and toroidal components. The dominant mode is a poloidal dipole flow field.

141
\[ \langle (\nabla \times \mathbf{u}_m^m)^2 \rangle \]

<table>
<thead>
<tr>
<th></th>
<th>( \mathbf{u}_2^0 )</th>
<th>( \mathbf{u}_4^0 )</th>
<th>( \mathbf{u}_6^0 )</th>
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<tbody>
<tr>
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<td>0.027</td>
<td>0.001</td>
<td>( \sim 10^{-5} )</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{u}_1^0 )</td>
<td>( \mathbf{u}_3^0 )</td>
<td>( \mathbf{u}_5^0 )</td>
<td>( \mathbf{u}_7^0 )</td>
</tr>
<tr>
<td>2</td>
<td>0.942</td>
<td>0.056</td>
<td>0.002</td>
<td>( \sim 10^{-5} )</td>
</tr>
</tbody>
</table>

\[ \langle (\mathbf{B}_{T_i}^m)^2 \rangle \]

<table>
<thead>
<tr>
<th></th>
<th>( \mathbf{B}_{T_1}^0 )</th>
<th>( \mathbf{B}_{T_3}^0 )</th>
<th>( \mathbf{B}_{T_5}^0 )</th>
<th>( \mathbf{B}_{T_7}^0 )</th>
<th>( \mathbf{B}_{T_9}^0 )</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>0.974</td>
<td>0.026</td>
<td>( \sim 10^{-4} )</td>
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<td>0</td>
</tr>
<tr>
<td></td>
<td>( \mathbf{B}_{T_1}^1 )</td>
<td>( \mathbf{B}_{T_3}^{-1} )</td>
<td>( \mathbf{B}_{T_5}^{r-1} )</td>
<td>( \mathbf{B}_{T_7}^1 )</td>
<td>( \mathbf{B}_{T_9}^{r1} )</td>
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<td>0.244</td>
<td>0.098</td>
<td>0.073</td>
<td>0.050</td>
</tr>
</tbody>
</table>

Table 7.10. The leading components of enstrophy for \( \mathbf{u}_m^m \) and magnetic energy for \( \mathbf{B}_{T_i}^m \) for the optimal transient solution. 1) axisymmetric \( E^S \) flow, 2) axisymmetric \( E^A \) flow.

### 7.9 Cube and sphere comparison

In this thesis project we have studied various optimal models in both Cartesian and spherical geometry. We found cases with only one optimal branch as well as cases with several branches. Generally speaking, the percentage of random start that launched on the optimal branch is around 60%—the \( E^S \) flow and quadrupole family \( B \) has 70%, NNT case has 66%, axisymmetric \( E^A \) case has 62%—with the exception of NTT case has 32% but it still produces the same three branches as the NNT case.

Among all optimal branches, we see that the cube optimum and the sphere optimum have quite different properties. To understand better why this is the case, we want to have a direct comparison of their field structures. One choice would be to make the size of the cube and the sphere comparable, then “cut off the corners” so one could fit most of the flow inside one other. But this creates artificial edges in an otherwise smooth flow, which then distorts the original optimal structure. Instead, we put a whole cube with the maximal side length \( 2/\sqrt{3} \) inside a sphere with radius 1, then run a forward model to see how the magnetic field evolves. We use the dominant NTT optimal flow and its magnetic eigenvector at \( Rm_{c,min} \) as the test case. Both fields remain smooth, normalized and satisfy the solenoidal condition inside a cube, which is now a subdomain of the sphere. For example, the \( x \) component of the vector basis is now given by

\[
U_x(m_x, m_y, m_z) = \frac{2}{\sqrt{3\pi}} \sin(m_x \frac{\sqrt{3\pi}}{2}) \cos(m_y \frac{\sqrt{3\pi}}{2}) \cos(m_z \frac{\sqrt{3\pi}}{2}),
\]

\[
B_x(m_x, m_y, m_z) = \cos(m_x \frac{\sqrt{3\pi}}{2}) \cos(m_y \frac{\sqrt{3\pi}}{2}) \cos(m_z \frac{\sqrt{3\pi}}{2}).
\]

The corresponding spectral coefficients are given in Table 7.11. The gap between the cube and sphere is padded with zero vector field. Only the four corners of the cube with zero velocity touch the spherical surface so the no-slip boundary conditions of the sphere is respected.
Table 7.11. Dominant spectral coefficients used to reconstruct the NTT optimum in the sphere.

Numerically however it is not ideal to introduce “de facto” boundaries inside another domain. Here the shape of the cube causes ringing when transferred to the spherical domain. Nevertheless, we can still get the dominant structures reproduced inside the sphere, see Figure 7.17 a)-b). We also test the flow structures by running a forward model at $Rm \gg Rm_{c,min}$ and check if the magnetic field lines follow the fluid motion, see Figure 7.16.

Figure 7.16. a) The optimal NTT magnetic field on Cartesian grids for comparison. b) The reproduced dominant NTT magnetic field on spherical grids.

The time evolution of the magnetic field generated by NTT flow is shown in Figure 7.18 a)-b). We see the field strength decays away very quickly, and the optimal structures also deform with time. The resulting asymptotic growth rate
A test run at $Rm \gg Rm_{c,\text{min}}$ shows the streamlines of the magnetic field at later times follow the flow field, just as expected from the frozen flux approximation; we used $Rm = 600$, $\Delta t = 10^{-4}$, $(l_{\text{max}}, n_{\text{max}}) = (24, 12)$, and $B_T$ from the NTT case as the initial field. Here the magnetic streamlines are plotted at $t = 0.3$.

The time evolution of the NTT optimal magnetic field. a) Streamlines at $t = 0.1$ diffusion time. b) Streamlines at $t = 0.3$ diffusion time. We use $B_T$ from NTT case as the initial field here, then run a forward model at $Rm = 55$ as if it is still inside a cube with side length $2/\sqrt{3}$ at $Rm_{c,\text{min}}$.

$\gamma$ is negative. Considering that the volume of a cube with side length $2/\sqrt{3}$ is still smaller than the volume of a sphere with radius 1, increasing $Rm$ to $\sim 100$ in order to have the same effective normalization for the NTT flow as other spherical flows would not make $\gamma$ positive, either. If we use a random initial magnetic field in all space as the starting point, the growth rate at $Rm = 55$ is $\gamma \approx -10$, which is still not close to the sphere optimum. Note that although we can measure the value of $\gamma$ more precisely, its precision is in fact limited by the overall resolution of the cube optimum inside the sphere.

The loss of optimality here could be due to the different spatial distribution of magnetic diffusion in a sphere. The optimal fluid motion that can balance the overall magnetic diffusion in one geometry may not be optimal in general. Even if the fluid is not moving in some parts of the domain, it still has an effect on
the overall decaying rate. In other words, when transferring designs to a different geometry, there might be a mismatch between what is optimal locally without considering the boundaries and what is optimal globally taking the boundary into account.

7.10 Conclusions

In this chapter, we analyze several scenarios for dynamo action in a sphere. We want to find out how different symmetries affect the onset of a dynamo. We include five different symmetries in our study. (1) The optimal axisymmetric $u$ field (spherical harmonic order $m = 0$) for dynamo action. (2) The optimal $E^S$ flow field $u$ and $E^S$ magnetic field $B$ for dynamo action. (3) The optimal $E^S$ flow field $u$ and $E^A$ magnetic field $B$ for dynamo action. (4) The optimal axisymmetric $E^S$ flow field $u$ for dynamo action. (5) The optimal axisymmetric $E^A$ flow field $u$ (spherical harmonic order $m = 0$) for dynamo action. In set-up (1), we find $Rm_c = 96.37$; the $m = 1$ spherical harmonic order dictates the asymptotic growth of magnetic fields. We find $Rm_c = 79.16$ in set-up (3) and $Rm_c = 82.68$ in set-up (4), which shows a magnetic field in the dipole family is slightly easier to generate than that in the quadrupole family, but the difference is nugatory. This is also seen in the smaller scale KR flow optimization of Gubbins et al. [2000b]. They found $Rm_c$ in the quadruple family is slightly higher than the dipole family. Both (3) and (4) have the same $Rm_t = 30.21$ as in the unconstrained case. This is due to a common optimal flow field up to a rotational transformation. As a consequence, the $E^A$ flows that occupy the rest of parameter space must have a higher $Rm_t$. In set-up (5) we find $Rm_c = 114.51$ and $Rm_t = 31.74$; in set-up (6) we find $Rm_c = 138.37$ and $Rm_t = 36.08$. The $E^S$ flows are more favourable for dynamo actions than the $E^A$ flows if both are axisymmetric. The associated optimal flow field that maximizes the short-term magnetic energy growth in both set-up (5) and (6) has only poloidal components. In set-up (5) the optimal transient growth favours $m = 0$ magnetic field with only poloidal components, the flow field is dominated by $u^p_0$ components. In set-up (6), the $m = 1$ magnetic field is preferable with 16% of toroidal components for the same time window, the dominant flow component is $u^p_1$. Both $u^p_0$ and $u^p_0$ cannot sustain a dynamo alone at $Rm_t$, but they each produces an optimal transient growth for their corresponding symmetry class.
Chapter 8
Conclusions

In this thesis, we extended the study of Willis [2012] and identified the optimal kinematic dynamos generated by steady flows with various geometries, boundary conditions and symmetry classes. Given an enstrophy based $Rm$, the optimal solution is identified using a variational method. We define a Lagrangian that consists of an objective functional, normalization constraints, solenoidal constraints, and constraints for the time evolution of magnetic field $B$. Each constraint is multiplied with a Lagrange multiplier. By taking variational derivatives of the Lagrangian with respect to each variable (including the Lagrange multipliers) and setting each derivative to zero, one gets a coupled system of Euler-Lagrange (EL) equations. The optimal solution is the one that solves all EL equations. We searched numerically for the lower bound on the magnetic Reynolds number $Rm_{c,min}$ for the dynamo action, and analyzed the properties of the corresponding optimal velocity field $u(x)$ and magnetic eigenmode $B(x,T)$ at a prescribed time $T$. In some cases, we also studied the optimal transient growth and found the ultimate lower bound on non-negative instantaneous growth in magnetic energy $Rm_{t,min}$. No dynamos can occur below this bound even for a very short time period due to insufficient magnetic induction. We found mainly large scale structures in the optimized fluid flow and magnetic fields, yet the precise form differs from model to model.

In Cartesian coordinates, we identified the optimal kinematic dynamo for a flow confined in a cube. We tested four sets of magnetic boundaries NNT, NTT, NNN and TTT (T denotes superconducting boundary conditions and N denotes pseudo-vacuum boundary conditions on opposite sides of the cube, and the three letters represent the $x, y, z$ directions). We approach the optimum iteratively in an optimization loop using a spectral Galerkin method. The minimal magnetic Reynolds number for dynamo action is at least three times lower than ABC flows. Swapping the magnetic boundary conditions from T to N leaves the optimal magnetic energy growth nearly unchanged numerically. This swapping of boundary conditions corresponds to a symmetry transformation for the optimal flow field from $u$ to $-u$. For the mixed boundary cases NNT and NTT, we can represent the dominant optimal flow field at $Rm_{c,min}$ with three Fourier modes that each describe a 2D flow field. For the homogenous boundary cases NNN and TTT, we did not find a clear dominant structure. The dominant NNT/NTT flows have one main vortex plus two secondary vortices in each half of the domain as the
mean flow in the VKS experiment. But in the VKS experiment the two blades are counter-rotating, the direction of the flow and the resulting magnetic eigenmode do not match ours.

In spherical coordinates, we identified the optimal kinematic dynamo in a sphere with no-slip and insulating boundary conditions. We use a spectral Galerkin method with specially constructed Jacobi polynomials as the radial basis functions. The optimal flow field at \( Rm_{c,\text{min}} \) has a rotational symmetry of order 2 and a very concentrated structure near the centre. The dominant spherical harmonic modes are \((l, |m|) = (1, 0), (2, 2), (3, 2)\), when the rotational symmetry axis is aligned with the \( \hat{z} \) axis. Near the boundary, the optimal flow is very weak. The rms speed is much lower compared to the global shear magnitude or root mean enstrophy in the system. The associated magnetic eigenmode at \( Rm_{c,\text{min}} \) has dominantly dipolar structures. With respect to the rotational symmetry axis of \( \mathbf{u} \), the fastest growing magnetic field eigenmode has only odd \( m \) modes. Comparing the spatial structures to well-known flows such as DJ flows, our optimal flows in a sphere tend to concentrate in the bulk to form one or more strong spirals. Boundary flows are always weak. The value of critical transient magnetic Reynolds number \( Rm_{t,\text{min}} \) in this model is about half of \( Rm_{c,\text{min}} \).

We also studied spherical models with different boundary conditions and symmetry restrictions. The optimal kinematic dynamo in a sphere with free-slip and insulating boundary conditions shares many similarities with the no-slip case. The enstrophy based \( Rm_{c,\text{min}} \) and \( Rm_{t,\text{min}} \) are just slightly below that in the no-slip case. We use five different set-ups to further explore how the dynamo onset changes with symmetries, all with no-slip boundary conditions: (1) dynamos generated by axisymmetric flows, (2) dynamos with an equatorially anti-symmetric \((E^A)\) magnetic field (the dipole family) generated by \( E^S \) flows, (3) dynamos with an \( E^S \) magnetic field (the quadrupole family) generated by \( E^S \) flows, (4) dynamos generated by axisymmetric \( E^S \) flows, (5) dynamos generated by axisymmetric \( E^A \) flows. The dipole family has a slightly lower critical magnetic Reynolds number \( Rm_c \) than that of the quadrupole family, followed by the onset of a dynamo generated by axisymmetric flows, which is about 1.5 times higher compared to the unrestricted case. With additional symmetry restrictions, the last two cases (4) and (5) have even higher values of \( Rm_c \). The optimal transient solutions, however, are not necessarily linked to the optimal dynamo solutions. The optimal transient solution for the dipole family, quadrupole family and the unrestricted case are the same up to a rotation. The optimized transient magnetic field from set-up (4) has only \( m = 0 \) poloidal components, but from set-up (5) we have \( m = 1 \) magnetic eigenmode with both poloidal and toroidal components. The values of \( Rm_t \) for (4) and (5) remain the same order of magnitude as in the unrestricted case. A list of critical magnetic Reynolds numbers for all spherical models is also given below in Table 8.1 below.

As stated in the introduction, the kinematic model we used in this thesis does not consider the backreaction from the magnetic field to the conductive fluid flow via the Lorentz force. In reality, the Lorentz force may not be negligible and the velocity field is likely to have time dependence. At the present stage, our optimal solutions cannot capture the dynamical interactions between the flow and
Table 8.1. A list of critical magnetic Reynolds numbers and transient magnetic Reynolds numbers. 1) axisymmetric flow, 2) the flow \( \mathbf{u} \) has \( E^S \) symmetry and \( \mathbf{B} \) has \( E^A \) symmetry, 3) the flow \( \mathbf{u} \) has \( E^S \) symmetry and \( \mathbf{B} \) has \( E^S \) symmetry, 4) axisymmetric \( E^S \) flow, 5) axisymmetric \( E^A \) flow, 6) unrestricted case. 7) free-slip boundary conditions for the flow field \( \mathbf{u} \). Cases 1) to 6) have no-slip boundary conditions for the flow field \( \mathbf{u} \).

<table>
<thead>
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<th></th>
<th>1)</th>
<th>2)</th>
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<th>4)</th>
<th>5)</th>
<th>6)</th>
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<td>61.62</td>
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<tr>
<td>( Rm_t )</td>
<td>-</td>
<td>30.21</td>
<td>30.21</td>
<td>31.74</td>
<td>36.08</td>
<td>30.21</td>
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</table>

the magnetic field at the onset of a dynamo. It would be interesting to extend our model to include these and other relevant effects. However, many challenges lie ahead both in studies related to experiments and numerical simulations. How can one apply an optimization method in a hydrodynamically turbulent regime? And how to identify the optimal initial conditions in a highly non-linear MHD model? Do we have fast algorithms for direct numerical simulations (DNS) in order to reach convergence with limited computational resources? Substantial progress in these directions seems necessary to truly understand the dynamical aspects of dynamos.
Appendices
Appendix A

Dynamo theory

A.1 Theoretical lower bounds on dynamo action

A.1.1 Backus bound

The Backus bound is a theoretical bound for dynamo action based on maximum strain rate. We show below the derivations in Backus [1958]. Let us consider a region $V$ filled with conducting fluid, surrounded by an external region $\hat{V}$. Taking the dimensional induction equation defined inside region $V$, then multiply it by $B$, we get

$$B \cdot \frac{\partial B}{\partial t} = B \cdot \nabla \times (u \times B) - B \cdot \eta \nabla^2 B. \quad (A.1)$$

The first term can be rewritten as,

$$\int_V B \cdot \frac{\partial B}{\partial t} \, dV = \frac{1}{2} \frac{\partial}{\partial t} \int_V B^2 \, dV. \quad (A.2)$$

When there is no contribution of magnetic induction from external region $\hat{V}$, we get

$$\frac{1}{2} \frac{\partial}{\partial t} \int_{V \cup \hat{V}} B^2 \, dV = \int_V \left[ B \cdot (B \cdot \nabla)u - \eta (\nabla \times B)^2 \right] \, dV. \quad (A.3)$$

The next step is to estimate the magnitude of magnetic induction,

$$\int_V B \cdot (B \cdot \nabla)u \, dV \leq S_{max} \int_V B \cdot B \, dV, \quad (A.4)$$

where the $S_{max}$ is the absolute maximum eigenvalue of the strain rate tensor,

$$S_{ij} = \frac{1}{2} (\nabla_i u_j + \nabla_j u_i). \quad (A.5)$$

Dynamo action requires non-negative value from LHS of (A.2). This translates to

$$\frac{S_{max}}{\eta} \geq \frac{\int_V (\nabla \times B)^2 \, dV}{\int_V B^2 \, dV} \quad (A.6)$$
In a sphere surrounded by insulating exterior \( \hat{V} \), the least decaying magnetic eigenmode for \( \nabla^2 \mathbf{B} \) is \( \pi^2/L^2 \) from a poloidal field with spherical harmonic degree \( l = 1 \), so we get
\[
\int_{\hat{V}} (\nabla \times \mathbf{B})^2 \, dV \geq \int_{\hat{V}} \mathbf{B} \cdot \nabla^2 \mathbf{B} \, dV \geq \frac{\pi^2}{L^2} \int_{V} \mathbf{B}^2 \, dV,
\]
(A.7)
where \( L \) is the dimensional radius. In terms of maximum strain rate based magnetic Reynolds number, the lower bound is
\[
Rm_s \geq \pi^2.
\]
(A.8)

### A.1.2 Childress bound

Childress bound uses maximal speed to estimate the contribution from the magnetic induction [Childress, 1969]. The energy equation in (A.3) can be rewritten as
\[
\frac{1}{2} \frac{\partial}{\partial t} \int_{V \cup \hat{V}} \mathbf{B}^2 \, dV = \int_{V} [(\nabla \times \mathbf{B}) \cdot (\mathbf{u} \times \mathbf{B}) - \eta (\nabla \times \mathbf{B})^2] \, dV.
\]
(A.9)
Then the estimated contribution from the velocity field \( \mathbf{u} \) has to be bounded above by
\[
\int_{V} (\nabla \times \mathbf{B}) \cdot (\mathbf{u} \times \mathbf{B}) \, dV \leq u_{\text{max}} \sqrt{\int_{V} (\nabla \times \mathbf{B})^2 \, dV} \sqrt{\int_{V} \mathbf{B}^2 \, dV}.
\]
(A.10)
In a sphere \( V \) with electrical insulating boundary conditions, this gives
\[
\frac{u_{\text{max}} L}{\eta} \geq \pi.
\]
(A.11)

### A.1.3 Proctor bound

The necessary condition for dynamo action by Backus [1958] is improved by Proctor [1977]. There is one additional term that gives contribution from the external region \( \hat{V} \), the magnetic energy equation becomes
\[
\frac{1}{2} \frac{\partial}{\partial t} \int_{V \cup \hat{V}} \mathbf{B}^2 \, dV = \int_{V} [\mathbf{B} \cdot (\mathbf{B} \cdot \nabla) \mathbf{u} - \eta (\nabla \times \mathbf{B})^2] \, dV - \eta \int_{V} \frac{1}{\gamma(r/L)} (\nabla \times \mathbf{B})^2 \, dV
\]
(A.12)
Here \( \eta/\gamma(r/L) \) is the magnetic diffusivity in region \( \hat{V} \), \( \gamma(x) \to \mathcal{O}(1/x) \) as \( x \to \infty \). The least decaying mode of magnetic field \( \mathbf{B} \) is found by minimizing a non-dimensionalized Lagrangian by length scale \( L \),
\[
\mathcal{L} = \int_{V} (\nabla \times \mathbf{B})^2 \, dV + \int_{V} \frac{1}{\gamma(r)} (\nabla \times \mathbf{B})^2 \, dV
\]
\[
- \alpha^2 (\int_{V} \mathbf{B}^2 \, dV - 1) - \int_{V \cup \hat{V}} \Pi_1 \nabla \cdot \mathbf{B} \, dV - \int_{V \cup \hat{V}} \Pi_2 \nabla \cdot \mathbf{J} \, dV
\]
\[
- \int_{V \cup \hat{V}} v(r) \hat{r} \cdot (\nabla \times \mathbf{B} - \mathbf{J}) \, dV
\]
(A.13)
The optimal solution as $r \to \infty$ gives

$$\frac{\int_V (\nabla \times \mathbf{B})^2 \, dV}{\int_{V \cup \hat{V}} \mathbf{B}^2 \, dV} \geq 12.29$$  \hspace{1cm} (A.14)

In terms of the maximum strain rate based magnetic Reynolds number, this is $Rm_s \geq 12.29$. 
Appendix B

Cubes

B.1 Coordinate system

In this section we introduce some bookkeeping index notations in order to show the derivations in the following sections. The index notation is used to label all array components in a concise way. Unless specified otherwise, in this section each index runs through the three numbers 1, 2, 3 which refer to the \(x, y, z\) directions respectively. If an index appears once in an upper position and once in a lower position, then this index is summed over. For example, the divergence of \(\mathbf{u}\) can be written like this:

\[
\nabla \cdot \mathbf{u} = \partial_i u^i
\]

(B.1)

In general, a scalar has no free indices, all indices have to be contracted like in the above example of the divergence of \(\mathbf{u}\). The total number of components equals the number of dimensions to the power of the number of free indices. For example, a tensor \(A_{ij}\) has \(3^2 = 9\) components.

In a general space, to lower or raise an index of a tensor we multiply it with the metric \(\eta_{jk}\) or its inverse \(\eta^{jk}\). For example, to raise one index in a tensor \(A_{ij}\) is done like this:

\[
A_{ij} \eta^{jk} = A^i_j
\]

(B.2)

Usually the metric measures how the spacetime is curved. In a flat 3-dimensional space with Cartesian coordinates, the metric is simply the identity matrix:

\[
\eta_{ab} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

(B.3)

where \(\eta^{ab}\) is called the inverse metric. It satisfies

\[
\eta_{ab} \eta^{ac} = \delta^c_a,
\]

(B.4)

so we get the identity matrix again,

\[
\eta^{ab} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

(B.5)
B.2 Equivalent norms

In this section we derive the equivalence of the global shear and the enstrophy norm $S = \omega^*$. We assume the flow $u$ satisfies 3 conditions:

1) $\nabla \cdot u = 0$, and
2) $u \cdot n \big|_{\Sigma} = 0$, and
3) $n \times (\nabla \times u) \big|_{\Sigma} = 0$,

where $\Sigma$ is the surface of the cube, $n$ is the unit normal vector pointing outward at each face of $\Sigma$, as shown in Figure B.1. First, we rewrite the three conditions on $u$ with index notation. Condition (1) is the incompressible condition,

$$\partial_i u^i = 0. \quad (B.6)$$

Conditions (2) is the impermeable boundary condition,

$$u_i n^i \big|_{\Sigma} = 0. \quad (B.7)$$

The additional boundary condition (3) can be written with index notation as follows:

$$\epsilon_{lkm} \epsilon^{ijk} n^l \partial_i u_j \big|_{\Sigma} = 0 \quad (B.8)$$

where the contraction of the Levi-Civita symbols gives two terms:

$$\epsilon_{lkm} \epsilon^{ijk} = -\epsilon_{lmk} \epsilon^{ijk} = -\delta_l^i \delta_m^j + \delta_l^j \delta_m^i \quad (B.9)$$

Then condition (3) can be simplified as:

$$n^l (\partial_m u_l - \partial_l u_m) \big|_{\Sigma} = 0 \quad (B.10)$$

where $n^i$ is non-zero only at the two sides of the cube $\Sigma_l$ along direction $l$. The expression inside the bracket in equation (B.10) is anti-symmetric. The flow is confined in a unit cube, $x, y, z \in [0, 1]$. The global shear is defined as

$$S = \sqrt{\langle 2S_{ij}S^{ij} \rangle}, \quad (B.11)$$

where $S^{ij} = S_{kl} \eta^{ki} \eta^{lj}$. The strain rate tensor $S_{ij} \eta^{kl}$ is defined as:

$$S_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i). \quad (B.12)$$
It measures how the symmetric part of the flow is distorted.

Claim (1): The strain rate tensor is symmetric.

\[ S_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i) = \frac{1}{2} (\partial_j u_i + \partial_i u_j) \]
\[ S_{ji} = \frac{1}{2} (\partial_j u_i + \partial_i u_j) \]  

So we get
\[ S_{ij} = S_{ji}. \]

Claim (2): \( S_{ij} \) and \( S^{ij} \) have the same components.

\[ S^{ij} = \begin{pmatrix} S_{11}^{11} & S_{12}^{12} & S_{13}^{13} \\ S_{21}^{21} & S_{22}^{22} & S_{23}^{23} \\ S_{31}^{31} & S_{32}^{32} & S_{33}^{33} \end{pmatrix} = S_{kl} \eta^{ki} \eta^{lj} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}. \]

This implies
\[ 2S_{ij} S^{ij} = 2(S_{11})^2 + 2(S_{12})^2 + 2(S_{13})^2 + 2(S_{21})^2 + 2(S_{22})^2 + \\
2(S_{23})^2 + 2(S_{31})^2 + 2(S_{32})^2 + 2(S_{33})^2 \]
\[ = 2(S_{11})^2 + 2(S_{22})^2 + 2(S_{33})^2 + 4(S_{12})^2 + 4(S_{13})^2 + 4(S_{23})^2. \]

Another way to compute this is to simplify each component,
\[ 2S_{ij} S^{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i) (\partial^j u^i + \partial^i u^j) \]
\[ = \frac{1}{2} (\partial_i u_j \partial^j u^i + \partial_j u_i \partial^i u^j + \partial_i u_j \partial^i u^j + \partial_j u_i \partial^j u^i) \]
\[ = \partial_i u_j \partial^j u^i + \partial_i u_j \partial^i u^j \]

We want to evaluate the average strain rate over the whole volume. The average is defined as
\[ \langle \cdots \rangle = \frac{1}{V} \int \cdots \, dv. \]

Claim (3): \( S^2 = \langle -u_j (\partial_i \partial^i u^j) \rangle \).

We have the following equalities:
\[ S^2 = \langle \partial_i u_j \partial^j u^i + \partial_i u_j \partial^i u^j \rangle \]
\[ = \langle \partial_i u_j \partial^j u^i \rangle + \langle \partial_i u_j \partial^i u^j \rangle \]
\[ = -\langle u_j (\partial_i \partial^i u^j) \rangle + \frac{1}{V} \int \partial_i (u_j \partial^i u^j) \, dV \]
\[ = -\langle u_j (\partial^i \partial_i u^j) \rangle + \frac{1}{V} \int n_i (u_j \partial^i u^j) \, d\Sigma \]
\[ = -\langle u_j (\partial_i \partial^i u^j) \rangle + \frac{1}{V} \int n_i (u_j \partial^j u^i) \, d\Sigma \]
\[ = -\langle u_j (\partial_i \partial^i u^j) \rangle + \frac{1}{V} \int n_i (u_j \partial^j u^i) \, d\Sigma \]
The flow is divergence free in all space, so we have
\[ \partial^j \partial_i u^i = 0 \] (B.22)
along any direction \( j \), and the first term in (B.20) must vanish. Let us look at the second term. Because of condition (2), on each side of the cube, \( \mathbf{u} \cdot \mathbf{n} = 0 \) and therefore does not depend on the other two directions perpendicular to \( \mathbf{n} \). So is we construct an arbitrary vector \( \mathbf{p} \) such that
\[ \mathbf{p}^i n_i \bigg|_{\Sigma} = 0 \] (B.23)
and
\[ p_j n_i \partial^i u^j \bigg|_{\Sigma} = 0 \] (B.24)
In fact, \( u_j \) is one specific example of \( p_j \), so the second term in (B.20) also vanishes. We get
\[ \langle p_i u_j \partial^i u^j \rangle = 0 \] (B.25)
Similarly, we can use condition (2) and (3) to simplify (B.21). The expression inside the bracket in equation (B.10) is anti-symmetric, so we can construct another arbitrary vector \( \mathbf{q} \) such that
\[ q^i n_i \bigg|_{\Sigma} = 0 \] (B.26)
and
\[ q^m n^j (\partial_m u_l - \partial_l u_m) \bigg|_{\Sigma} = 0 \] (B.27)
Combining with equation (B.24), the second term in (B.27) must be zero. So
\[ -q^m n^j \partial_l u_m \bigg|_{\Sigma} = -q_j n_i \partial^i u^j \bigg|_{\Sigma} = 0 \] (B.28)
Again let \( \mathbf{u} \) being a specific example of \( \mathbf{q} \), the second term in (B.21) also vanishes. We have one term left:
\[ \langle \partial_i u_j \partial^i u^j \rangle = -\langle u_j (\partial_i \partial^i u^j) \rangle \] (B.29)
In Cartesian coordinates,
\[ \nabla^2 = \partial_i \partial^i \] (B.30)
So
\[ \langle \partial_i u_j \partial^i u^j \rangle = -\langle u_j (\partial_i \partial^i u^j) \rangle = \langle -\mathbf{u} \cdot \nabla^2 \mathbf{u} \rangle \] (B.31)
Now using the standard vector calculus notation, we can rewrite the enstrophy norm as:
\[ \langle (\nabla \times \mathbf{u})^2 \rangle = \langle \left( \nabla \times \mathbf{u} \right) \cdot (\nabla \times \mathbf{u}) \rangle = \langle \nabla \cdot (\mathbf{u} \times (\nabla \times \mathbf{u})) + \mathbf{u} \cdot (\nabla \times (\nabla \times \mathbf{u})) \rangle = \langle \nabla \cdot (\mathbf{u} \times (\nabla \times \mathbf{u})) \rangle + \langle \mathbf{u} \cdot (\nabla \times (\nabla \times \mathbf{u})) \rangle \] (B.32)
We have condition (3), so
\[
\langle \nabla \cdot (u \times (\nabla \times u)) \rangle = \frac{1}{v} \int \nabla \cdot (u \times (\nabla \times u)) \, dv = \frac{1}{v} \int \nabla \cdot (u \times (\nabla \times u)) \, d\Sigma = \frac{1}{v} \int u \cdot ((\nabla \times u) \times n) \, d\Sigma = 0
\] (B.33)

and
\[
\langle u \cdot (\nabla \times (\nabla \times u)) \rangle = \langle u \cdot \nabla (\nabla \cdot u) - u \cdot \nabla^2 u \rangle = \langle -u \cdot \nabla^2 u \rangle
\] (B.34)

Now we get three equivalent definitions of the enstrophy norm in the cube:
\[
\langle (\nabla \times u)^2 \rangle = \langle -u \cdot \nabla^2 u \rangle = S^2
\] (B.35)

So the \( L_2 \) norm is the same,
\[
\langle (\nabla \times u)^2 \rangle^{1/2} = \langle -u \cdot \nabla^2 u \rangle^{1/2} = S = 1.
\] (B.36)
Appendix C

Spheres

C.1 Coordinate system

In this section, we introduce the index notations to be used in the next section for the derivation of the equivalence of norms. The geometry of the optimization problem is described by the coordinate system. The spherical coordinates are the most natural choice for geodynamo modelling. We use the following convention: 

\[ r \in [0, 1], \theta \in [0, \pi] \text{ and } \phi \in [0, 2\pi]. \]

They are related to the usual Cartesian coordinates as

\[
\begin{align*}
    r &= \sqrt{x^2 + y^2 + z^2}, \\
    \theta &= \cos^{-1}\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \\
    \phi &= \tan^{-1}\left(\frac{y}{x}\right).
\end{align*}
\] (C.1)

See Figure C.1 for the illustration of the relation above.

After the coordinates are fixed, we can define a set of basis vectors. There are two choices: coordinate basis and non-coordinate basis. We use the non-coordinate basis, which follows the usual conventions in the literature. The three basis vectors are:

\[
\begin{align*}
    e_r &= \frac{\partial}{\partial r}, \quad e_\theta = \frac{1}{r} \frac{\partial}{\partial \theta}, \quad e_\phi = \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}.
\end{align*}
\] (C.2)
The commutation coefficients \( c^\lambda_{\mu\nu} \) of a given basis set is defined as
\[
[e_\mu, e_\nu] = c^\lambda_{\mu\nu} e_\lambda.
\] (C.3)
In this case, we get six non-zero components:
\[
\begin{align*}
&c^{\theta}_{r\theta} = -\frac{1}{r}, & c^{\theta}_{\theta r} = \frac{1}{r}, \\
&c^{\phi}_{r\phi} = -\frac{1}{r}, & c^{\phi}_{\phi r} = \frac{1}{r}, \\
&c^{\phi}_{\theta\phi} = -\frac{\cot \theta}{r}, & c^{\phi}_{\phi\theta} = \frac{\cot \theta}{r}.
\end{align*}
\] (C.4)
The dual one-form basis for \( e_\mu \) is denoted \( v^\nu \), and it is given by
\[
v^\nu(e_\mu) = \delta^\nu_\mu.
\] (C.5)
So we get
\[
\begin{align*}
&v^r = dr, & v^\theta = r\, d\theta, & v^\phi = r\sin \theta\, d\phi
\end{align*}
\] (C.6)
The metric is constructed from the one-form basis \( v_i \) as
\[
g_{\mu\nu} v^\mu \otimes v^\nu,
\] (C.7)
then we get a flat metric \( \eta_{\mu\nu} \),
\[
g_{\mu\nu} = \eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\] (C.8)
The inverse metric \( \eta^{\mu\nu} \) can be derived from the metric according to the relation:
\[
\eta_{\mu\nu} \eta^{\nu\rho} = \delta^\rho_\mu
\] (C.9)
To rise or lower an index, we can use the inverse metric or the metric:
\[
A^\mu = A_\nu \eta^{\nu\mu}, \quad A_\lambda = A^\rho \eta_{\rho\lambda} \tag{C.10}
\]
Since the metric is flat, lowering or raising indices will not change the quantity.

Now we can finally define the differential operator \( \nabla \). For a scalar function \( f \), the gradient is
\[
\nabla_\mu f = \partial_\mu f
\] (C.11)
Written explicitly, it is
\[
\nabla f = \frac{\partial f}{\partial r} dr + \frac{\partial f}{\partial \theta} d\theta + \frac{\partial f}{\partial \phi} d\phi
\]
\[
= \frac{\partial f}{\partial r} v_r + \frac{1}{r} \frac{\partial f}{\partial \theta} v_\theta + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} v_\phi
\] (C.12)
When \( \nabla \) acts on one-form, it picks up a correction term in addition to the derivatives as
\[
\nabla_\nu A_\mu = \partial_\nu A_\mu - \Gamma^\lambda_{\mu\nu} A_\lambda
\] (C.13)

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\( \Gamma^\lambda_{\mu
u} \) are the covariant connection coefficients defined by

\[
\Gamma^\lambda_{\mu
u} = \frac{1}{2} g^{\lambda\rho} \left( \partial_\mu g_{\rho\nu} + \partial_\nu g_{\rho\mu} - \partial_\rho g_{\mu\nu} \right) + \frac{1}{2} \left( \Gamma^\rho_{\lambda\mu} + \Gamma^\mu_{\rho\lambda} - \Gamma^\rho_{\mu\lambda} \right) \tag{C.14}
\]

Since the metric is flat, all Christoffel symbols are zero. The covariant connection coefficients are made of commutation coefficients only, they are

\[
\Gamma^\theta_{r\theta} = \frac{1}{r}, \quad \Gamma^r_{\theta\theta} = -\frac{1}{r} \quad \Gamma^\phi_{r\phi} = \frac{1}{r}, \quad \Gamma^r_{\phi\phi} = -\frac{1}{r} \quad \Gamma^\phi_{\theta\phi} = \cot \theta \quad \Gamma^\theta_{\phi\phi} = -\frac{\cot \theta}{r} \tag{C.15}
\]

In components, this gives

\[
\begin{align*}
\nabla_r A_r &= \frac{\partial A_r}{\partial r}, \quad \nabla_\theta A_r &= \frac{1}{r} \frac{\partial A_r}{\partial \theta} - \frac{A_\theta}{r}, \quad \nabla_\phi A_r &= \frac{1}{r} \frac{\partial A_r}{\partial \phi} - \frac{A_\phi}{r} \\
\nabla_r A_\theta &= \frac{\partial A_\theta}{\partial r}, \quad \nabla_\theta A_\theta &= \frac{1}{r} \frac{\partial A_\theta}{\partial \theta} + \frac{A_r}{r}, \quad \nabla_\phi A_\theta &= \frac{1}{r} \frac{\partial A_\theta}{\partial \phi} - \frac{\cot \theta}{r} A_\phi \\
\nabla_r A_\phi &= \frac{\partial A_\phi}{\partial r}, \quad \nabla_\theta A_\phi &= \frac{1}{r} \frac{\partial A_\phi}{\partial \theta}, \quad \nabla_\phi A_\phi &= \frac{1}{r} \frac{\partial A_\phi}{\partial \phi} + \frac{A_r}{r} \cot \theta + \frac{1}{r} \frac{\sin \theta}{\sin \phi} A_\theta
\end{align*}
\]

(C.16)

One can check this definition is consistent with the familiar formulas in vector calculus. For example, we get the divergence of a vector field as:

\[
\nabla \cdot A = \frac{\partial A_r}{\partial r} + 2 A_r + \frac{1}{r} \frac{\partial A_\theta}{\partial \theta} + \frac{\cot \theta A_\theta}{r} + \frac{1}{r} \frac{\sin \theta}{\sin \phi} \frac{\partial A_\phi}{\partial \phi} \tag{C.17}
\]

C.2 Equivalent norms

Note we can check the equivalence of global shear and enstrophy \( S = \omega^* \) in spherical coordinates. We assume the same three conditions for the flow field \( \mathbf{u} \) just as in §B.2. First we write down the components of \( S \),

\[
S^2 = \langle 2 S_{ij} S^{ij} \rangle = \left\langle \frac{1}{2} \left( \nabla_i u_j + \nabla_j u_i \right) \left( \nabla^i u^j + \nabla^j u^i \right) \right\rangle = \frac{1}{2} \left( \left( \nabla_i u_j \right) \left( \nabla^i u^j \right) + \left( \nabla_j u_i \right) \left( \nabla^j u^i \right) \right) + \frac{1}{2} \left( \left( \nabla_i u_j \right) \left( \nabla^i u^j \right) + \left( \nabla_j u_i \right) \left( \nabla^j u^i \right) \right) = \left\langle \left( \nabla_i u_j \right) \left( \nabla^i u^j \right) \right\rangle + \left\langle \left( \nabla_i u_j \right) \left( \nabla^j u^i \right) \right\rangle \tag{C.18}
\]

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Then it follows that

\[
\langle (\nabla_i u_j)(\nabla^i u^j) \rangle = \langle \nabla_i (u_j \nabla^i u^j) \rangle - \langle u_j (\nabla_i \nabla^i u^j) \rangle
\]

\[
= \frac{1}{v} \int \nabla_i (u_j \nabla^i u^j) \ dv - \langle u_j (\nabla_i \nabla^i u^j) \rangle
\]

\[
= \frac{1}{v} \int u_j (\nabla^i u^j) \ d\Sigma - \langle u_j (\nabla_i \nabla^i u^j) \rangle
\]

\[
= \langle -u_j (\nabla_i \nabla^i u^j) \rangle ,
\]

(C.19)

because the velocity field \( u \) vanishes at the boundary. For the other term, we have

\[
\langle (\nabla_i u_j)(\nabla^j u^i) \rangle = \langle \nabla_i (u_j \nabla^j u^i) \rangle - \langle u_j (\nabla_i \nabla^j u^i) \rangle
\]

\[
= \frac{1}{v} \int \nabla_i (u_j \nabla^j u^i) \ dv - \langle u_j (\nabla_i \nabla^j u^i) \rangle
\]

\[
= \frac{1}{v} \int u_j (\nabla^j u^i) \ d\Sigma - \langle u_j (\nabla_i \nabla^j u^i) \rangle
\]

\[
= - \langle u_j (\nabla^j(\nabla_i u^i)) \rangle = 0,
\]

(C.20)

because the velocity field \( u \) is also solenoidal. So \( S^2 = \langle -u \cdot (\nabla^2 u) \rangle \).

We can also rewrite the enstrophy norm as:

\[
\langle (\nabla \times u)^2 \rangle = \langle (\nabla \times u) \cdot (\nabla \times u) \rangle
\]

\[
= \langle \nabla \cdot (u \times (\nabla \times u)) + u \cdot (\nabla \times (\nabla \times u)) \rangle
\]

\[
= \langle \nabla \cdot (u \times (\nabla \times u)) \rangle + \langle u \cdot (\nabla \times (\nabla \times u)) \rangle .
\]

(C.21)

The total derivative vanishes because we get,

\[
\langle \nabla \cdot (u \times (\nabla \times u)) \rangle = \frac{1}{v} \int \nabla \cdot (u \times (\nabla \times u)) \ dv
\]

\[
= \frac{1}{v} \int \mathbf{r} \cdot (u \times (\nabla \times u)) \ d\Sigma
\]

\[
= \frac{1}{v} \int u \cdot ((\nabla \times u) \times \mathbf{r}) \ d\Sigma = 0.
\]

(C.22)

So

\[
\langle u \cdot (\nabla \times (\nabla \times u)) \rangle = \langle u \cdot \nabla (\nabla \cdot u) - u \cdot \nabla^2 u \rangle
\]

\[
= \langle -u \cdot \nabla^2 u \rangle .
\]

(C.23)

Now we get three equivalent definitions of the enstrophy norm again just as in the cube:

\[
\langle (\nabla \times u)^2 \rangle = \langle -u \cdot \nabla^2 u \rangle = S^2.
\]

(C.24)
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