Robust multiscale finite volume method based iterative schemes

Author(s):
Cortinovis, Davide

Publication Date:
2016

Permanent Link:
https://doi.org/10.3929/ethz-a-010705725

Rights / License:
In Copyright - Non-Commercial Use Permitted
ROBUST MULTISCALE FINITE VOLUME METHOD BASED ITERATIVE SCHEMES

A thesis submitted to attain the degree of

DOCTOR OF SCIENCES of ETH ZURICH

(Dr. sc. ETH Zurich)

presented by

DAVIDE CORTINOVIS

MSc. ETH in Mechanical Engineering, ETH Zurich
born on 03.05.1985
citizen of BASEL (BS) and ITALY

accepted on the recommendation of

Prof. Dr. Patrick Jenny
Dr. Seong Hee Lee

2016
Abstract

The multiscale finite-volume (MSFV) method was designed to compute approximate solutions of large systems of equations arising from the discretization of elliptic partial differential equations (PDE). Later, MSFV based iterative (i-MSFV) schemes were introduced in order to increase and control the accuracy of the solutions. Unfortunately, the presence of highly heterogeneous coefficients in the PDEs severely affects convergence rates and robustness of these methods. In this thesis, robust MSFV method based iterative schemes with enhanced convergence rates are presented.

The proposed iterative Galerkin-enriched MSFV (i-Ge-MSFV) method is based on a selective enrichment of the MSFV coarse-space. The coarse-space of the classical MSFV method, spanned by so-called basis function, is augmented by enrichment functions aiming at capturing fine-scale effects not included in the standard MSFV coarse-space. As a consequence, additional coarse-scale constraints must be introduced in order to close the i-Ge-MSFV coarse-scale system. To this end, a novel hybrid Petrov-Galerkin / Galerkin coupling approach is introduced. The hybrid formulation allows for a straightforward coupling of enrichment functions, while preserving the ability of the classical MSFV method to enforce conservative coarse-scale solutions. Moreover, the enrichment approach adopted in the i-Ge-MSFV method requires only minor modifications of the classical MSFV algorithm and therefore, previously developed MSFV extensions can easily be incorporated into the new method. Hence, besides featuring enhanced convergence rates and superior robustness properties, the i-Ge-MSFV method retains the capabilities of its predecessors. The performance of the i-Ge-MSFV method was tested in a series of very challenging test-cases and compared to previous MSFV based schemes. The results demonstrate the greatly improved convergence properties of the proposed method.

The i-Ge-MSFV method shares some conceptual similarities with previously developed extensions of the MSFV method. In particular, the treatment of complex wells, fractured porous media and coarse-space enrichment rely on the same concept: special basis functions with support in a subset of the domain are introduced either to model the effect of interest (wells, fractures) or to be able to include missing fine-scale information in the coarse-scale problem (enrichment).
Another new concept introduced in this thesis is the zonal MSFV (zMSFV) framework, which introduces the notion of zones, zonal functions and extended zonal functions. The framework describes in a unified way how to couple regions governed by different mathematical models, or which are discretized in different ways, to the MSFV method. A special definition of zones and zonal functions is used to derive a variant of the zMSFV framework suitable for the solution of subsurface flow and transport problems. The resulting zMSFV method is recast in algebraic form and a zMSFV based preconditioner is derived. Numerical tests demonstrate that the zMSFV preconditioner delivers contrast independent convergence rates.
Sintesi

Il metodo "Multiscale Finite-Volume" (MSFV) è stato ideato per calcolare soluzioni approssimate di sistemi di equazioni lineari derivanti dalla discretizzazione di equazioni differenziali alle derivate parziali (PDE) di tipo ellittico. In seguito sono stati proposti metodi iterativi MSFV (i-MSFV) con l'intento di aumentare e controllare l'accuratezza delle soluzioni. Purtroppo la presenza di coefficienti altamente eterogenei nelle PDE influenza gravemente la velocità di convergenza e la robustezza di questi metodi. In questa tesi vengono discussi metodi iterativi con caratteristiche simili ai metodi classici i-MSFV, ma con proprietà di convergenza, flessibilità e robustezza superiori a tutti i suoi predecessori.

Il metodo "iterative Galerkin-enriched MSFV" (i-Ge-MSFV) proposto in questa tesi si basa su un arricchimento selettivo dello spazio grezzo (coarse-space) generato da funzioni di base caratteristiche del metodo MSFV. Ciò avviene tramite le cosiddette funzioni di arricchimento, volte a catturare gli effetti presenti su scala fine non ancora inclusi nello spazio grezzo. Ne consegue la necessità di inserire ulteriori vincoli al fine di ottenere un sistema di equazioni determinato. A tal proposito viene introdotto un approccio ibrido Petrov-Galerkin / Galerkin per la chiusura del sistema di scala grezza. Questo tipo di formulazione ibrida consente di introdurre un numero indeterminato di funzioni di arricchimento, mantenendo la capacità del metodo MSFV classico di calcolare soluzioni conservative su scala grezza. Inoltre, l’approccio di arricchimento adottato per il metodo i-Ge-MSFV, è formulato in modo tale da richiedere solo piccole modificazioni dell’algoritmo utilizzato per l’implementazione del metodo MSFV classico. Di conseguenza, tutte le estensioni del metodo MSFV proposte nel recente passato possono essere facilmente incorporate nel nuovo metodo presentato un questa tesi. Quindi, oltre ad esibire proprietà di convergenza e robustezza superiori, il metodo i-Ge-MSFV mantiene tutte le capacità dei suoi predecessori. Le prestazioni del metodo i-Ge-MSFV sono state rilevate in una serie di test numerici ad alto tasso di difficoltà e comparati con le prestazioni di precedenti versioni di metodi iterativi basati su MSFV. I risultati dimostrano chiaramente la superiorità del nuovo metodo sia in termini di robustezza che in termini di velocità di convergenza.

Il metodo i-Ge-MSFV condivide alcune somiglianze concettuali con estensioni precedentemente sviluppate per il metodo MSFV. In particolare, il trattamento di pozzi complessi, materiali rocciosi fratturati e arricchimento dello
spazio grezzo si basano sullo stesso concetto: funzioni di base con supporto compatto vengono introdotte sia per modellare effetti di interesse (pozzi, fratture) che per includere le informazioni mancati nello spazio grezzo (arricchimento).

Un altro nuovo metodo presentato in questa tesi è il metodo MSFV zonale (zMSFV) che introduce il concetto di zone, funzioni zonali e funzioni zonali estese. Il metodo descrive in modo unificato la procedura utilizzata per congiungere diversi modelli matematici e discretizzazioni varie con il metodo MSFV classico. Tramite l’utilizzo di una particolare definizione delle zone e delle funzioni zonali, è possibile derivare un metodo particolarmente adatto per la simulazione di problemi riguardanti il flusso di uno o più fluidi in mezzi porosi presenti nel sottosuolo. Questa variante del metodo zMSFV viene riformulata in forma algebrica e utilizzata come precondizionatore per metodi di Krylov. I test numerici considerati in questa tesi dimostrano che il precondizionatore zMSFV permette di ottenere velocità di convergenza indipendenti dal contrasto presente nei coefficienti delle equazioni differenziali.
Acknowledgement

First and foremost, I would like to express my sincere gratitude to my advisor Prof. Patrick Jenny for giving me the great opportunity to work under his supervision. I really enjoyed his continued support, encouragement and the many illuminating advices.

I would also like to thank Dr. Seong Lee for accepting to be the co-advisor and for the many inspiring discussions during my stay in San Ramon and Houston. My thanks go also to the Chevron/Schlumberger Intersect Alliance for the financial support of my PhD project.

Special thanks go to my dear colleagues, which I consider to be my friends, from the Institute of Fluid Dynamics (IFD). In particular to Dr. Hossein Gorji, whose support and friendship have been of inestimable importance during the past four years, to Karim Khayrat for the nice discussions on MSFV and numerical methods, to Thomas for the juicy updates, to Franca Schmid for the lovely cakes, the spreading of good mood and the ”uncovered swords”, to Adrien Lücker for the fruitful mathematical discussions and the even more enjoyable discussions on classical music, to Dr. Dimitrios Karvounis for our intense discussions on football, to Rajdeep Deb for being a great officemate, to Stephan Küchlin for the most well-timed jokes I have ever heard, to Robert Tritarelli for his help and advices during my teaching assistant duties, to Nemanja Andric for being part of the ”hood” and the nice Hawaii present, to Valentin Giddey for continuing the ”plus/minus list” and for taking my beloved coffee breaks very seriously, and to Dr. Daniel Meyer, Philipp Weiss, Bianca Maspero, Sonia Atkinson and Hans Peter Caprez for their support.

Working on a PhD thesis is a demanding task. This work would have not been possible without the help and support of many people outside of ETH. Special thanks go to Stéphanie, Gian, Gerhard, Margaretha and Francesca for their support during difficult times and to Roberto, Lajko, Emanuel and Fabian for being such amazing friends. My heartfelt gratitude goes to my parents for all their support throughout the years. You never stopped believing in me, and for that I am incredibly blessed and thankful. Finally, and most importantly, I would like to thank Rahel for her love, encouragement and unconditional support over so many years.
Contents

I Introduction 1

1 Multiphase flow in porous media 3
  1.1 General considerations 3
  1.2 Mathematical model for immiscible two-phase flow 5
  1.3 IMPES scheme for incompressible flow 5

2 Implications for linear system solvers 8

3 Multiscale methods 11

4 Motivation of the thesis 13

II MSFV method and i-MSFV method 15

5 Introduction 17

6 General multiscale method formulation 18

7 Classical MSFV method 21
  7.1 Construction of basis and correction functions 21
  7.2 Coarse-scale coupling 23
  7.3 Reconstruction of conservative fine-scale solutions 24
  7.4 Remarks 24

8 Classical i-MSFV method 25
  8.1 Iterative scheme 25
  8.2 Limitations 26

III Iterative Galerkin-enriched MSFV method 29

9 Introduction 31

10 i-Ge-MSFV method 33
  10.1 Main concepts 33
  10.2 Construction of basis functions and related coarse space 34
  10.3 Coarse-scale coupling 35
  10.4 Enrichment strategies 38
10.4.1 Adaptive enrichment ........................................ 38
10.4.2 A-priori enrichment ....................................... 42

11 Numerical results .............................................. 46
  11.1 A-priori enrichment ........................................ 46
  11.2 Adaptive enrichment and mixed approach .............. 52
  11.3 3D problems ................................................ 59

12 The i-Ge-MSFV method for special grids ................. 61
  12.1 Non-conforming coarse grids ............................. 61
    12.1.1 Problem statement and i-Ge-MSFV approach ........ 61
    12.1.2 Numerical results .................................... 65
  12.2 Inactive cells .............................................. 68

13 Conclusion .................................................... 71

IV Zonal MSFV framework ....................................... 73

14 Introduction .................................................. 75

15 Framework description ...................................... 76
  15.1 Zonal MSFV approximation ................................. 76
  15.2 Basis and extended zonal basis functions .............. 77
  15.3 Coarse-scale system ....................................... 79
  15.4 Remarks .................................................... 80

16 Zonal MSFV method for high-contrast problems .......... 82
  16.1 Specification of zones and related zonal functions .... 82
  16.2 Algebraic formulation and zonal MSFV preconditioner ... 83
  16.3 Selection of zones ......................................... 89

17 Numerical results ............................................. 91
  17.1 High-contrast media ....................................... 91
  17.2 SPE10 ...................................................... 98

18 Conclusion .................................................... 101

V Conclusion and Outlook .................................... 103
List of Figures

1  Primary coarse grid $\mathcal{T}^C$ (solid lines) and dual coarse grid $\mathcal{T}^D$ (dashed green lines) defining coarse-scale partitions of $\Omega$. The blue and gray regions show the support domains for the basis functions associated with two coarse-scale DoF locations (black and red dots, respectively). The underlying fine-scale grid is not shown. ........................................... 19

2  MSFV method grids: Primary coarse partition (solid, blue lines), dual coarse partition (dashed, green lines) and fine-scale partition (solid, black lines). .................................................. 22

3  Permeability field containing two shale layer formations (solid, black), with superimposed coarse grid (dotted, blue) and the dual coarse grid (dotted, green). ................................. 27

4  The convergence histories of the i-MSFV method for different numbers of smoothing steps ($n_\star$); shown is the base-10 logarithm of the residual infinity norm. The test-case is based on the permeability field shown in Fig. 3. ...................... 28

5  Nodal basis functions of the standard MSFV method (top figures) associated to the dual CV containing the L-shaped shale layers shown in Fig. 3. Nodal basis functions (4 center figures) after the insertion of two additional DoF. The corresponding enrichment functions are shown in the bottom figures. ....... 36

6  (a) Development of $||r||_\infty$ (solid, red line) during the adaptive detection of additional DoF. The square symbols indicate the detection ($TOL_{rate} = 0.1$) and addition of new DoF. The underlying permeability field and the location of insertion of additional DoF (red dots) is shown in (b). ..................... 40

7  Convergence history (bottom figure) of the mixed a-priori / adaptive enrichment algorithm for different numbers of a-priori ("P") selected DoF locations. The black squares indicate, if the insertion of a new DoF was performed after a detection loop (iteration). Coarse grid (blue lines, $14 \times 5$ CVs), dual grid (green) and permeability field considered are shown in the top figure. The red dots mark the location of all additional DoF resulting from the "P30-A21-GeMSFV" run. Note that the prefix "Px-Ay" employed in the legend stands for: "x" DoF were selected a-priori and "y" DoF were selected adaptively. 45
8 Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. Two initial configurations with 81 (a) and 9 (b) basis functions are considered. Coarse (blue) and dual coarse (green) grids are shown on top of the corresponding convergence maps. The location of the first 50 additional DoF are marked with red dots.

9 Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. Two initial configurations with 81 (a) and 9 (b) basis functions are considered. Coarse (blue) and dual coarse (green) grids are shown on top of the corresponding convergence maps. The locations of the first 50 additional DoF are marked with red dots.

10 Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. The test-case employs the same configuration used for the simulations shown in Fig. 9. The only difference is given by the fine-scale grid aspect ratio ($\alpha = 10$) used to emulate the effects of anisotropic permeability tensors.

11 Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) for two coarse-spaces initially spanned by 70 (a) and 30 (b) basis functions. The corresponding coarse grids (blue), with respectively $14 \times 5$ and $10 \times 3$ CVs, are shown in the top figures. The red dots mark the locations of the first 50 DoF in the created a-priori lists.

12 Convergence histories of i-MSFV (pink lines) and i-Ge-MSFV methods with $n_s = 6$ (a) and $n_s = 20$ (b). The employed permeability field and grids are shown in Fig. 8(a). Note that the prefix ”Px-Ay” employed in the legend stands for: ”x” DoF were selected a-priori and ”y” DoF were selected adaptively.

13 Convergence histories of i-MSFV (pink lines) and i-Ge-MSFV methods with $n_s = 6$ (a) and $n_s = 20$ (b). The employed permeability field and grids are shown in Fig. 9(a). Note that the prefix ”Px-Ay” employed in the legend stands for: ”x” DoF were selected a-priori and ”y” DoF were selected adaptively.
Convergence histories of i-MSFV and i-Ge-MSFV methods with \( n_s = 6 \) (a) and \( n_s = 20 \) (b). The employed permeability field and grids are shown in Fig. 11(a) (top figure).

Convergence histories of the i-Ge-MSFV method resulting from different choices of \( n_s \) and numbers of a-priori selected DoF ("P") locations. In (b), \( n_s = 20 \) is fixed while the number of a-priori selected DoF varies between 15 and 75. The employed permeability field and grids are shown in Fig. 11(a) (top figure).

Fine-scale reference solution \( p_f \) obtained for three different well configurations (a). Configuration 1: \( p_w(192, 43) = 1, p_w(15, 10) = 0 \); configuration 2: \( p_w(51, 10) = 1, p_w(203, 3) = 1, p_w(16, 36) = 0, p_w(96, 36) = 0, p_w(114, 42) = 0 \); configuration 3: \( p_w(16, 27) = 1, p_w(34, 16) = 1, p_w(201, 3) = 1, p_w(33, 39) = p_w(127, 33) = 0 \). Figure (b) illustrates the saturation distribution (injected fluid) obtained after 100, 2000 and 5000 time steps \( (t^n) \) of a two-phase problem simulation (well configuration 1). The distributions are used as "initial" condition in the i-Ge-MSFV method convergence studies in Fig. 17(b).

Convergence histories of the i-Ge-MSFV method (P30-A24) for different well locations (a) and saturation fields (b). The corresponding pressure and saturation fields are shown in Fig. 16. Adaptive enrichment was performed based on well configuration 1.

Permeability fields: (a) \( \mu_{ln(K)} = 0, \sigma^2_{ln(K)} = 4 \), (b) SPE10 benchmark. Fine-scale grids: (a) \( 88 \times 88 \times 88 \), (b) \( 60 \times 220 \times 85 \) coarse grid: (a) \( 8 \times 8 \times 8 \), (b) \( 12 \times 20 \times 5 \). The convergence history of the i-Ge-MSFV method with purely adaptive enrichment \( (TOL_{rate} = 0.1, TOL_1 = 10^{-7}) \) is shown for different aspect-ratios \( \alpha \).

MSFV grids for faulted reservoirs: classical structured MSFV coarse grid a) and non-conforming structured MSFV coarse grid (b). The fine-scale CVs which compose the dual CV boundaries are coloured in red, while green fine-scale CVs represent locations of coarse-scale DoF.

MSFV grids for faulted reservoirs: "unstructured" MSFV grid (a) and extended dual CV for the fault region.
i-Ge-MSFV grids for faulted reservoirs: a) interaction region across fault and b) dual CVs for the i-Ge-MSFV method. The locations of additional coarse-scale DoF are shown in blue. 64

Results for 2D faulted reservoir: base-10 logarithm of the permeability field (a), converged pressure solution (b) and convergence history for the i-Ge-MSFV method (c). 66

Results for 3D faulted reservoir: base-10 logarithm of the permeability field (a), converged pressure solution (b) and convergence history for the i-Ge-MSFV method (c). 67

Inactive CVs are shown in black. Locations of coarse-scale DoF for the classical MSFV method are shown green, while additional coarse-scale DoF locations used by the Ge-MSFV method are shown in blue. 68

Test-case with inactive cells: a) distribution of inactive cells (black), standard coarse-scale DoF (green) and added coarse-scale DoF (blue) on the dual CV boundary (red). In (b) the converged i-Ge-MSFV pressure solution is depicted. The convergence history for the i-Ge-MSFV method is shown in (c). 70

a) Classical MSFV method grids: skeleton $\mathcal{S}$ of the dual-grid (red dashed lines) and primary grid (solid black lines). A primary coarse CV and a dual coarse CV are highlighted in red and green, respectively. b) Two zones (blue regions) are introduced together with the zonal DoF (dots). In addition, a DoF associated to the dual grid vertices $x_V^i$ is shown. The maximum possible support of the extended zonal functions associated to $\Omega^P_i$ is represented by the light blue region. 78

a) Classical MSFV method partitioning with coloured CVs: black squares represent dual CV vertices, red squares dual CV edges and white squares are dual CV interior CVs. b) zMSFV partitioning with 5 zones, where the largest two are adjacent to each other. Zonal-boundary CVs are shown in blue, zonal-interior CVs in yellow and zonal-vertex CVs in green. 84

a) High-contrast permeability field with values $K_{\text{channels}}$ in the channels (red) and 1 otherwise. b) Dual coarse grid with zones for the zMSFV method. 92

Spectrum of the iteration matrix $G$ for to the preconditioned Richardson method (109) with zMSFV-G (a) MSFV-G (b) and MSFV-PG (c) preconditioners. The permeability field is shown in Fig. 28(a), where $K_{\text{channels}} = 10^4$ was used. 94
30 Convergence history of the preconditioned GMRES method with the zMSFV-G preconditioner for different numbers $N$ of zonal coarse-scale unknowns. The permeability field is shown in Fig. 28(a), where $K_{\text{channels}} = 10^4$ was used. b) Convergence histories of GMRES with MSFV-G preconditioner for $K_{\text{channels}} = 10^3$ (squares) and $K_{\text{channels}} = 10^4$ (crosses). The solid line corresponds to the convergence history of zMSFV-G with $N = 97$ in figure a). 

31 a) Permeability field of SPE10 bottom layer. b-e) Dual grid and zones of the zMSFV method for $\gamma = 10^1, 10^2, 10^3$ and $10^4$, respectively. 

32 Convergence histories of GMRES with zMSFV-G preconditioner for different threshold values $\gamma_{\text{min}}$. The underlying permeability field is displayed in Fig. 31(a). Also shown are the convergence histories for the MSFV-G preconditioner (red line) and for the MSFV-G preconditioner applied to a homogeneous permeability field with the same dimensions, boundary conditions and grid sizes as for the other runs.

List of Tables

1 Number of iterations required to reduce the $l^2$ norm of the residual to $10^{-8}$ with the stationary preconditioned Richardson method. If the scheme did not converge within 2000 iterations, the residual after the 2000th iteration is given in parenthesis, while (-) denotes diverging iterations. The total number $N_C$ of coarse-scale unknowns is reported in parenthesis. The tested permeability field is shown in Fig. 28(a). 

2 Number of GMRES iterations required to achieve $||\epsilon_{\text{rel}}||_2 < 10^{-8}$ for the three preconditioners. The tested permeability field is shown in Fig. 28(a). 

3 Number of zones ($N_B$), dual CV related DoF ($N_v$), zonal DoF ($N_V$) and total number of coarse DoF ($N_C$) for different choices of $\gamma$. The related grids and zones are depicted in Fig. 31.
Part I

Introduction
1 Multiphase flow in porous media

1.1 General considerations

Multiphase flow in porous media plays an important role in many scientific disciplines and is highly relevant for a broad spectrum of industrial applications including petroleum reservoir management, groundwater flow modelling and enhanced geothermal power extraction.

Despite the large interest in multiphase flow and transport in porous media, the understanding of many of the physical phenomena involved is still limited. Furthermore, the physical phenomena of interest are too complex to be described exactly by a single mathematical model. Therefore, mathematical models based on some simplification of the underlying physics have been proposed for different scenarios. In the petroleum industry, the selection of the appropriate mathematical model is guided by the reservoir state. During the early stage of oil production (primary recovery), oil motion is governed by the natural decompression of the reservoir and a single-phase flow model is generally sufficient to describe the main features of the flow accurately. During the secondary oil recovery water is injected in the reservoir and hence, at least two distinct phases must be considered in the mathematical formulation. Additional problems arise in enhanced oil recovery applications, where thermal effects, compressibility, chemical reactions and mass transfer between phases require the introduction of complex multicomponent multiphase flow models.

The aforementioned mathematical models are generally formulated in terms of a set of partial differential equations (PDE) derived from conservation of mass, momentum and energy, and by using a set of constitutive relations where required. Unfortunately, analytical solutions are rare and only obtainable by introducing strong assumptions which tend to oversimplify the nature of the problem. Similarly the numerical solution of the full set of conservation laws is generally unfeasible due to the high computational power required to
resolve the pore-scale structures, resulting in billions of unknowns already for domains with a characteristic size several orders of magnitude lower than the reservoir scale. Darcy's Law is widely employed to reduce the (spatial) complexity of the resulting PDEs. The introduced linear relationship between pressure gradient and velocity substitutes the rather complex momentum conservation equation. At the same time, a macroscopic description of variables and parameters (e.g. intrinsic permeability) is implicitly introduced, resulting in a continuum description of the porous medium.

Despite the simplifications introduced by Darcy's Law, the resulting set of PDEs does not allow for general analytical solutions. However, their numerical solution for relevant real-field scenarios, i.e. physical domains with an extension in the order of kilometres, becomes more feasible from a computational point of view. A multitude of numerical solution strategies has been developed in the context of reservoir simulations. Most strategies are designed to exploit particular features of a model with the aim of optimizing computational efficiency. In most cases, however, the solution of a discretized mathematical model is obtained by solving a linear system of equations.

In practical applications, the solution of linear systems takes up to 90% of the total CPU time spent for a large-scale simulation, and thus, efficient linear solvers delivering either exact or accurate approximate solutions are of paramount importance for the simulation of real-field problems.

In this PhD work, the focus is set on the efficient solution of large linear systems of equations obtained from discretized elliptic PDEs. Elliptic PDEs arise naturally in the simulation of multiphase flow in porous media. For example, the so-called IMPES formulation of incompressible and immiscible two-phase flow in porous media results in a coupled system of elliptic and hyperbolic PDEs, which must be solved repeatedly. The mathematical model describing the flow of two incompressible, immiscible phases in a porous medium and the related IMPES strategy are presented in the next section.
1.2 Mathematical model for immiscible two-phase flow

The conservation of mass for each phase in an immiscible two-phase flow is given by

\[ \frac{\partial (\phi S_i \rho_i)}{\partial t} = -\nabla \cdot (\rho_i u_i) + q_i, \quad i \in \{1, 2\}, \quad (1) \]

where \( \phi \) is the porosity of the medium, \( S_i \) the saturation of phase \( i \), \( \rho_i \) its density and \( q_i \) represents a source term. The velocity \( u_i \) of each phase is given by Darcy’s law:

\[ u_i = -\frac{k_{r,i}}{\mu_i} \mathbf{K} (\nabla p_i - \rho_i g \nabla z), \quad (2) \]

where \( \mu_i, k_{r,i} \) and \( p_i \) are viscosity, relative permeability and pressure of phase \( i \), respectively, while \( g \) represents the gravitational acceleration, \( z \) the depth and \( \mathbf{K} \) is the intrinsic permeability tensor describing the ability of a fluid to flow through the porous medium. It is assumed that the fluids completely fill the void spaces of the porous medium, which implies

\[ S_1 + S_2 = 1. \quad (3) \]

Additionally, a relation for the pressure difference between the fluids is expressed in terms of the macroscopic capillary pressure

\[ p_c(S_1) = p_1 - p_2, \quad (4) \]

which is given as an empirical function of the wetting phase (here \( S_1 \)). Similarly, functions depending on pressure and saturation are used to model \( k_{r,i}, \mu \) and \( \phi \). Different mathematical formulations which depend on the selected primary variables (two out of four unknowns) can be used to obtain a solution to the problem considered. Not all formulations are equally suited for numerical computations. A widely used approach in reservoir simulations is the IMPES scheme for incompressible, immiscible two-phase flow, which is introduced in the next section.

1.3 IMPES scheme for incompressible flow

Incompressibility of the fluids is enforced by considering the phase density \( \rho_i \) to be constants. Additionally, capillary forces are neglect and hence, Eq. (4) reduces to the simple relation \( p_1 = p_2 = p \). In addition, the porosity is assumed to be only dependent on the spatial coordinate, i.e. \( \phi = \phi(x) \). Under these assumptions, Eq. (1) can be rewritten as

\[ \phi \frac{\partial S_i}{\partial t} = -\nabla \cdot u_i + \frac{q_i}{\rho_i}, \quad i \in \{1, 2\}. \quad (5) \]
The definitions of the phase mobilities

\[ \lambda_i = \frac{k_{r,i}}{\mu_i} \]  

(6)

and the total mobility

\[ \lambda_{tot} = \lambda_1 + \lambda_2, \]  

(7)

together with Darcy’s Law (2) are substituted in the expression resulting from the summation of the mass conservation equations for the two phases. This leads to

\[ -\nabla \cdot (\Lambda \cdot \nabla p) = q \]  

(8)

with

\[ \Lambda = \lambda_{tot} K \]  

(9)

and

\[ q \equiv \frac{q_1}{\rho_1} + \frac{q_2}{\rho_2} - \nabla \cdot K (\lambda_1 \rho_1 + \lambda_2 \rho_2) g \nabla z. \]  

(10)

Equation (8) is the conservation of total mass expressed in terms of the pressure variable. The same equation can be easily expressed in a form which closely resembles the mass conservation equation for incompressible flows found in classical fluid mechanics textbooks, i.e.

\[ \nabla \cdot \mathbf{u}_{tot} = \frac{q_1}{\rho_1} + \frac{q_2}{\rho_2}, \]  

(11)

where \( \mathbf{u}_{tot} \) is the total velocity defined as

\[ \mathbf{u}_{tot} = \mathbf{u}_1 + \mathbf{u}_2 = -K \cdot (\lambda_{tot} \nabla p - (\lambda_1 \rho_1 + \lambda_2 \rho_2) g \nabla z). \]  

(12)

In the IMPES (implicit pressure, explicit saturation) scheme, as the name already implies, the pressure equation is solved implicitly using saturation values from a previous time step (or initial conditions for the very first computation). The computed pressure field is used to compute the total velocity (12), which is by construction divergence free, and thus, mass conservative. Then, the saturation equation (5) for one phase, say \( S_1 \), is solved with an explicit integration scheme in order to obtain the saturation field at the new time-step. Hereby, a fractional flow formulation for the phase velocity is employed, i.e.

\[ \mathbf{u}_i = f_i \mathbf{u}_{tot} + K \cdot (f_1 \lambda_2 (\rho_1 - \rho_2) g \nabla z), \]  

(13)
1.3 IMPES scheme for incompressible flow

with the fractional flow functions defined as

\[ f_i = \frac{\lambda_i}{\lambda_{tot}}. \]  \hspace{1cm} (14)

The updated saturation field is then fed back to the pressure equation to update the phase mobilities and a new pressure solution is computed.

Clearly, the computational bottleneck of the IMPES scheme is the numerical solution of the pressure equation (8). Equation (8) is an elliptic PDE with highly oscillating coefficients \( \Lambda \) and therefore it often results in a stiff linear system to be solved for the pressure at each time step. The computational cost for solving the non-linear hyperbolic saturation equation is generally much smaller compared to the one required by the linear solver for pressure. Therefore, efficient numerical methods for the solution of large linear stiff systems are of great interest.
2 Implications for linear system solvers

The solution of a large sparse system of linear equations is a task encountered in many numerical simulations involving physical phenomena. They generally arise from the discretization of PDEs or directly from a large set of algebraic equations (e.g. electrical circuits, chemical processes, economic models, structural engineering applications). A linear system of equations is of the form

\[ Ax = b, \]

where \( A \) is a non-singular, sparse coefficient matrix of size \( N \times N \), and \( x \) and \( b \) vectors of length \( N \) representing the solution and the right-hand side (rhs) of the system, respectively. Here, only cases where the linear system has a unique solution are considered.

Two main types of methods exist for the solution of linear systems: direct methods and iterative methods. Direct methods [14], generally based on some ideas related to classical Gauss elimination, have the appealing property that an exact solution of the system (up to rounding errors) can be found after a finite number of operations. Additionally, high-level direct solvers are robust and reliable and therefore widely used in industrial applications. The major drawback of direct methods consists in their poor scalability with respect to the problem size. Thus, computational time and memory requirements become unaffordable as soon as the size of the coefficient matrix is increased.

As discussed previously, the system of equations arising in reservoir simulation are typically extremely large. Frequently, high-resolution geological models require a discretization containing millions or even billions of equations. For this class of problems, the use of an iterative method is mandatory. Iterative methods solve linear systems of equations by computing a sequence of increasingly more accurate approximate solutions. They are less expensive than direct methods in terms of memory requirements and often also with respect to the number of operations required to obtain the solution, in particular if only an approximate solution is required. There exist two main
classes of iterative methods for linear systems: stationary iterative schemes and Krylov subspace methods. Stationary schemes like Jacobi, Gauss-Seidel and Successive Overrelaxation methods are extremely easy to implement and analyse. However, convergence is not guaranteed (except for special types of coefficient matrices) and the convergence speed is unsatisfactorily slow for many practical applications. Krylov subspace methods such as conjugate gradients (CG) [32, 55, 44], biconjugate gradients (BICG, BiCGSTAB) [62] and generalized minimal residual [57] (GMRES) methods, overcome most of the limitations of stationary schemes and are among the most widely used iterative schemes. The main reason for the success of these methods, is that a solution can be found in a finite number of steps. More precisely, Krylov subspace methods obtain a converged solution in at most $N$ iterations in exact arithmetic. However, in practical applications the number of iterations is lower than $N$, if the problem is well-conditioned [55]. Therefore, in the presence of an ill-conditioned system, preconditioning techniques must be used to accelerate the convergence of the method.

Besides the truly iterative methods mentioned previously, two additional iterative approaches are often used for the solution of linear systems: multigrid methods and domain decomposition methods. Both techniques can be either used as stand-alone linear solvers or as preconditioner in a Krylov subspace method. Multigrid methods (MG) [8, 9, 23], and the closely related algebraic multigrid (AMG) methods [10, 59], were initially introduced for the solution of second-order elliptic equations and later extended for other types of problems. They rely on the fundamental fact that the low-frequency error component seen on a given grid results in a high-frequency error on a coarser grid. Thus, MG approaches combine basic stationary iterative methods, which are very efficient at reducing (smoothing) high-frequency error components, with a cascade of successively coarser grids, on which the error is injected and smoothed repeatedly. A similar procedure is performed during the prolongation steps, i.e. during the successive interpolation from the coarsest to the finest-grid. For some types of systems AMG is very efficient but it is more difficult to parallelize and has a higher set-up cost than other iterative solvers. Domain decomposition (DD) methods [61, 56] are a class of iterative approaches designed for the solution of boundary value problems on parallel computers. They rely on a divide and conquer strategy, i.e. on a subdivision of the computational domain into smaller subdomains, in which discrete problems can be solved independently of each other. The iterative component of DD methods appears via the exchange of information required to couple the local solutions. Unfortunately, the convergence rate of classical DD methods depends on the number of subdomains used and hence, these
methods are not scalable. As a remedy, a coarse level operator allowing for a global exchange of information is introduced, and the resulting two-level methods are used as a preconditioners in Krylov subspace methods.

The above discussion underlines the different ranges of applicability for classical linear system solvers. It can be expected that some methods will be very efficient for some problems, but terribly inadequate for others. With respect to the systems of equations discussed in the previous section, the following considerations have to be made. The size of the system of interest, i.e. the discrete version of Eq.(8), is generally orders of magnitude larger than the one which could be handled by direct solvers, making the use of iterative schemes mandatory. For the same reason, a high degree of parallelism and good scalability are highly desirable features to be considered when selecting an iterative scheme. Additionally, the presence of rapidly oscillating coefficients ($\Lambda$) in the pressure equation results in very ill-conditioned coefficient matrices and thus, in a severe loss of convergence speed for almost all classical iterative schemes. Nevertheless, state-of-the-art parallel AMG solvers and two-level DD preconditioners [21] for Krylov subspace methods are capable of handling most of the problems discussed so far. Their main disadvantage, however, is related to the iterative nature of the methods. Iterative methods are extremely efficient in delivering an approximate solution of a system of equations, i.e. the iteration process is stopped once a given tolerance is reached. Unfortunately, Eq.(11) requires a fully converged solution in order to guarantee a conservative velocity field and thus avoid mass balance errors in the solution of the transport problem (5). As already mentioned in the previous section, at each time-step the saturation dependent parameters (phase mobilities) in the pressure equation must be updated and a new system of equations must be assembled and solved. Furthermore, the change in parameters is required only in small subregions of the domain of interest, due to the hyperbolic character of the transport equation. Therefore, a large gain in computational efficiency can be obtained by designing numerical methods capable of delivering accurate approximate conservative solutions and displaying a high degree of space-time adaptivity. Some of the multiscale methods discussed in the next section possess exactly these features.
3 Multiscale methods

The extremely high computational cost inherent to numerical solutions of large-scale second-order elliptic PDEs with heterogeneous coefficients (A) arising in the simulation of flow and transport in porous media motivated the development of a new class of (approximate) linear system solvers: so-called multiscale (MS) methods.

MS methods are closely related to upscaling methods [19, 4], which represent the first attempt to reduce the computational complexity of the problem. Upscaling methods compute effective coarse-scale parameters incorporating the fine-scale coefficients. The former solves the (upscaled) problem at a coarser scale. Thus, computational efficiency is obtained by reducing the number of degrees of freedom (DoF) required to describe the geological problem and hence, by solving a system with a coefficient matrix of smaller size. However, these methods rely on averaging fine-scale parameters. As a result, the capability of obtaining a solution with the same resolution as the initial fine-scale model is lost. Furthermore, the accuracy of the coarse-scale model is generally case-dependent and difficult to predict. In addition, it appears undesirable to sacrifice the high-resolution description of the soil properties available in modern geological models.

Multiscale methods [33, 34, 35, 36, 6, 65, 3, 54, 16] overcome some limitations of upscaling methods by introducing a set of *numerically computed basis functions with local support* designed to capture the fine-scale information at the highest resolution possible. Similar to upscaling methods, a coarse-scale problem with a strongly reduced number of DoF is assembled and solved. However, MS methods allow us to reconstruct *approximate* fine-scale solutions by interpolating the coarse-scale solution back to the fine-scale via the basis functions. Besides accounting for fine-scale heterogeneity in an appropriate way in the coarse-scale problem, basis functions can be computed independently from each other, making multiscale methods amenable to massively parallel implementations. Furthermore, the required update of
saturation dependent parameters can be performed locally. Thus, the set of basis functions computed at the beginning of the simulation can be updated in an adaptive way, i.e. only basis functions with support in regions with a significant change of the parameter values are recomputed. The high computational efficiency of MS methods is therefore due to the small size of the coarse-scale system solved, the space-time adaptive nature of the method and the inherent high level of parallelism.

The different multiscale modelling approaches can be subdivided into three main categories: the multiscale finite-element (MSFE) methods [33, 18], the multiscale mixed finite-element (MSMFE) methods [4, 11, 5, 2, 1, 39], and the multiscale finite-volume (MSFV) methods [36, 60, 31, 68, 46, 43, 53, 58, 7]. These three approaches share the peculiarity of introducing sets of basis functions obtained from numerical solutions in localized subdomains. They differ from each other mainly in the way how the basis functions are coupled to form a coarse-scale system. However, only the MSMFE method and the MSFV method provide conservative velocity fields, which is a crucial property, if transport problems have to be addressed in addition to the flow problem.
4 Motivation of the thesis

In the last two decades the range of applicability of the MSFV method, which was initially designed for the solution of second-order elliptic equations, was extended to parabolic equations [28, 45, 68], complex physics [49], complex well modelling [38] and fractured porous media [30]. Many published results (e.g. [40, 41]) underline the capability of such MS methods to deliver accurate approximate solutions for a wide range of challenging scenarios. Nonetheless, major deviations from the reference fine-scale solution can be observed for permeability fields involving strong contrast and long coherent structures, which may become very pronounced for the MSFV method [48, 64]. In order to increase the accuracy [24] of the MSFV method solutions, MSFV method based iterative schemes have been proposed in the past [26, 51, 69, 63].

However, the robustness of the classical iterative MSFV (i-MSFV) method [26] and the convergence rate of MSFV based preconditioned Krylov subspace methods [51] [63] are still negatively affected by the presence of high-contrast coefficients in the governing PDEs. Hence, the main motivation for this PhD thesis is to develop robust MSFV based iterative solvers for the solution of elliptic equations with high-contrast coefficients. Furthermore, the main concepts employed to develop such robust iterative schemes are shown to be closely related to other MSFV method extensions. The generalization of these ideas results in the zonal MSFV framework, which includes most of the previously introduced MSFV extensions, and introduces a framework for coupling additional models to the classical MSFV method.

The classical MSFV method and the limitations of the classical i-MSFV method are discussed in Part II of the thesis. Part III is entirely dedicated to the i-Ge-MSFV method. The zonal MSFV framework is presented in Part IV. Part V includes concluding remarks and suggestions for future works.
Part II

MSFV method and i-MSFV method
This part of the thesis is adapted from "Iterative Galerkin-Enriched Multiscale Finite-Volume Method" by Cortinovis and Jenny [13], that is, text, figures and equations in this chapter are identical with the publication. In particular, § 6 and § 7 are based on section two of the paper, and § 8 is based on section three of the same publication.
5 Introduction

This part of the thesis is devoted to the explanation of the main concepts of MS methods. A general formulation of multiscale methods is proposed first. The classical MSFV method [36] is then introduced in the light of the new formulation in order to establish a relationship between the MSFV method and classical finite element methods. The reason for introducing a more general formulation than the one found in the standard MSFV literature is that the same formulation can be used to introduce in a straightforward way the enrichment approaches discussed in the next part of the thesis. In §8, the classical i-MSFV method [26] is briefly introduced and its limitations are discussed based on an enlightening test-case.
6 General multiscale method formulation

As mentioned earlier, in the numerical investigation of subsurface flow problems involving one or multiple phases, the main computational cost is related to the repeated solution of the governing pressure equation (mass conservation). Recall that mass conservation is expressed in terms of the elliptic equation

\[ \nabla \cdot (\Lambda \cdot \nabla p) = \nabla \cdot h + q \quad \text{in } \Omega \]  

where \( p \) is the pressure, \( \Lambda \) the positive definite mobility tensor, \( q \) the volumetric source term, \( h \) a vector accounting for the influence of gravity and capillary pressure, and \( \Omega \) the domain of interest. The 2nd order tensor \( \Lambda \) incorporates soil structure information described by the permeability tensor \( K(x) \), and therefore tends to have a complex spatial distribution involving a wide range of scales. Furthermore, the mobility tensor also depends on the local saturation values (via the relative permeabilities \( k_{r,i}(S) \) and the viscosities \( \mu_i \) of the different phases \( i \)), and will therefore vary in time, if transport problems are considered. Finally, heterogeneous distributions may also be encountered for the terms on the rhs of Eq. (16). Consequently, an appropriate high-resolution discretization of Eq. (16) by means of standard numerical methods involves many DoF and results in large systems of algebraic equations to be solved many times during simulations.

Multiscale methods aim at obtaining high-resolution solutions of elliptic and parabolic equations by solving the problem at a coarser scale. The coarse-scale solution is mapped to the fine-scale via a set of basis functions. At the same time, basis functions ensure that the effects of fine-scale heterogeneities are included in the coarse-scale formulation of the problem. The methods considered here approximate the fine-scale solution \( p_f \) as a superposition of basis functions \( \{\Phi_k\}_{k=1}^{N_C} \) scaled by the corresponding coarse-scale unknowns \( \{\hat{p}_k\}_{k=1}^{N_C} \) and a correction function \( \Phi \), accounting for the heterogeneity of the rhs terms in Eq. (16). Thus, the multiscale approximation \( p_{MS} \)
The fine-scale solution reads
\[
p_{MS}(x) = \sum_{k=1}^{N_C} \Phi_k(x) \bar{p}_k + \tilde{\Phi}(x) \approx p_f(x), \quad \forall x \in \Omega.
\] (17)

The \(N_C\) coarse-scale unknowns are determined by solving the coarse-scale linear system of equations arising from the constraints
\[
\int_{\Omega} \Theta_k (L(p_{MS}) - w) \, dV = 0, \quad \forall k \in \{1, \ldots, N_C\},
\] (18)

where \(L(f) \equiv \nabla \cdot (\Lambda \cdot \nabla f)\) is the elliptic operator in Eq. (16), \(w \equiv \nabla \cdot h + q\) the corresponding total rhs and \(\{\Theta_k\}_{k=1}^{N_C}\) is a set of test functions. The functions \(\{\Phi_k\}_{k=1}^{N_C}\) and \(\{\Theta_k\}_{k=1}^{N_C}\) have local support (see Fig. 1). Furthermore, \(\{\Phi_k\}_{k=1}^{N_C}\) is guaranteed to be a partition of unity in \(\Omega\), i.e. \(\sum_{k=1}^{N_C} \Phi_k(x) \equiv 1, \quad \forall x \in \Omega\). Therefore, the multiscale method resulting from the superposition (17) and the constraints (18) is strongly reminiscent of a standard finite element method stemming from a weighted residual method formulation. The main difference between the class of methods described here and a classical FEM formulation is that the basis functions in the former are numerically computed functions incorporating fine-scale information, in contrast to the analytical basis functions in the latter. The construction of the multiscale
basis functions and the choice of test functions in the classical MSFV method are discussed in the next section.
7 Classical MSFV method

7.1 Construction of basis and correction functions

The MSFV method reduces the number of coupled DoF required for the solution of Eq. (16) on a domain $\Omega$ with respect to an arbitrary fine-scale discretization, while retaining the same level of resolution. For illustration, a 2D example with orthogonal fine-scale and coarse-scale grids is shown in Fig. 2.

The fine-scale control volumes (CV) $\{\Omega^F_i\}_{i=1}^{N_F}$ define a non-overlapping partition of $\Omega$, i.e. $\Omega = \bigcup_{i \in \{1, \ldots, N_F\}} \Omega^F_i$, $\Omega^F_i \cap \Omega^F_j = \emptyset$ for any $i \neq j$. Furthermore, the unknowns $\{p^F_i\}_{i=1}^{N_F}$ are associated to the fine-scale CV centres $\{x^F_i\}_{i=1}^{N_F}$.

The reduction of DoF is achieved by introducing a primary coarse-scale partition with coarse-scale CVs $\{\Omega^P_k\}_{k=1}^{N_P}$ ("coarse CV" from here on) and coarse-scale unknowns associated to the coarse-scale CV centres $\{x^P_k\}_{k=1}^{N_P}$. In order to retain the same level of resolution, a dual coarse-scale partition with dual coarse-scale CVs $\{\Omega^D_h\}_{h=1}^{N_D}$ ("dual CV" from here on) is constructed by connecting the CV centres of neighbouring coarse CVs. The dual CVs are used to compute two sets of functions, that is, $\{\phi_{k,h}\}_{k=1,h=1}^{N_P,N_D}$ and $\{\tilde{\phi}_h\}_{h=1}^{N_D}$, incorporating the fine-scale information.

The functions $\phi_{k,h}$ are numerical solutions of the homogeneous part of Eq. (16) restricted to $\Omega^D_h$, $\forall h \in \{1, \ldots, N_D\}$. The restriction is obtained by solving

\begin{align}
\nabla \cdot (\Lambda \cdot \nabla \phi_{k,h}) &= 0 \quad \text{in } \Omega^D_h \\
\nabla \perp \cdot (\Lambda \cdot \nabla \perp \phi_{k,h}) &= 0 \quad \text{on } \partial \Omega^D_h \\
\phi_{k,h}(x^F_i) &= \delta_{kl} \\
\phi_{k,h}(x) &= 0 \quad \forall x \in \Omega \setminus \overline{\Omega^D_h},
\end{align}

where $\nabla \perp f = n_h (n_h \cdot \nabla f)$ and $n_h$ is the unit normal vector at $\partial \Omega^D_h$ pointing outwards. The functions $\tilde{\phi}_h$ represent particular solutions of Eq. (16) and
satisfy the local problems:

\[
\nabla \cdot (\Lambda \cdot \nabla \tilde{\phi}_h) = \nabla \cdot \mathbf{h} + q \quad \text{in } \Omega^D_h \quad (23)
\]

\[
\nabla_\perp \cdot (\Lambda \cdot \nabla_\perp \tilde{\phi}_h) = \nabla_\perp \cdot \mathbf{h} \quad \text{on } \partial \Omega^D_h \quad (24)
\]

\[
\tilde{\phi}_h(x^P_l) = 0 \quad (25)
\]

\[
\tilde{\phi}_h(x) = 0 \quad \forall x \in \Omega \setminus \overline{\Omega^D_h}. \quad (26)
\]

Localization is introduced implicitly via the boundary conditions (Eqs. (20) and (24)) first proposed in [33], i.e. by neglecting the contribution of fluxes perpendicular to a given dual CV boundary or, as an equivalent interpretation, by solving 1D reduced problems (2D reduced problems for 3D cases) on \( \partial \Omega^D_h \) and using the solutions as Dirichlet boundary condition for the solution in \( \Omega^D_h \). The local problems can be solved with any appropriate numerical scheme yielding conservative solutions. In the present case, the fine-scale solutions are obtained based on a standard finite-volume discretization. By superposition of the computed local solutions, one obtains the correction function \( \Phi \) and the basis functions \( \{\Phi_k\}_{k=1}^{N_P} \), i.e.

\[
\Phi = \sum_{h=1}^{N_D} \tilde{\phi}_h \quad (27)
\]
7.2 Coarse-scale coupling

and

\[ \Phi_k = \sum_{h=1}^{N_D} \phi_{k,h}, \]  

(28)

which can now be used for the general multiscale approximation \( p_{MS} \) in Eq. (17), with \( N_C = N_P \) being the number of unknowns of the coarse-scale problem. Note that, by construction, \( \{\Phi_k\}_{k=1}^{N_P} \) is a partition of unity.

7.2 Coarse-scale coupling

In the classical MSFV method formulation the coarse-scale system is constructed by inserting Eq. (17) into Eq. (16) and integrating the resulting expression over the coarse CVs \( \{\Omega^P_k\}_{k=1}^{N_P} \). After application of Gauss' theorem, the resulting linear system of equations can be compactly expressed as

\[ A \cdot p = b \]  

(29)

with the coefficients of \( A \) and \( b \) given by

\[ a_{lk} = \int_{\partial \Omega^P_l} (\Lambda \cdot \nabla \Phi_k) \cdot n_l ds, \]  

(30)

and

\[ b_l = \int_{\Omega^P_l} q dV + \int_{\partial \Omega^P_l} h \cdot n_l ds - \int_{\partial \Omega^P_l} (\Lambda \cdot \nabla \tilde{\Phi}) \cdot n_l ds, \]  

(31)

respectively. Note that one can reformulate the MSFV method's coarse-scale coupling in the more general form given in Eq. (18) by defining the "top-hat" functions \( \{H_k\}_{k=1}^{N_P} \), i.e.

\[ H_k(x) = \begin{cases} 1 & \text{if } x \in \Omega^P_k \\ 0 & \text{otherwise}, \end{cases} \]  

(32)

and by setting \( \Theta_k = H_k, \forall k \in \{1, \ldots, N_P\} \) in Eq. (18). Thus, the standard MSFV method relies on a Petrov-Galerkin FEM formulation of the coarse-scale problem with numerically computed nodal basis functions and test functions chosen such that conservative solutions are enforced at the coarse-scale.
7.3 Reconstruction of conservative fine-scale solutions

The pressure field $p_{MS}$ yields conservative velocity fields at the fine-scale except for all fine-scale CVs crossed by dual CV boundaries. In order to avoid severe mass balance errors when solving transport problems at the fine-scale, the reconstruction of conservative fine-scale velocity fields is of great importance. The required reconstruction step can be performed locally in each coarse CV $\Omega^P_k$ by solving

$$\nabla \cdot (\Lambda \cdot \nabla p_k') = \nabla \cdot h + q \quad \text{in } \Omega^P_k$$

$$\nabla p_k' \cdot n_k = \nabla p_{MS} \cdot n_k \quad \text{on } \partial \Omega^P_k$$

for $p_k'$ and writing the fine-scale total velocity (flux) $u'$ as

$$u' = \begin{cases}
-(\Lambda \cdot \nabla p_k' - h) & \text{in } \Omega^P_k \\
-(\Lambda \cdot \nabla p_{MS} - h) & \text{on } \partial \Omega^P_k.
\end{cases}$$

In order to overcome the strict time-step size limitations generally encountered for the classical IMPES scheme (cf. § 1.3), an adaptive fully implicit MSFV method was presented in [37]. The idea is to solve the elliptic pressure equation with the MSFV method, while the non-linear hyperbolic transport problems (5) is discretized implicitly and solved with Newton’s method. Due to the possibility of solving the transport problem for each Newton iteration using simple domain decomposition methods (Schwarz alternating procedures [56]) based on the natural block structure of the MSFV coarse grid, the overall algorithm is particularly efficient.

7.4 Remarks

The steps outlined above represent the key ingredients of the MSFV method. Building on these ideas, the method was further enhanced to deal with gravity and compressibility effects [47, 45], complex wells [66, 45, 38], compositional processes [25] and flow in fractured media [29]. Additionally, a MSFV method formulation for hyperbolic transport problems was introduced in [67]. Despite the capability of the classical MSFV method to deliver accurate approximate solutions for a wide range of scenarios [40], highly heterogeneous anisotropic permeability fields can cause a deterioration of the quality of the solution. This behaviour led to the development of the i-MSFV method, which is outlined in the next section.
8 Classical i-MSFV method

8.1 Iterative scheme

The iterative multiscale finite-volume method introduced by Hajibeygi et al. [26] aims at improving the MSFV method approximation to any desired level of accuracy. The central idea in developing the iterative improvement is as follows. The fine-scale reference solution and the MSFV method approximation differ from each other only due to the applied localization boundary condition in Eq. (24). They would coincide if

$$\nabla \cdot (\Lambda \cdot \nabla \phi_h) = \nabla \cdot (\Lambda \cdot \nabla p_f) \text{ on } \partial \Omega_h^D$$

(36)

was used instead. Unfortunately, the fine-scale field $p_f$, which represents the reference fine-scale solution, is not known; hence an alternative field must be used in order to improve the estimate of the rhs of Eq. (36).

The i-MSFV method introduces an iterative improvement of the localization assumption (24) used for the computation of the local functions $\phi_h$ composing the correction function, which is replaced by

$$\nabla \cdot (\Lambda \cdot \nabla \phi_h^{(\nu)}) = \nabla \cdot (\Lambda \cdot \nabla p_s^{(\nu)}) \text{ on } \partial \Omega_h^D$$

(37)

with $\nu$ and $p_s^{(\nu)}$ denoting the iteration step and the smoothed pressure solution after $\nu$ iterations, respectively. Denoting as $\mathcal{W}$ any convergent iterative scheme (smoother) which can be used for the solution of the system of linear equations arising from a fine-scale discretization of Eq. (16), the smoothed pressure solution at each iteration step $\nu$ can be written as

$$p_s^{(\nu)} = \mathcal{W}(p_{MS}^{(\nu-1)}, n_s),$$

(38)

where $n_s$ is the number of smoothing steps performed and $p_{MS}^{(\nu-1)}$ is the i-MSFV method approximation at the previous iteration level used as an initial guess in the $\nu$-th iteration. In particular, $p_{MS}^{(0)}$ refers to the MSFV
method approximation obtained without iterations, i.e. by employing the standard localization assumption (24) for the computation of the local correction terms. After the computation of the improved correction function

\[ \tilde{\Phi}^{(\nu)} = \sum_{h=1}^{N_D} \tilde{\phi}^{(\nu)}_h, \]  

(39)

the coarse-scale system (29) is assembled and solved, delivering the multiscale solution \( p_{MS}^{(\nu)} \) at the \( \nu \)-th iteration level. Note that only the rhs of the system in Eq. (29) needs to be recomputed after each iteration, since the iterative improvement proposed in Eq. (37) affects the correction function only. It should be remarked that conservative fine-scale velocity fields can be computed after each i-MSFV method iteration by substituting \( p_{MS} \) with \( p_{MS}^{(\nu)} \) in Eqs. (34) and (35). Therefore, the i-MSFV method iteration loop may be terminated well before convergence is reached without compromising mass conservation, which is a crucial property for transport problems. However, the classical MSFV method results in a stable iterative scheme only if enough smoothing steps are applied, but unfortunately the required number of steps is not known a-priori.

8.2 Limitations

In general the i-MSFV method requires only few smoothing steps and MSFV iterations to recover the converged fine-scale reference solution. However, for really complex permeability fields with highly oscillating coefficients (e.g. in the presence of shale layers or channels), the global convergence rate of the method may become unsatisfactorily slow.

As an illustrative example the artificial isotropic permeability field depicted in Fig. 3 is considered. Two shale layer formations representing channels are positioned such that they cut dual CV boundaries in three distinct regions: an ”in-channel” segment and two ”out-channel” segments. The shale permeability is \( k_{\text{shale}} = 10^{-6}k_{bg} \) (black), where \( k_{bg} \) is the background permeability (white). No-flow conditions are applied at all boundaries and two wells are positioned in the fine-scale CVs \((3,3)\) and \((57,57)\) with constant pressures \( p = 1 \) and \( p = 0 \), respectively. Line-relaxation is used as a smoother like in the original paper on the i-MSFV method [26]. Convergence histories of the i-MSFV method are shown in Fig. 4 for different numbers of smoothing steps \( n_s \). In order to achieve convergence, at least \( n_s = 1300 \) smoothing steps per i-MSFV method iteration (not shown) are required and for acceptable convergence rates \( n_s \) has to be at least 1500. The required number of smoothing
8.2 Limitations

Figure 3: Permeability field containing two shale layer formations (solid, black), with superimposed coarse grid (dotted, blue) and the dual coarse grid (dotted, green).

steps is so high, since already a small deviation from the correct source term \((\nabla_\perp \cdot (\Lambda \cdot \nabla_\perp p_f))\) leads to strong oscillations of the correction function in dual CVs with boundaries traversed by multiple shale-layers. This instability is the result of solving the reduced problem (37) with inaccurate correction terms for fine-scale CVs in the "in-channel" region. The locally introduced error affects the global solution via the coarse-scale coupling, i.e. the correction function introduces an incorrect high flux in the coarse-scale balance equations (last term in Eq. (31)), which has to be compensated by scaling the basis functions with appropriate \(\{\hat{p}_k\}\) values to fulfil the coarse-scale constraints. Therefore, the computational cost for obtaining good i-MSFV method convergence rates may increase dramatically due to the required accuracy of the transverse fluxes in such critical regions.

In the next part of the thesis, a general strategy to improve both robustness and convergence rate of the i-MSFV method is presented. The new approach nicely fits into the already developed MSFV/i-MSFV method framework.
Figure 4: The convergence histories of the i-MSFV method for different numbers of smoothing steps ($n_s$); shown is the base-10 logarithm of the residual infinity norm. The test-case is based on the permeability field shown in Fig. 3.
Part III
Iterative Galerkin-enriched MSFV method
Some chapters in this part of the thesis are adapted from "Iterative Galerkin-Enriched Multiscale Finite-Volume Method" by Cortinovis and Jenny [13], that is, text, figures and equations in these chapters are identical with the publication. In particular, §9 is based on section one of the publication, §10 on section three, §11 on section four and §13 on section five of the publication.
9 Introduction

As discussed earlier, the major reason for the drastic reduction of computational efficiency experienced by the classical i-MSFV method is due to the high sensitivity of the correction function to contrast variation along the dual CV boundaries. Additionally, the stability of the i-MSFV method is only guaranteed, if enough smoothing steps are performed.

MSFV based iterative schemes aiming at improving the stability of the i-MSFV method were proposed in [51, 69, 63]. The three approaches are similar in the sense that the MSFV method is recast in an algebraic formulation and that the resulting algebraic operators are used to derive a MSFV method preconditioner. The MSFV preconditioner is then used in combination with a Krylov subspace method in order to stabilize the iteration and hence, to obtain an unconditionally stable MSFV based iterative scheme. The main difference is that in [51] the correction function operator is used, while in [69, 63] the correction function operator is substituted by a different local solver, and a Galerkin-type of coarse-scale coupling is used instead. The latter approach, i.e. the substitution of the correction function and the selection of a Galerkin based coarse-scale coupling, results in an unconditionally stable algorithm even without using Krylov subspace methods for stabilizing the iterations. Nevertheless, both approaches will still suffer a significant deterioration of convergence rates in the presence of high-contrast fields.

In this part of the thesis the focus is set on developing a robust version of the classical i-MSFV method with greatly improved convergence rates in the presence of high-contrast: the iterative Galerkin-enriched MSFV (i-GeMSFV) method. The presented concepts result in a straightforward extension of the already established MSFV/ i-MSFV methods presented in sections 6 – 8, hence the previous developments of the method [37, 47, 45, 42, 46] do not require substantial modifications. The improvement is achieved by the selective enrichment of the coarse-space spanned by standard MSFV method basis functions, i.e. by introducing additional DoF and related functions at
selected locations along dual CV boundaries. By construction it is ensured that the resulting augmented set of basis functions forms a partition of unity over the entire computational domain. In order to close the system of equations at the coarse scale, an additional constraint is required for each additional DoF. The classical MSFV method approach would involve the creation of additional arbitrarily shaped coarse CVs overlapping the standard coarse grid. In order to avoid this ambiguous procedure, a more general strategy for the coarse-scale coupling of the local solutions is introduced. Like its predecessor, the resulting i-Ge-MSFV method ensures conservative coarse-scale solutions and allows to reconstruct conservative fine-scale velocity fields.

In order to avoid repetitions, no algebraic version of the i-Ge-MSFV method is presented here, since the very general zonal MSFV framework formulation discussed in the next part of thesis (and its algebraic version) can be easily modified to obtain the i-Ge-MSFV method as a special case of the framework. Hence, the performance of the Ge-MSFV based preconditioner in combination with a Krylov subspace method is discussed in art 13 of the thesis.
10 i-Ge-MSFV method

10.1 Main concepts

In order to increase the convergence rate of the i-MSFV method, two main approaches can be followed: (i) improving the coarsening strategy and (ii) developing coarse-space enrichment strategies. The former aims at selecting dual coarse grids such that the resulting dual CV boundaries do not contain disconnected regions (e.g. shale layers cutting dual CV boundaries as displayed in Fig. 3) or intersect with highly conducting channel structures. Here, we follow the second approach and formally consider the enrichment of a given initial coarse-space with additional basis functions assembled from local enrichment functions \( \{ \psi_{e,h} \}_{e=1,h=1}^{N_A,N_D} \) (\( N_A \): number of added DoF; \( N_D \): number of dual CVs), aiming at better capturing the fine-scale effects due to channels and disconnected regions. Additional coarse DoF must be introduced in order to couple the enrichment functions to the coarse-scale system. Consequently, the i-Ge-MSFV method consists of two main steps: the determination of critical fine-scale CVs on dual CV boundaries, for which additional DoF need to be introduced, and the coarse-scale coupling of the new DoF. The outlined idea clearly aims at counteracting the problems discussed in §8.2: the additional DoF will allow for a direct control of the coarse-scale flux contribution stemming from critical regions on dual CV boundaries via the coarse-scale system. Consequently, the enriched coarse-scale operator improves the accuracy of transverse fluxes in sensitive regions and thus has better convergence properties with less smoothing steps per i-Ge-MSFV method iteration.

A similar approach has successfully been tested for a MSFE method [17, 15, 21, 20]. The authors describe the mathematically rigorous creation of an enhanced coarse space capable of capturing the influence of ”inclusions” (high permeability values encapsulated in a low permeability region within a coarse grid block) and channels (high permeability channels connecting two or more coarse grid CVs) at the coarse scale. While the effect of in-
Inclusions is already captured by multiscale basis functions (analogous to the MSFV method basis functions), additional functions are required to capture the effect of channels. To this end, selected eigenvectors (“spectral basis functions”) computed from locally defined homogeneous Neumann eigenvalue problems are assigned to the corresponding coarse nodes after multiplication with the nodal basis function. As a consequence, the augmented set of functions does not form a partition of unity. Additionally, the solution of the eigenvalue problems is computationally rather expensive.

Conceptually the strategies explained in the following are similar to the aforementioned enriched MSFE method approach. However, besides the intrinsic difference between the methods (MSFV vs. MSFE), three main distinctions must be made. First, in contrast to the enriched MSFE method [17], the augmented set of basis functions constructed and employed by the i-Ge-MSFV method is a partition of unity, where each enrichment function is associated with an additional DoF located on a dual CV boundary and second, in the i-Ge-MSFV method the detection of new DoF locations is either based on a heuristic, but computationally cheap preprocessing step or a slightly more expensive adaptive enrichment strategy. Finally, the i-Ge-MSFV method computes coarse-scale conservative solutions and allows for the reconstruction of conservative fine-scale solutions after each iteration.

10.2 Construction of basis functions and related coarse space

The computation of the local solutions $\psi_{e,h}$, $\phi_{k,h}$ and $\tilde{\phi}_h$ for the i-Ge-MSFV method is similar to the procedure already outlined for the standard MSFV method. After having defined the $N_A$ additional DoF locations $\{x_{e}^{A}\}_{e=1}^{N_A}$, the functions $\phi_{k,h}$ can be computed from

\begin{align}
\nabla \cdot (\Lambda \cdot \nabla \phi_{k,h}) &= 0 \quad \text{in } \Omega_h^D \\
\n\nabla_\perp \cdot (\Lambda \cdot \nabla_\perp \phi_{k,h}) &= 0 \quad \text{on } \partial \Omega_h^D \\
\phi_{k,h}(x_{e}^{P}) &= \delta_{kl} \\
\phi_{k,h}(x_{i}^{A}) &= 0 \\
\phi_{k,h}(x) &= 0 \quad \forall x \in \Omega \setminus \Omega_h^D,
\end{align}
while \( \overline{\phi}^{(v)} \) (including iterative improvements of the localization assumption) now satisfy
\[
\nabla \cdot (\Lambda \cdot \nabla \overline{\phi}^{(v)}) = \nabla \cdot \mathbf{h} + q \quad \text{in } \Omega_h^D \tag{45}
\]
\[
\nabla_\perp \cdot (\Lambda \cdot \nabla_\perp \overline{\phi}^{(v)}) = \nabla_\perp \cdot (\Lambda \cdot \nabla_\perp p_s^{(v)}) \quad \text{on } \partial \Omega_h^D \tag{46}
\]
\[
\overline{\phi}^{(v)}(x_P) = 0 \tag{47}
\]
\[
\overline{\phi}^{(v)}(x_A) = 0 \tag{48}
\]
\[
\overline{\phi}^{(v)}(x) = 0 \quad \forall x \in \Omega \setminus \overline{\Omega}_h^D. \tag{49}
\]

Finally, the local enrichment functions associated with the additional DoF locations are numerical solutions of
\[
\nabla \cdot (\Lambda \cdot \nabla \psi_{e,h}) = 0 \quad \text{in } \Omega_h^D \tag{50}
\]
\[
\nabla_\perp \cdot (\Lambda \cdot \nabla_\perp \psi_{e,h}) = 0 \quad \text{on } \partial \Omega_h^D \tag{51}
\]
\[
\psi_{e,h}(x_P) = 0 \tag{52}
\]
\[
\psi_{e,h}(x_A) = \delta_{e\ell} \tag{53}
\]
\[
\psi_{e,h}(x) = 0 \quad \forall x \in \Omega \setminus \overline{\Omega}_h^D \tag{54}
\]
computed in each dual CV with at least one additional DoF located somewhere on its boundary.

The correction function \( \overline{\Phi}^{(v)} \) is assembled exactly as for the standard i-MSFV method (cf. Eq. (39)), while the \( N_C = N_P + N_A \) basis functions in Eq. (17) are now given by
\[
\Phi_k = \begin{cases} 
\sum_{h=1}^{N_D} \phi_{k,h} & \text{if } k \leq N_P \\
\sum_{h=1}^{N_D} \psi_{e=k-N_P,h} & \text{if } k > N_P
\end{cases} \tag{55}
\]
Note that Eqs. (42), (43), (52) and (53) ensure that \( \{\Phi_k\}_{k=1}^{N_C} \) forms a partition of unity in \( \Omega \).

### 10.3 Coarse-scale coupling

The insertion of \( N_A \) additional DoF requires \( N_A \) additional coarse-scale constraints of the form of Eq. (18). As a straightforward extension of the original MSFV method, additional constraints can simply be obtained by introducing new CVs (and thus additional top hat-functions \( \mathcal{H} \)) enclosing each of the additional DoF. This approach has one major drawback as it introduces ambiguity to the i-Ge-MSFV method formulation. Control volume size and
Figure 5: Nodal basis functions of the standard MSFV method (top figures) associated to the dual CV containing the L-shaped shale layers shown in Fig. 3. Nodal basis functions (4 center figures) after the insertion of two additional DoF. The corresponding enrichment functions are shown in the bottom figures.
shape may be chosen without many restrictions, but at the same time the solution and convergence rates depend on both. Further, the automatic creation of suitable CVs may become challenging, if regions with agglomeration of additional DoF are present.

As the name implies, the coarse-scale coupling formulation of the i-Ge-MSFV method is based on a hybrid Galerkin / Petrov-Galerkin method approach: the test functions used in the MSFV method are retained to ensure conservative coarse-scale solutions, while the additionally required \( N_A \) test functions belong to the set of basis functions \( \{ \Phi_k \}_{k=1}^{N_C} \). In particular, we select the basis functions related to the additional DoF and consequently, the test functions of the i-Ge-MSFV method are given by

\[
\Theta_k = \begin{cases} 
\mathcal{H}_k & \text{if } k \leq N_P \\
\Phi_k & \text{if } k > N_P
\end{cases}.
\]

This approach combines the advantages of the two methods, i.e. the intrinsic conservation properties of finite-volume methods arising from a Petrov-Galerkin formulation of the coarse-scale problem (MSFV method), and the flexibility and residual minimization properties of the Galerkin based weighted residual approach. It should be noticed that the presented selection of additional test functions is not the only possible one. For example, one may select basis functions related to the coarse CV centres, i.e. \( \Theta \in \{ \Phi_k \}_{k=N_P+1}^{N_P+N_A} \), but then attention must be paid in order to avoid a linearly dependent coarse-scale system. Furthermore, the number of DoF that can be added like this is restricted to \( N_P \). Note that it is also possible to obtain a pure Galerkin FEM method formulation of the coarse-scale problem by using \( \{ \Phi_k \}_{k=1}^{N_C=N_P+N_A} \) as test functions instead of the previously defined top hat-functions. However, the resulting coarse-scale fluxes are not conservative and an additional step is required to enforce this condition \([69, 63]\). Selecting test functions as in Eq. (56) is a very natural choice, since each additional \( \Phi_k \) can be coupled at the coarse-scale without any restriction posed on the number of DoF that may be added.

The system of equations resulting from Eq. (18) with test functions and basis functions as defined in Eqs. (56) and (55), respectively, is given by

\[
Ap = b
\]

with the coefficients of \( A \) and \( b \) reading

\[
a_{lk} = \begin{cases} 
\int_{\partial \Omega \cap P} (\Lambda \cdot \nabla \Phi_k) \cdot n_l ds & \text{if } l \leq N_P \\
\int_{\Omega} \Phi_l (\nabla \cdot \Lambda \cdot \nabla \Phi_k) dV & \text{if } l > N_P
\end{cases}.
\]
and

\[ b_l = \begin{cases} 
\int_{\Omega_l^P} q dV + \int_{\partial\Omega_l^P} h \cdot n_l ds - \int_{\partial\Omega_l^P} (\Lambda \cdot \nabla \Phi) \cdot n_l ds & \text{if } l \leq N_P \\
\int_{\Omega_l} \Phi_l (q + \nabla \cdot h) dV - \int_{\Omega_l} \Phi_l (\nabla \cdot \Lambda \cdot \nabla \Phi) dV & \text{if } l > N_P.
\end{cases} \] (59)

Note that Gauss’ theorem was used for the derivation of the elements \( a_{lk} \) and \( b_l \) for \( l \in \{1, ..., N_P\} \).

### 10.4 Enrichment strategies

The last task to be addressed is the identification of fine-scale CVs, for which the introduction of an additional coarse-scale DoF results in an enhanced convergence rate, or alternatively, in a reduction of the number of smoothing steps per i-Ge-MSFV iteration. For simple permeability fields, like the synthetic field in Fig. 3, such locations can easily be determined. Obviously the introduction of additional DoF within the shale layer formations will enhance the convergence rate, since the local errors can be controlled directly as part of the coarse-scale problem. However, for generic permeability fields an automatic detection of suitable locations is preferable and often the only practical way. Two enrichment approaches are considered in the next sections: a heuristic a priori detection strategy and an adaptive one. Both strategies can be used as a stand alone procedure, but may also be combined. It should be remarked that the a priori strategy is not ensured to be optimal with respect to the number of additional DoF introduced, and as a consequence, may introduce more DoF than needed for a specified convergence rate.

#### 10.4.1 Adaptive enrichment

The adaptive enrichment approach places additional DoF during the first iteration loop by using the residual distribution as an indicator for the most suitable location. The residual vector after the \( \nu \)-th i-Ge-MSFV method iteration is given by

\[ r^{(\nu)} = b_F - A_F p_{MS}^{(\nu)} \] (60)

with \( A_F \) and \( b_F \) obtained from a fine-scale finite-volume discretization of Eq. (16) and \( p_{MS}^{(\nu)} \) representing the i-Ge-MSFV method solution vector at
the same iteration level. In this context, each detection loop consists of three main operations:

1. the i-Ge-MSFV method iteration,

2. the residual based selection of new DoF, and

3. the computation of enrichment functions and adaptation of basis and enrichment functions influenced by the new DoF.

These operations are performed repeatedly until a predefined convergence criterion of the form \( \|r^{(\nu)}\| < TOL_1 \) is fulfilled for some vector norm and user defined tolerance \( TOL_1 \). The just outlined adaptive enrichment strategy can therefore be seen as an integral part of the i-Ge-MSFV method, since each DoF detection loop is simply an enrichment step between two succeeding i-Ge-MSFV method iterations. The addition of new DoF may become unnecessary, if the i-Ge-MSFV method already exhibits satisfying convergence rates. Therefore, new DoF are only added between two subsequent iterations, if

\[
\frac{\|r^{(\nu)}\|_{\infty}}{\|r^{(\nu-1)}\|_{\infty}} \geq TOL_{rate},
\]

where \( TOL_{rate} \) is a specified parameter. Operations 1 and 3 have been outlined in the preceding sections and will not be discussed again here. The second operation, i.e. the residual based selection of additional DoF, represents a crucial step of the adaptive enrichment strategy and requires further elaboration. Obvious candidates for the introduction of additional DoF are fine-scale CVs with high absolute residual values. It should be remarked that the residual vanishes up to machine accuracy for all fine-scale CVs inside dual CVs, since \( p^{(\nu)}_{MS} \) is a superposition of functions locally satisfying the governing equation (cf. Eqs. (40), (45) and (50)). This is a good motivation to choose the residual distribution as an indicator for suitable DoF locations on dual CV boundaries. The simplest possible residual based selection criterion reads

\[
x^* = \arg \max_{\{x_F^i\}_{i=1}^N} r^{(\nu)}(x_{F_i}^F)
\]

with \( r^{(\nu)}(x_l) = |r_l| \), i.e. the l-th element of the residual vector, and for simplicity it is assumed that Eq. (62) is well-defined (for the very remote case of multiple fine-scale CVs with equal maximal residual values, one could simply select a single CV out of the candidates). Applying Eq. (62) results in a single DoF addition per detection loop and, as a consequence, the number of detection loops required to achieve good convergence rates depends
on the number of channels and shale layer formations present in the domain and on how they intersect with the dual CV boundaries. This behaviour is illustrated in Fig. 6, where the parameters $n_s = 10$ and $TOL_{rate} = 0.2$ were used for the DoF detection algorithm. Initially, the solutions diverge since $n_s \ll 1500$ (compare with Fig. 4) and, as expected, convergence is only obtained after adding 4 DoF at appropriate locations. Large domains with highly channelized permeability fields therefore require substantially more detection loops, and thus, more computational work. Clearly, adding multiple DoF per iteration would reduce the number of required detection loops. However, the selection of multiple DoF per detection loop can lead to ambiguity and sub-optimal choices, and therefore this is not recommended here. Also note that this adaptive detection of additional DoF may only be applied once at the beginning of a simulation. A very crude extension of the presented adaptive enrichment allowing for multiple DoF detection is used for the 3D test-cases in §11.3. Nevertheless, to reduce the total number of detection loops, instead of starting with the original set of MSFV basis functions, one can apply an a-priori enrichment strategy to ”precondition” the coarse space before adding more DoF based on the residual based detection approach. The resulting algorithm is summarized in Algorithm 1. In the following, the mentioned a-priori selection strategy is explained.

Figure 6: (a) Development of $||r||_\infty$ (solid, red line) during the adaptive detection of additional DoF. The square symbols indicate the detection ($TOL_{rate} = 0.1$) and addition of new DoF. The underlying permeability field and the location of insertion of additional DoF (red dots) is shown in (b).
Algorithm 1: Adaptive enrichment.

1: set $n_s$, $TOL_1, TOL_{rate}$
2: $\nu \leftarrow 0$
3: if "a-priori detection" then
4: \hspace{1cm} run Algorithm 2
5: \hspace{1cm} $\{x^A_e\}_{e=1}^{N_A} \leftarrow$ a-priory detected additional DoF locations
6: end if
7: compute $\{\phi_{k,h}\}, \{\psi_{e,h}\}, \{\tilde{\phi}_h^{(\nu=0)}\}$ \hspace{1cm} $\triangleright$ local problem solutions
8: assemble and solve coarse system \hspace{1cm} $\triangleright$ Eqs. (57) - (59)
9: $p_{MS}^{(\nu)} := \sum_{k=1}^N \Phi_k \hat{p}_k + \Phi^{(\nu)}$
10: compute $r^{(\nu)} = b_F - A_F p_{MS}^{(\nu)}$
11: while $\|r^{(\nu)}\| > TOL_1$ do
12: \hspace{1cm} $\nu \leftarrow \nu + 1$
13: \hspace{1cm} compute $p_{s}^{(\nu)}$, update $\tilde{\phi}_h^{(\nu)}$
14: \hspace{1cm} compute $p_{MS}^{(\nu)}$
15: \hspace{1cm} if $\frac{\|r^{(\nu)}\|_\infty}{\|r^{(\nu-1)}\|_\infty} > TOL_{rate}$ then \hspace{1cm} $\triangleright$ convergence speed check
16: \hspace{1cm} \hspace{1cm} $N_A \leftarrow N_A + 1$
17: \hspace{1cm} \hspace{1cm} $x^* \leftarrow \arg \max \ r^{(\nu)}(x_F^i) \hspace{1cm} \triangleright$ DoF location detection
18: \hspace{1cm} \hspace{1cm} $(x_F^i)_{i=1}^{N_F}$
19: \hspace{1cm} add $x^*$ to set the of DoF locations $\{x^A_e\}_{e=1}^{N_A}$
20: \hspace{1cm} compute new enrichment functions
21: \hspace{1cm} update $\{\phi_{k,h}\}, \{\psi_{e,h}\}$ influenced by DoF addition
22: end while
### 10.4.2 A-priori enrichment

Given the skeleton $S$ of the dual grid, i.e. $S = \bigcup_{i,j \in \{1,\ldots,N_D\}, i \neq j} (\Omega^D_i \cap \Omega^D_j)$, the idea is to solve

\begin{equation}
\nabla_{\parallel} \cdot (K \cdot \nabla p^G) = -q^D \quad \text{on } \Gamma^D \tag{63}
\end{equation}

\begin{align}
p^G(x^P) &= 0 \tag{64} \\
p^G(x_A) &= 0 \tag{65} \\
p^G(x) &= 0 \quad \text{in } \Omega \setminus \Gamma^D, \tag{66}
\end{align}

where $\nabla_{\parallel} = \nabla - n_{\Gamma} (n_{\Gamma} \cdot \nabla)$ is the tangential nabla operator, $n_{\Gamma}$ the unit vector normal to $\Gamma$ and $K$ the absolute permeability tensor. Further, the source term on the rhs of Eq. (63) is given as

\begin{equation}
q^D \equiv C (n_{\Gamma}^T \cdot K \cdot n_{\Gamma})^2 \quad \text{on } \Gamma^D, \tag{67}
\end{equation}

where the constant $C$ ensures dimensional consistency in Eq. (63). Equations (63)-(66) are considered in each detection loop $\zeta$, after which the $N_e$ locations $\{x_m\}_{m=1}^{N_e}$ where $p^G$ attains a local extremum $p^*$ and violates

\begin{equation}
p^G(x_m) \leq \beta \tag{68}
\end{equation}

are added to the set of additional DoF locations $\{x_A^A\}$. Note that $\beta$ is a threshold parameter, which has to be defined. Detection loops are repeated with the augmented set of additional DoF locations until Eq. (68) is fulfilled for all $m \in \{1,\ldots,N_e\}$. Thereby the indexing convention is that

\begin{equation}
p^*(x^A_1) \geq p^*(x^A_2) \geq \cdots \geq p^*(x^A_{N_A}) \tag{69}
\end{equation}

holds after each loop. As a consequence, an ordered list of locations on dual CV boundaries is obtained, which can be used to assign additional DoF in the i-Ge-MSFV method. Clearly, if all fine-scale CVs have been added to the ordered list of additional DoF, one will be required to select a subset of locations from it.
Algorithm 2: A-priori enrichment.

1. define $\beta_{(\zeta)}$ for all $\zeta$ \hspace{1cm} $\triangleright$ DoF acceptance condition
2. $\zeta \leftarrow 1$
3. compute $q_{\Gamma}(x) := (n_{\Gamma}^T \cdot K(x) \cdot n_{\Gamma})^2$
4. repeat
5. $p_{\Gamma}(x) \leftarrow 0$; $\forall x \in \{$DoF locations$\}$. 
6. $q_{\Gamma}(x) \leftarrow 0$; $\forall x \in \{$DoF locations$\}$. 
7. solve $\nabla \cdot K \nabla p_{\Gamma}(x)_{(\zeta)} = -q_{\Gamma}(x)$
8. $\{x_{j}^{*}\}_{\zeta=1}^{N_{e}} \leftarrow$ detect the $N_{e}$ extrema of $p_{\Gamma}(\zeta)$
9. for $j = 1 \rightarrow N_{e}$ do
10. \hspace{1cm} if $p_{\Gamma}(x_{j}^{*}) > \beta_{(\zeta)}$ then
11. \hspace{2cm} add location $x_{j}^{*}$ to collection of DoF locations $\{x_{e}^{A}\}_{e=1}^{N_{A}}$
12. \hspace{1cm} end if
13. end for
14. $\zeta \leftarrow \zeta + 1$
15. until no new DoF location detected.
16. output: ordered DoF location list $\{x_{e}^{A}\}_{e=1}^{N_{A}}$

The idea underlying the procedure described above is to mimic the influence of wrong correction terms $(\nabla_{\perp} \cdot (\Lambda \cdot \nabla_{\perp} p_{s}^{(\nu)}) \neq \nabla_{\perp} \cdot (\Lambda \cdot \nabla_{\perp} p_{f}))$ on the multiscale solution, and thus to determine locations on dual CV boundaries particularly sensitive to an inaccurate computation of the transverse fluxes. The rhs term of Eq. (67), which approximates the local transverse flux contribution at some iteration level, is a deviation from the optimal value $(\nabla_{\perp} \cdot (\Lambda \cdot \nabla_{\perp} p_{f}))$ and it is given by a quadratic scaling of the local permeability coefficients. This choice is motivated by fluxes being the product of permeability coefficient and pressure gradient, and thus errors introduced by inaccurate gradients are amplified by the corresponding coefficient. The quadratic dependence of the local source term on the corresponding coefficient is introduced to identify highly conducting regions and to populate them with additional DoF. By solving the reduced problem in Eq. (63) and detecting the location of extrema, the locations most sensitive to the input source terms are determined. The algorithm is independent of any problem specific quantity (e.g. wells) and only requires knowledge of the dual grid and permeability field. Therefore it can be implemented as a pure preprocessing step. Further, the computational cost is very low, as it only requires the solution of one-dimensional problems.

As an illustrative example, the permeability field and grids as shown in Fig. 7 (top figure) are considered, leading to an initial coarse-space spanned by 70
basis function. The parameters used in Algorithm 2 and Algorithm 1 are: \( \beta = 0, n_s = 20, TOL_1 = 10^{-8} \) and \( TOL_{rate} = 0.2 \). Figure 7 (bottom) shows the convergence history for the mixed a-priori/adaptive DoF detection algorithm (Algorithm 1) with different choices of a-priori selected DoF locations. The nomenclature used for the i-Ge-MSFV runs with different numbers of a-priori selected DoF is as follows: "P20-A10-iGeMSFV" means that 20 DoF were added with the a-priori detection algorithm (Algorithm 2), while 10 DoF were selected adaptively (Algorithm 1). The black square symbols indicate, if insertion of a new basis function took place during a detection loop (iterations). Clearly, the pre-enriched coarse-spaces reduce the number of detection loops required to satisfy the chosen convergence tolerance. The i-Ge-MSFV method based on a pure adaptive approach, which detects 53 additional DoF and requires 70 iterations to converge ("P0-A53-iGeMSFV", yellow line), exhibits similar convergence rates as the pre-enriched variants. Thus, the number of detection loops is reduced significantly without suffering deterioration of convergence speed.
10.4 Enrichment strategies

Figure 7: Convergence history (bottom figure) of the mixed a-priori / adaptive enrichment algorithm for different numbers of a-priori ("P") selected DoF locations. The black squares indicate, if the insertion of a new DoF was performed after a detection loop (iteration). Coarse grid (blue lines, 14 × 5 CVs), dual grid (green) and permeability field considered are shown in the top figure. The red dots mark the location of all additional DoF resulting from the "P30-A21-iGeMSFV" run. Note that the prefix "Px-Ay" employed in the legend stands for: "x" DoF were selected a-priori and "y" DoF were selected adaptively.
11 Numerical results

In this section, the capabilities of the i-Ge-MSFV method are investigated for three different permeability fields with highly oscillating coefficients. In addition, the influence of expanding saturation fronts and well locations is investigated to assess the robustness of the method. For simplicity, the effects of capillary pressure and gravity are neglected \((h = 0)\), and no-flow boundary conditions are used. Unless stated otherwise, Cartesian uniform fine-scale grids with a unity CV aspect ratio \(\alpha (\alpha = \frac{\delta x}{\delta y} \text{ in 2D}; \alpha = \frac{\delta x}{\delta y} = \frac{\delta y}{\delta z} \text{ in 3D})\) are employed; together with an isotropic permeability field.

11.1 A-priori enrichment

The first set of test-cases is dedicated to the evaluation of the performance of the i-Ge-MSFV method with the application of the pure a-priori placement strategy (Algorithm 2). For all test-cases \(B^{(\zeta)} = 0, \forall \zeta\) is used (line 1 in Algorithm 2) and a complete list of DoF location candidates is created. The convergence maps below show the influence of number of additional DoF used and number of smoothing steps on the mean convergence rate given by

\[
\mathcal{R}_m = \left( \frac{\|\epsilon^{(\nu^*)}\|_{\infty}}{\|\epsilon^{(0)}\|_{\infty}} \right)^{\frac{1}{\nu^*}} = \left( \frac{||P_{MS}^{(\nu^*)} - P_F||_{\infty}}{||P_{MS}^{(0)} - P_F||_{\infty}} \right)^{\frac{1}{\nu^*}},
\]

where \(\nu^*\) is the number of iterations needed for obtaining convergence. For all cases considered the convergence criterion is \(||r||_{\infty} < TOL = 10^{-7}\).

In the first numerical example a permeability field (top figures in Fig. 8) with mean \(\mu_{\ln(K)} = 3\) and variance \(\sigma^2_{\ln(K)} = 2\) is considered.
Figure 8: Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. Two initial configurations with 81 (a) and 9 (b) basis functions are considered. Coarse (blue) and dual coarse (green) grids are shown on top of the corresponding convergence maps. The location of the first 50 additional DoF are marked with red dots.

The fine-scale grid used for the discretization of the problem contains $99 \times 99$ CVs. Three wells located in the fine-scale CVs $(14,3)$, $(94,77)$ and $(43,92)$ with constant well pressures $p_w(14, 3) = 1$, $p_w(94, 77) = 0$ and $p_w(43, 92) = 0$, respectively, were considered. Figure 8 shows the resulting convergence maps for two different coarse grids resulting in initially 81 (Fig. 8(a)) and 9 (Fig. 8(b)) basis functions, respectively. Compared to the standard i-MSFV method (0 additional DoF), the i-Ge-MSFV method achieves significantly improved convergence rates, independently of the considered initial coarse-space. For the rather smooth permeability field considered, the a-priori strategy performs well, which is demonstrated by the convergence rates improving steadily as the number of additional DoF increases. The same configurations, i.e grids, well locations and well pressures, were used for the permeability field
shown in Fig. 9. The field has the same one-point statistics as the previous example with the difference that now conducting channels are present and aligned in a 30 degree angle from the y-axis. The convergence map of the case with 81 initial basis functions (Fig. 9(a)) shows an almost constant $R_m$ between 5 and 40 additional DoF and an abrupt decrease after the addition of 45 DoF. This is an indication that the a-priori algorithm inaccurately estimates the importance of some DoF locations. The same behaviour cannot be observed for the coarser initial space (Fig. 9(b)), where an increased number of DoF leads to a smooth improvement of $R_m$. Further, a comparison between the two convergence maps shows that a simple refinement of the coarse grids may not necessarily lead to greatly improved convergence rates. The third numerical example (Fig. 10) investigates the influence of anisotropic fields by considering a numerical analogon, i.e by increasing the aspect ratio $\alpha$ of the fine-scale CVs. The test-case configuration used to obtain the results shown in Fig. 9 is used in combination with $\alpha = 10$. The convergence rates obtained for the anisotropic case (Fig. 10) deteriorate slightly for the coarse-space initially spanned by 81 basis functions, but they remain almost unchanged in the case of 9 initial basis functions. In the last numerical example the SPE 10 bottom layer [12] is adapted to a $210 \times 45$ fine-scale grid ($\alpha = 1$). The fine-scale CVs located at (15,10) and (192,43) are perforated by two wells with constant well pressures, that is, $p_w(15,10) = 0$ and $p_w(192,43) = 1$. Two initial coarse-spaces, spanned by 70 and 30 basis functions, respectively, are considered. The enriched coarse-spaces again yield considerably enhanced convergence rates (Fig. 11) for both initial configurations. However, the number of additional DoF needed to obtain convergence is considerably higher than in the previous numerical examples, which is due to the highly channelized structure of the underlying permeability field.
Figure 9: Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. Two initial configurations with 81 (a) and 9 (b) basis functions are considered. Coarse (blue) and dual coarse (green) grids are shown on top of the corresponding convergence maps. The locations of the first 50 additional DoF are marked with red dots.
Figure 10: Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) of the i-Ge-MSFV method, employing a pure a-priori enrichment approach. The test-case employs the same configuration used for the simulations shown in Fig. 9. The only difference is given by the fine-scale grid aspect ratio ($\alpha = 10$) used to emulate the effects of anisotropic permeability tensors.
Figure 11: Shown at the bottom are convergence rate maps (blue: slow convergence; red: fast convergence) for two coarse-spaces initially spanned by 70 (a) and 30 (b) basis functions. The corresponding coarse grids (blue), with respectively $14 \times 5$ and $10 \times 3$ CVs, are shown in the top figures. The red dots mark the locations of the first 50 DoF in the created a-priori lists.
Numerical Results

11.2 Adaptive enrichment and mixed approach

In this subsection, the performance of the i-Ge-MSFV method using purely adaptive and mixed (a-priori/adaptive) DoF detection strategies is investigated. The test-case configurations described in the previous section, (permeability fields, grids and well configurations) hold also here, unless mentioned differently. Furthermore, the coarse grids with higher resolution are used to construct the initial coarse-space (Fig. 8(a)- 10(a)) for the mixed approach. For all test-cases the parameters \( TOL_{rate} = 0.1 \) and \( TOL_1 = 10^{-8} \) are used in Algorithm 1 and a single adaptive enrichment step is performed. Further, if a-priori enrichment is considered, the same tentative DoF location lists created for the numerical example in the previous section are employed. For simulations with mixed a-priori/adaptive enrichment, a pre-enrichment degree (ratio between additional DoF and initial DoF number) between 0.25 and 0.6 is selected. Note that the convergence histories shown in the figures below refer to simulations performed after termination of the enrichment step.
11.2 Adaptive enrichment and mixed approach

The first test-case is based on the grids and permeability field shown in Fig. 8(a). The convergence history \( \epsilon_{rel} = \frac{||p^{(x)}_{MS} - p_F||_{\infty}}{||p_F||_{\infty}} \) obtained for two different choices of \( n_s \) (6 and 20) are given in Figs. 12(a) and 12(b), respectively. In both cases all enrichment strategies deliver greatly improved convergence rates compared to the standard i-MSFV method (pink lines) (not converging, if \( n_s = 6 \) is used) and match almost perfectly for \( n_s = 20 \). However, the number of additional DoF required for the pure adaptive strategy (green lines) is reduced by at least a factor of two compared to both the mixed (red lines) and the pure a-priori (blue lines) approaches. The increase of \( n_s \) has the effect of decreasing the number of adaptively detected additional DoF and at the same time, convergence rates are enhanced.

A similar behaviour is observed for the grids and permeability fields shown in Fig. 9(a), where convergence is obtained in 25 (Fig. 13(a)) and 15 iterations (Fig. 13(b)). Slower convergence rates are obtained for the coarse-space enriched by 60 a-priori computed basis functions (blue line), confirming the inappropriate utilization of the algorithm as a standalone approach. Compared to the previous example, a higher degree of coarse-space enrichment is

Figure 13: Convergence histories of i-MSFV (pink lines) and i-Ge-MSFV methods with \( n_s = 6 \) (a) and \( n_s = 20 \) (b). The employed permeability field and grids are shown in Fig. 9(a). Note that the prefix ”Px-Ay” employed in the legend stands for: ”x” DoF were selected a-priori and ”y” DoF were selected adaptively.
obtained for the adaptive and mixed strategy due to the highly-conductive channelized structures present in the permeability field considered. The convergence rates achieved by the two methods are very similar for both numbers of smoothing steps employed, whereas the total number of DoF is slightly higher for the mixed strategy with \( n_s = 20 \).

The importance of pre-enrichment by means of an a-priori strategy can be seen in Figs. 14(a) and 14(b), where the SPE 10 bottom layer test-case (Fig. 11(a)) was investigated. The number of DoF added adaptively in the pure adaptive approach is about 3 times larger than for the mixed approach using 30 a-priori detected DoF locations, independent of the choice of \( n_s \) (10, 20). The obtained convergence rates are similar, while the total number of DoF employed is higher for the pure adaptive strategy. A comparison with the standard i-MSFV method using \( n_s = 1000 \) shows that the i-Ge-MSFV method has greatly improved convergence rates and at the same time the required number of smoothing steps per iteration is reduced by factors of 100 and 50, depending on \( n_s \).

Based on the same test-case configuration (Fig. 11(a)) we investigated the influence of pre-enrichment degree and variation of \( n_s \) on the convergence behaviour. An increase of \( n_s \) (Fig. 15(a)) reduces the number of DoF placed adaptively, while convergence rates are similar for all configurations, with exception of the slightly slower converging P30-A29-iGeMSFV run (\( n_s = 6 \)). The influence of the pre-enrichment degree on the convergence rates is shown in Fig. 15(b). The convergence rates achieved by the mixed enrichment approach are similar to the one obtained for the pure adaptive approach (pink line), while the number of total DoF increases slightly with higher degree of pre-enrichment.
11.2 Adaptive enrichment and mixed approach

Figure 14: Convergence histories of i-MSFV and i-Ge-MSFV methods with $n_s = 6$ (a) and $n_s = 20$ (b). The employed permeability field and grids are shown in Fig. 11(a) (top figure).

Figure 15: a) Convergence histories of the i-Ge-MSFV method resulting from different choices of $n_s$ and numbers of a-priori selected DoF ("P") locations. In (b), $n_s = 20$ is fixed while the number of a-priori selected DoF varies between 15 and 75. The employed permeability field and grids are shown in Fig. 11(a) (top figure).
NUMERICAL RESULTS

All test-cases considered so far underline the robustness of the i-Ge-MSFV method with respect to the heterogeneity of the underlying permeability field. For pure adaptive and mixed a-priori/adaptive coarse-space enrichment, convergence is generally obtained after 15 to 20 iterations. The last two numerical examples are devoted to the investigation of the i-Ge-MSFV method robustness properties with respect to the variation of the mobility coefficient \( \Lambda \) induced by a time-dependent two-phase flow problem (quadratic relative permeabilities, equal viscosities) and change of well locations. To this end, an initial i-Ge-MSFV method configuration is computed based on given initial (saturations field) and boundary conditions (wells) and used for simulations with different initial and boundary conditions. It is important to remark that no additional enrichment step is performed after selection of an enriched coarse-space. We select the previously used ”P30-24-iGeMSFV” set-up (green line in Fig. 15(b)), obtained by performing adaptive enrichment based on the well configuration ”Conf.1” (resulting fine-scale pressure field: top figure in Fig. 16(a)) and on a the reservoir initially saturated by one phase. Figures 16(a) and 16(b) show the different pressure fields and saturation distribution considered. The latter stems from solutions of a full flow and transport problem after 100, 2000 and 5000 time-steps \( (t^n) \) of a simulation with wells dictating a pressure field as shown in the top figure of Fig. 16(a)). The results clearly demonstrate that the convergence properties of the i-Ge-MSFV method are almost unaffected by strong variations of the applied boundary conditions (Fig. 17(a)) and initial conditions (Fig. 17(b)).

It should be remarked that in a real application of the i-Ge-MSFV method one would use the i-Ge-MSFV solution from the previous time-step as an initial guess for the subsequent iterations, and thus, compared to the results presented above, reduce the number of iterations needed to converge to the reference fine-scale solution.
11.2 Adaptive enrichment and mixed approach

Figure 16: Fine-scale reference solution $p_f$ obtained for three different well configurations (a). configuration 1: $p_w(192, 43) = 1$, $p_w(15, 10) = 0$; configuration 2: $p_w(51, 10) = 1$, $p_w(203, 3) = 1$, $p_w(16, 36) = 0$, $p_w(96, 36) = 0$, $p_w(114, 42) = 0$; configuration 3: $p_w(16, 27) = 1$, $p_w(34, 16) = 1$, $p_w(201, 3) = 1$, $p_w(33, 39) = p_w(127, 33) = 0$. Figure (b) illustrates the saturation distribution (injected fluid) obtained after 100, 2000 and 5000 time steps ($t^n$) of a two-phase problem simulation (well configuration 1). The distributions are used as "initial" condition in the i-Ge-MSFV method convergence studies in Fig. 17(b).
Figure 17: Convergence histories of the i-Ge-MSFV method (P30-A24) for different well locations (a) and saturation fields (b). The corresponding pressure and saturation fields are shown in Fig. 16. Adaptive enrichment was performed based on well configuration 1.
11.3 3D problems

The extension of the i-Ge-MSFV method to 3D is straightforward and is only outlined here. In the three dimensional case the i-Ge-MSFV method requires the computation of 1D (edges) and 2D (faces) reduced problems in order to restrict the governing equation to each dual CV. Following the previous reasoning, additional DoF may be needed on faces, if channelized formations are present. The DoF detection algorithms can easily be generalized to the 3D case by taking into account the dual CV faces. As stated previously, the major drawback of the adaptive detection approach is that only one DoF is added after each iteration. For the following test-cases, a simple extension of Algorithm 1, which allows to detect and add multiple DoF, was used. Instead of selecting only the fine-scale CV location with the highest absolute residual, each edge and face present in the domain is considered a separate entity and one DoF is added for each of the first ”n” entities with the highest residuals. The performance of the i-Ge-MSFV method in 3D was tested for two permeability fields: a permeability field with $\mu_{ln(K)} = 0$ and $\sigma^2_{ln(K)} = 4$ (Fig. 18(a)), and the full SPE10 benchmark test-case (Fig. 18(b)). The smoother is based on a ILU(0) preconditioned Richardson iteration. A-priori enrichment was skipped, while each adaptive enrichment round involves the addition of $N_C/4$ additional DoF ($N_C$ is the dimension of the initial coarse space), if the strong reduction rate requirement is not achieved ($TOL_{rate} = 0.1$). For all configurations tested, the i-Ge-MSFV method converges within 5 to 25 iterations. The required number of additional DoF introduced is in general very moderate (Fig. 18(c)). As expected, a substantial increase of DoF is observed for the standard SPE10 case (Fig. 18(d), green line with circles) due to the almost impermeable layers in the third spatial dimension. More realistic grid aspect ratios reduce the number of added DoF, which tends to reach the limit of the isotropic version of the problem (red, dotted line).
Figure 18: Permeability fields: (a) $\mu_{\ln(K)} = 0$, $\sigma_{\ln(K)}^2 = 4$, (b) SPE10 benchmark. Fine-scale grids: (a) $88 \times 88 \times 88$, (b) $60 \times 220 \times 85$ coarse grid: (a) $8 \times 8 \times 8$, (b) $12 \times 20 \times 5$. The convergence history of the i-Ge-MSFV method with purely adaptive enrichment ($TOL_{rate} = 0.1$, $TOL_1 = 10^{-7}$) is shown for different aspect-ratios $\alpha$. 
12 The i-Ge-MSFV method for special grids

The classical MSFV method and the presented i-Ge-MSFV method were implemented and tested for structured coarse-scale and fine-scale grids. In general, the largest part of a reservoir can be described by structured grids and therefore both methods can be applied safely. Furthermore, structured grids are easier to handle and lead to computationally more efficient solvers than their unstructured counterparts. However, the presence of faults and/or inactive cells in a reservoir model may force the introduction of unstructured coarse grids. In the following it is shown how the i-Ge-MSFV method can be used to circumvent these problems and that the convergence rate of the method is hardly affected by the introduced modifications.

12.1 Non-conforming coarse grids

12.1.1 Problem statement and i-Ge-MSFV approach

It should be remarked that the focus of the discussion is on the coarse grids and hence, the fine-scale discretization for non-conforming grids is not discussed here. The main problem of the classical MSFV method applied to a faulted reservoir is depicted in Fig. 19 for the most simple case of a single vertical fault in 2D. The MSFV grids on both sides of the fault are structured (Fig.19(b)). However, problems arise at the fault interface, where the left and right coarse grids do not match. Intuitively, a proper MSFV dual-grid can be created by finding connections between left and right dual CV boundaries as shown in Fig. 20(a). This approach, which leads to unstructured dual-grids [52], is straightforward to apply to the simple case shown here, but will become much more complex (and cumbersome to implement) for multiple oblique faults in 3D. In [27] a different approach consisting in the creation of an extended dual CV for the fault region was proposed. The resulting dual CV is shown in Fig. 20(b). The major drawback of this approach is related to the size of the dual CVs, which must be introduced for large faults. In such cases, the computation of basis and correction functions
will be expensive and negatively impact the overall efficiency of the method.

So far, the placement of additional DoF on dual CV boundaries was considered only in the context of coarse-space enrichment. However, the placement of additional DoF can be used to allow for a more flexible creation of dual grids. The application of this idea to non-conforming coarse grids results in a simple strategy for the creation of structured dual CVs suited for the i-Ge-MSFV method. The strategy can be summarized as:

1. Delete non-conforming dual CV boundaries in the fault interaction region.
2. Connect the dual CVs at the boundaries of the interaction region with new boundaries.
3. Introduce additional DoF at the intersection dual CV boundaries.

Hereby, since no constraints are set on the shape of the new dual CV boundaries, one can choose them to be simple straight lines (or planes in 3D). Hence, structured grids can be obtained and the size of dual CVs can be controlled by the spacing between the lines. A possible dual CV topology resulting from this strategy is shown in Fig. 21.
12.1 Non-conforming coarse grids

Figure 19: MSFV grids for faulted reservoirs: classical structured MSFV coarse grid a) and non-conforming structured MSFV coarse grid (b). The fine-scale CVs which compose the dual CV boundaries are coloured in red, while green fine-scale CVs represent locations of coarse-scale DoF.

Figure 20: MSFV grids for faulted reservoirs: "unstructured" MSFV coarse grid (a) and extended dual CV for the fault region.
Figure 21: i-GeV-MSFV grids for faulted reservoirs: a) interaction region across fault and b) dual CVs for the i-GeV-MSFV method. The locations of additional coarse-scale DoF are shown in blue.
12.1 Non-conforming coarse grids

12.1.2 Numerical results

The first test-case is a 2D problem discretized on a $220 \times 60$ uniformly spaced fine-scale grid with $20 \times 12$ coarse CVs. Two wells are located in the CVs $(15, 10)$ and $(193, 43)$ with fixed pressure values $p_w(15, 10) = 0$ and $p_w(193, 43) = 1$. The permeability field used corresponds to the SPE10 bottom layer with the addition of a single fault (vertical dislocation equivalent to 41.8 fine-scale CVs), as shown in Fig. 22(a). Equally spaced new boundaries are introduced, resulting in four intersections and an equal number of additional DoF. Further, adaptive enrichment is performed, resulting in 79 new DoF. For each iteration, 10 smoothing steps are performed with an ILU(0) preconditioned Richardson scheme. The convergence history shown in Fig. 22(c) is nearly identical to the one from the non-faulted case considered in the previous section (cf. Fig. 14). The same behaviour can be seen for the full 3D SPE10 isotropic test-case with a single fault (horizontal dislocation equivalent to 23.2 fine-scale CVs) shown in Fig. 23(a). The grid size is identical to the one employed for the case depicted in Fig. 18(b). The introduction of planes connecting the dual CVs across the faults has no impact on the convergence of the i-Ge-MSFV method, which was used in combination with 50 ILU(0) smoothing steps and $10^4$ enrichment DoF.
Figure 22: Results for 2D faulted reservoir: base-10 logarithm of the permeability field (a), converged pressure solution (b) and convergence history for the i-Ge-MSFV method (c).
12.1 Non-conforming coarse grids

Figure 23: Results for 3D faulted reservoir: base-10 logarithm of the permeability field (a), converged pressure solution (b) and convergence history for the i-Ge-MSFV method (c).
12.2 Inactive cells

Reservoir models often contain a large amount of cells with almost vanishing porosity values. The solution of the flow problem becomes irrelevant for such regions, since fluids will not be able to flow through them. A widely used approach to save memory and computational power, is to define cells with very low permeability as inactive cells. However, this approach easily results in very intricate distributions of active and inactive cells throughout the domain. The consequence for the MSFV method is that classical straight dual CV boundaries will eventually lead to a breakdown of the algorithm even for simple Cartesian grids. The situation depicted in Fig. 24, exposes the main problem: inactive cells (black) cutting the dual boundaries can lead to boundary segments disconnected from the coarse-scale DoF (green). As a consequence, the solution of the reduced problem in the disconnected regions is unique only up to a constant, which results in an ill-posed problem for the computation of basis and correction functions.

The i-Ge-MSFV method offers a simple remedy to the problem. By introducing additional coarse-scale DoF on disconnected boundary segments as shown in Fig. 24, a uniquely defined solution within each segment is obtained. Furthermore, given an algebraic formulation of the method as described in a later part of the thesis, it is possible to detect and fix the disconnected boundaries in an automated way. The robustness of this approach is demonstrated for a mildly heterogeneous permeability field with the addition of
some inactive cells creating barriers in the domain. The obtained configuration of additional DoF and standard coarse DoF is shown in Fig. 25(a) together with the inactive cells. Note that the locations of some standard coarse DoF have been moved (automatically) due to the presence of inactive cells at their natural position, i.e., the intersection of dual boundaries. The convergence history (Fig. 25(c)) demonstrates that inactive cells can be successfully treated by the i-Ge-MSFV method without modifying the dual grids.
Figure 25: Test-case with inactive cells: a) distribution of inactive cells (black), standard coarse-scale DoF (green) and additional coarse-scale DoF (blue) on the dual CV boundary (red). In (b) the converged i-Ge-MSFV pressure solution is depicted. The convergence history for the i-Ge-MSFV method is shown in (c).
13 Conclusion

In this part of the thesis, the i-Ge-MSFV method was introduced. The method relies on a coarse-space spanned by partition of unity functions and on a mixed Galerkin/ Petrov-Galerkin coarse-scale coupling. By neglecting enrichment functions, the i-Ge-MSFV method becomes identical to the standard MSFV/ i-MSFV method. The i-Ge-MSFV method ensures mass conservative coarse-scale solutions after each iteration via the Petrov-Galerkin constraints, whereas the enrichment functions are responsible for including important fine-scale features in the coarse-scale operator. The location of new DoF can either be determined a-priori or adaptively during the (first) iteration procedure. While the former requires less computational effort, the latter leads to better convergence rates and lower dimensional coarse-spaces. The combination of the two approaches leads to the best results in terms of computational efficiency and achieved convergence rates.

Even for the most challenging test-cases considered, a dramatic improvement of the convergence rates of the i-Ge-MSFV method over the standard i-MSFV method convergence rates was observed. Furthermore, a reduction of the number of smoothing steps per MSFV iteration was achieved. The robustness of the method with respect to the heterogeneity of the underlying permeability fields, changes of boundary (wells) and initial conditions (saturation fields) was demonstrated. Clearly, extreme scenarios will require a substantial enrichment of the initial coarse-space and therefore, the computational cost of solving the coarse-scale system will not be negligible. The problem can partially be attenuated by combining coarsening and enrichment strategies.

In addition, the i-Ge-MSFV method was shown to be capable of handling some grid related problems (i.e. non-conformal grids and inactive cells) in a systematic way. The proposed approaches avoid the introduction of unstructured coarse grids and do not affect the convergence rate of the method. In particular, given the same coarse-scale grid, the proposed treatment of inac-
tive cells allows to solve problems for which the classical MSFV algorithm would fail.
Part IV
Zonal MSFV framework
This part of the thesis is adapted from the paper "Zonal Multiscale Finite-Volume Framework" by Cortinovis and Jenny (submitted to JCP), that is, text, figures and equations in § 14-18 are identical with the paper.
In this section, the zonal MSFV (zMSFV) framework is introduced as a generalization of some of the aforementioned MSFV method extensions. In particular, the treatment of wells [38], fractures [30] and the coarse-space enrichment strategies described in the previous part rely on the same concept: special basis functions with support in a subdomain are introduced in order to model the effect of interest (wells, fractures) or to be able to include missing fine-scale features in the coarse-scale problem (enrichment). The zMSFV framework generalizes the concept by introducing the notion of zones and zonal basis functions, giving the possibility to split the domain into subregions of arbitrary size and shape requiring a particular numerical approach, which might differ from the rest of the domain. The ultimate aim is to be able to include different models (e.g. pore networks) directly in the MSFV method. Here, however, besides introducing the zMSFV framework formulation, the flexibility of the zMSFV methodology is demonstrated by applying a specialized version of it to the iterative solution of high-contrast problems. To this end, an algebraic formulation of the method is used to derive zMSFV based preconditioners, similar to previously introduced algebraic MSFV versions [50, 69, 51]. Unlike classical MSFV preconditioners, the zMSFV preconditioner can provide permeability-contrast independent convergence rates by including missing fine-scale dependencies in the coarse-scale problem.
15 Framework description

15.1 Zonal MSFV approximation

Let \( \{ \Omega^A, \Omega^B_1, ..., \Omega^B_{N_B} \} \) be a decomposition of \( \Omega \subset \mathbb{R}^d \), \( d = 2 \) or \( 3 \), into \( N_B + 1 \) non-overlapping subdomains. The zMSFV framework is illustrated based on the numerical solution of

\[
L^A(p) = q \quad \text{in } \Omega^A \tag{71}
\]

\[
L^B_i(p) = q \quad \text{in } \Omega^B_i \tag{72}
\]

subject to some boundary conditions on \( \partial \Omega \) and interface conditions on the interfaces \( \partial \Omega^B_i \cap \partial \Omega^A_i \) (\( i \in \{1, ..., N_B\} \)) and \( \partial \Omega^B_i \cap \partial \Omega^B_j \) (\( i \neq j \wedge i, j \in \{1, ..., N_B\} \)) where \( L^A \) and \( L^B_i \) are second-order linear elliptic operators and \( q(x) \) is a rhs term.

In the following discussion it is assumed that the solution in \( \Omega^B_i \) ("zone" from here on), or an approximation of it, is given by a superposition of known zonal basis functions \( \hat{\Psi}_{i,j} (i \in \{1, ..., N_B\} \wedge j \in \{1, ..., M_i\}) \) with compact support, i.e. \( \text{supp}(\hat{\Psi}_{i,j}) \subset \Omega^B_i \), \( \forall j \in \{1, ..., M_i\} \), where \( M_i \) denotes the number of zonal basis functions defined in \( \Omega^B_i \). The zMSFV method approximation \( p_{zms} \) to the solution of Eqs. (71) and (72) reads

\[
p_{zms}(x) = \sum_{i=1}^{N_V} a_i \Phi_i(x) + \sum_{i=1}^{N_B} \sum_{j=1}^{M_i} b_{i,j} \Psi_{i,j}(x) + \tilde{\Phi}(x), \quad \forall x \in \Omega, \tag{73}
\]

where the coefficients \( a_i \) (\( i \in \{1, ..., N_V\} \)) and \( b_{i,j} \) (\( i \in \{1, ..., N_B\} \wedge j \in \{1, ..., M_i\} \)) represent coarse-scale unknowns, \( \Phi_i (i \in \{1, ..., N_V\}) \), basis functions, \( \Psi_{i,j} (i \in \{1, ..., N_B\} \wedge j \in \{1, ..., M_i\}) \) extended zonal basis functions and \( \tilde{\Phi} \) is a correction function. Thus, the zMSFV coarse-space is spanned by basis and extended zonal basis functions. Note that \( \hat{\Psi}_{i,j} \neq \Psi_{i,j} \) and that \( N_V \) is a grid dependent number, as explained later in detail. The construction...
of basis and extended zonal basis functions and the derivation of the coarse-scale system employed to determine the coefficients in Eq. (73) are described in the following subsection.

15.2 Basis and extended zonal basis functions

Let $\Omega^P_i (i \in \{1, \ldots, N_P\})$ be the primary coarse-scale partition of $\Omega$ into $N_P$ CVs, $\Omega^D_i (i \in \{1, \ldots, N_D\})$ the dual coarse-scale partition of $\Omega^A$ into $N_D$ dual CVs and $x^V_i (i \in \{1, \ldots, N_V\})$ the $N_V$ vertices of the dual CVs. Further, $\Gamma_{i,j} = \partial \Omega^D_i \cap \partial \Omega^D_j$ denotes the common face of two adjacent dual coarse CVs and $\mathcal{S} = \cup_{i,j} \mathcal{S}_{\Gamma_{i,j}}$, the skeleton of the dual grid. Note that the primary coarse CVs partition the entire domain $\Omega$, while all other CVs constitute partitions of $\Omega^A$. In order to facilitate the explanation of the method it is assumed that $N_P = N_V + N_B$ primary coarse CVs are introduced such that each $\Omega^B_i$ is a primary CV, while the remaining $N_V$ CVs constitute a suitable (for MSFV) decomposition of $\Omega^A$ with $x^V_i$ as the CV centres. Conceptually, the described partitions can be obtained by creating classical MSFV partitions, defining zones in a second step and finally modifying the initial partitions, i.e. merging primary coarse CVs (if required) and deleting portions of the dual CVs intersected by a zone. Note that the primary coarse-scale partition is only required to enforce coarse-scale conservative solutions and does not influence the computation of $\Phi_i$ and $\Psi_{i,j}$.

Basis functions are computed numerically and satisfy

\[
L^A(\Phi_i) = 0 \quad \text{in } \Omega^A \setminus \mathcal{S} \tag{74}
\]
\[
\mathcal{R}(\Phi_i) = 0 \quad \text{on } \mathcal{S} \tag{75}
\]
\[
\Phi_i(x^V_j) = \delta_{ij} \quad \forall j \in \{1, \ldots, N_V\} \tag{76}
\]
\[
\Phi_i = 0 \quad \text{in } \Omega \setminus \Omega^A, \tag{77}
\]

$\forall i \in \{1, \ldots, N_V\}$, subject to interface conditions on $\partial \Omega^A \cap \partial \Omega^B_l$, $\forall l \in \{1, \ldots, N_B\}$, where $\delta_{ij}$ is the Kronecker delta and $\mathcal{R}(\Phi)$ abstractly denotes the reduced problem to be solved on $\mathcal{S}$ (cf. Eq. (20)). Equations. (77) and (76), besides defining $\Phi_i$ locally, act as boundary condition for the reduced problem on $\mathcal{S}$. 
Figure 26: a) Classical MSFV method grids: skeleton $\mathcal{S}$ of the dual-grid (red dashed lines) and primary grid (solid black lines). A primary coarse CV and a dual coarse CV are highlighted in red and green, respectively. b) Two zones (blue regions) are introduced together with the zonal DoF (dots). In addition, a DoF associated to the dual grid vertices $x_i^V$ is shown. The maximum possible support of the extended zonal functions associated to $\Omega_1^B$ is represented by the light blue region.
The correction function is a solution of
\[ L^A(\tilde{\Phi}) = q \quad \text{in } \Omega^A \backslash S \] (78)
\[ R(\tilde{\Phi}) = R(q) \quad \text{on } S \] (79)
\[ \tilde{\Phi}(x^j_V) = 0 \quad \forall j \in \{1, \ldots, N_V\} \] (80)
\[ \tilde{\Phi} = 0 \quad \text{in } \Omega \backslash \Omega^A. \] (81)

It can be regarded as a particular solution of the problem solved in \( \Omega^A \) as it is the case for the classical MSFV method [49]. The extended zonal basis functions are solutions of
\[ L^A(\Psi_{i,j}) = 0 \quad \text{in } \Omega^A \backslash S \] (82)
\[ R(\Psi_{i,j}) = 0 \quad \text{on } S \] (83)
\[ \Psi_{i,j}(x^j_V) = 0 \quad \forall j \in \{1, \ldots, N_V\} \] (84)
\[ \Psi_{i,j} = \hat{\Psi}_{i,j} \quad \text{in } \Omega^B \subseteq \{1, \ldots, N_B\}, \] (85)
\[ \forall i \in \{1, \ldots, N_V\} \text{ and } \forall j \in \{1, \ldots, M_i\}, \text{ subject to interface conditions on each interface } \partial \Omega^A \cap \partial \Omega^B, \forall l \in \{1, \ldots, N_B\} \text{ and } \partial \Omega^B \cap \partial \Omega^B, \forall l, k \in \{1, \ldots, N_B\} \land l \neq k. \] Provided that the zonal basis function \( \hat{\Psi}_{i,j} \) form a partition of unity within all \( \Omega^B_i \), the interface conditions, which govern the coupling between adjacent subdomains, can be chosen such that
\[ \sum_{i=1}^{N_V} \Phi_i(x) + \sum_{i=1}^{N_B} \sum_{j=1}^{M_i} \Psi_{i,j}(x) = 1, \quad \forall x \in \Omega. \] (86)

15.3 Coarse-scale system

The unknown coefficients in Eq. (73) are determined by solving the coarse-scale system
\[ \int_{\Omega^A} \Theta_k \left( L^A(p_{zms}) - q \right) dV \]
\[ + \sum_{l=1}^{N_B} \int_{\Omega^B_l} \Theta_k \left( L^B_l(p_{zms}) - q \right) dV = 0, \quad \forall k \in \{1, \ldots, N_C\}, \] (87)
where \( N_C = N_V + \sum_{i=1}^{N_B} M_i \) is the total number of coarse-scale unknowns and \( \Theta_k \ (k \in \{1, \ldots, N_C\}) \) are test functions. Two obvious options are available for the selection of the test functions. The first one is
\[ \Theta_k = \begin{cases} \Phi_k & \text{if } k \leq N_V \\ \Psi \in \{\Psi_{i,j}\}_{i=1,j=1}^{N_B,M_i} \backslash \{\Theta_l\}_{l=1}^{k-1} & \text{if } k > N_V \end{cases}, \] (88)
which leads to a Galerkin method. If conservative coarse-scale solutions are required, a different selection of test functions must be used. By choosing \( \Theta_k = \mathcal{H}_k, \forall k \in \{1, \ldots, N_P\} \), where

\[
\mathcal{H}_k^P(x) = \begin{cases} 
1 & \text{if } x \in \Omega_k^P \\
0 & \text{otherwise}
\end{cases},
\]

one obtains \( N_P \) coarse-scale constraints guaranteeing conservative coarse-scale solutions. Additional test functions may be required in order to close the coarse-scale system, if multiple zonal basis functions are used in some \( \Omega_i^B \). In this case, \( N_C - N_P \) extended zonal functions \( \Psi_{i,j} \) are selected to obtain

\[
\Theta_k = \left\{ \begin{array}{ll}
\mathcal{H}_k^P & \text{if } k \leq N_P \\
\Psi \in \{\Psi_{i,j}\}_{i=1,j=1}^{N_B,M} \setminus \{\Theta_l\}_{l=1}^{k-1} & \text{if } k > N_P
\end{array} \right.,
\]

which results in a Galerkin / Petrov-Galerkin method formulation of the coarse-scale problem and ensures conservative coarse-scale solutions, provided that a conservative fine-scale discretization of Eqs. (74)-(77) and (82)-(85) is adopted. Conservative fine-scale solutions can then be constructed in a similar fashion as described for the classical MSFV method (cf. §7.3).

### 15.4 Remarks

The zMSFV framework can be seen as a generalization of the previously introduced MSFV method and related works. In particular, with an appropriate selection of the operators in Eqs. (71) and (72) and corresponding interface conditions, one recovers the formulation employed to include complex wells [38] and, by additionally defining zones to be lower dimensional manifolds, fractures [30]. Also, the Ge-MSFV method [13] can be recovered by restricting the zone-extent to single CVs located on the skeleton \( \mathcal{S} \). The zMSFV framework additionally offers a framework for coupling models (e.g. pore network simulators) to the MSFV method and introduces an additional level of adaptivity to the MSFV method. In particular, zones can be introduced without any restrictions on size or geometry in the entire computational domain. Thus, the zonal formulation can also be interpreted as a framework for MSFV grid refinement. For example, zones containing a MSFV dual-grid a fine-scale grid resolution which differs from the one in the surrounding dual CVs can be introduced at any location in the domain. Furthermore, it is not required the dual CVs match at the zone interface, since the extension (82)-(85) of the zonal functions to the surrounding dual CVs does not dependent on the underlying grid. This can be advantageous for reservoir models, in which large portions of the computational domain can
be described by structured grids, except for small regions (e.g. around faults or wells) which may require a different type of grid and/or discretization.

In the following, the main features of the zMSFV framework are exploited to derive robust zMSFV preconditioners aiming at counteracting the deterioration of the convergence rate experienced by MSFV method based iterative schemes in the presence of high-contrast permeability fields.
16 Zonal MSFV method for high-contrast problems

In this section, the solution of the elliptic problem

$$\nabla \cdot (\Lambda \cdot \nabla p) = q \quad \text{in } \Omega$$  \hspace{1cm} (91)

with a zMSFV method based iterative scheme is considered. Similar to previous sections, $\Lambda$ is assumed to exhibit complex long-range coherent structures combined with a strong variation of the coefficients over a very short distance (e.g. highly conductive channels, shales, fractures). In the remainder of this section the application of the zMSFV methodology to the iterative solution of high contrast problems is presented. The method will be recast in an algebraic form in order to derive a zMSFV method based preconditioner.

16.1 Specification of zones and related zonal functions

In order to apply the zMSFV method, the subdomains $\Omega_i^B$, the associated zonal basis functions $\hat{\Psi}_{i,j}$ and the interface conditions must be specified. The specification of interface conditions is not required for the present case, since the same equation is considered in $\Omega$ and hence, also on the boundaries of the different zones. The selection of zones will mainly be dictated by the permeability field $K$ instead of being related to different types of operators, as it was the case for the more abstract general formulation (72) in the previous section. Furthermore, Eq. (91) is discretized on a fine-scale grid composed of fine-scale CVs $\Omega_i^F$ ($i \in \{1, ..., N_F\}$) covering the entire domain $\Omega$ and each $\Omega_i^B$ is an agglomeration of some $\Omega_i^F$. A simple algorithm for the selection of the zones is introduced later.

The solution space within each zone is spanned by the zonal basis functions $\hat{\Psi}_{i,j}$. Theoretically, the choice of $\hat{\Psi}_{i,j}$ is free (e.g. piecewise constant functions). Here, the zonal basis function are computed numerically by solving Eq. (91) in each zone with $q = 0$, similar to the equations solved for the basis
functions (74)-(77) and extended zonal basis function (82)-(85), such that the oscillatory behaviour of the underlying permeability field is honoured. For this purpose, a boundary is defined in each zone (Fig. 27(b)) and zonal coarse-scale DoF associated to the $\tilde{\Psi}_{i,j}$ are placed on it. However, the placement of coarse DoF is not restricted by any means to the zonal boundary itself and all CVs within a zone can be defined as coarse-scale DoF location. Furthermore, some zones may only contain a few $\Omega^F_i$, such that a distinction between the boundary and the interior of a zone becomes somewhat obsolete (see Fig. 27(b)). As a convention, all $\Omega^F_i$ forming such a zone are defined as zonal boundary CVs.

Note also, that the support of the correction functions presented in the previous section is confined to $\Omega^A$. Here, the correction function computations can be extended to the zones as well, since the same problem and the same underlying discretization is considered in the entire domain $\Omega$. This extension naturally arises in the algebraic formulation described next.

16.2 Algebraic formulation and zonal MSFV preconditioner

The algebraic formulation of the zMSFV method shares many similarities with previously introduced algebraic MSFV formulations [50, 69]. However, the correct treatment of zones in the algebraic context requires a substantial modification of the classical formulation. For simplicity, a similar notation as in [50] is used whenever possible and, without loss of generality, the formulation is restricted to a 2D Cartesian fine-scale grids with a 5-point discretization stencil.

Consider the linear system arising from a finite-volume discretization of Eq. (91), i.e.

$$Ap = q,$$  \hspace{1cm} (92)

where $A \in \mathbb{R}^{N_F \times N_F}$ is the coefficient matrix, $p \in \mathbb{R}^{N_F}$ the vector of unknowns, $q \in \mathbb{R}^{N_F}$ the corresponding rhs vector and $N_F$ is the total number of unknowns.

The dual and the zonal partitions of the zMSFV method subdivide the fine-scale unknowns into the categories dual-interior (i), dual-edge (e), dual-vertex (v), zonal-interior (I), zonal-edge (E) and zonal-vertex (V). Figure 27(b) shows a colouring of associated fine-scale CVs. For the reordering, the permutation matrix $P \in \mathbb{R}^{N_F \times N_F}$ is introduced, such that the permuted
Figure 27: a) Classical MSFV method partitioning with coloured CVs: black squares represent dual CV vertices, red squares dual CV edges and white squares are dual CV interior CVs. b) zMSFV partitioning with 5 zones, where the largest two are adjacent to each other. Zonal-boundary CVs are shown in blue, zonal-interior CVs in yellow and zonal-vertex CVs in green.
16.2 Algebraic formulation and zonal MSFV preconditioner

The fine-scale system can be written as

\[
\begin{bmatrix}
\tilde{A}_{ii} & \tilde{A}_{ie} & 0 & \tilde{A}_{IE} & \tilde{A}_{IV} & 0 \\
\tilde{A}_{ei} & \tilde{A}_{ee} & 0 & \tilde{A}_{eE} & \tilde{A}_{eV} & \tilde{A}_{ev} \\
0 & 0 & \tilde{A}_{ii} & \tilde{A}_{IE} & \tilde{A}_{IV} & 0 \\
\tilde{A}_{Ei} & \tilde{A}_{Ee} & \tilde{A}_{EI} & \tilde{A}_{EE} & \tilde{A}_{EV} & \tilde{A}_{Ev} \\
\tilde{A}_{Vi} & \tilde{A}_{Ve} & \tilde{A}_{VI} & \tilde{A}_{V} & \tilde{A}_{VV} & \tilde{A}_{Vv} \\
0 & 0 & \tilde{A}_{ve} & 0 & \tilde{A}_{vE} & \tilde{A}_{vV} & \tilde{A}_{vv}
\end{bmatrix}
\begin{bmatrix}
\tilde{p}_i \\
\tilde{p}_e \\
\tilde{p}_I \\
\tilde{p}_E \\
\tilde{p}_V \\
\tilde{p}_v
\end{bmatrix}
= 
\begin{bmatrix}
\tilde{q}_i \\
\tilde{q}_e \\
\tilde{q}_I \\
\tilde{q}_E \\
\tilde{q}_V \\
\tilde{q}_v
\end{bmatrix}.
\] (93)

Each submatrix \( \tilde{A}_{kl} \in \mathbb{R}^{N_k \times N_l} \) accounts for the contribution of the \( N_l \) unknowns of category \( l \in \{i,e,v,I,E,V\} \) to the equations related to the \( N_k \) unknowns of category \( k \in \{i,e,v,I,E,V\} \). Note that some blocks disappear due to the assumed 5 point-stencil discretization. Further, it is assumed that the permutation matrix \( P \) reorders the unknowns CV-wise (for both dual and zonal CVs) within each category and that CVs, edges and vertices are in lexicographic order. Under these assumptions, \( \tilde{A}_{ii}, \tilde{A}_{ee} \) and \( \tilde{A}_{II} \) are block diagonal matrices, while \( \tilde{A}_{EE} \) is block diagonal only if all zones are non-adjacent. The zMSFV method approximates \( p = A^{-1}q \) by solving

\[
M y = r,
\] (94)

where \( M \in \mathbb{R}^{N_F \times N_F} \) is the zMSFV method system matrix, \( r \) the corresponding rhs and \( y \) the zMSFV method solution (from now dimensions are only denoted if they are not already easily deducible from the context). The matrix \( M \), is obtained by modifying \( \tilde{A} \) and reads

\[
M = \begin{bmatrix}
\tilde{A}_{ii} & \tilde{A}_{ie} & 0 & \tilde{A}_{IE} & \tilde{A}_{IV} \\
0 & M_{ee} & 0 & \tilde{A}_{eE} & \tilde{A}_{eV} \\
0 & 0 & \tilde{A}_{ii} & \tilde{A}_{IE} & \tilde{A}_{IV} \\
0 & 0 & 0 & M_{EE} & M_{Ev} \\
0 & 0 & 0 & 0 & M_{cc}
\end{bmatrix},
\] (95)

where a block denoted by \( M_{ij} \) represents a modified submatrix \( \tilde{A}_{ij} \). Moreover, the categories "v" and "V" are now merged into the new category coarse-scale unknowns ("c"), which results in lumping together the last two rows and columns of \( \tilde{A} \) (e.g. \( \tilde{A}_{sc} = \begin{bmatrix} \tilde{A}_{eV} & \tilde{A}_{ev} \end{bmatrix} \)), prior to applying the modifications described in the following. The representation of the reduced problem operator ((75),(83)) in the algebraic context is obtained by discarding the influence of dual-interior unknowns on the solution of the reduced
problems [50], i.e. \( M_{ei} = 0 \) in (95), and by defining
\[
M_{ee} = \tilde{A}_{ee} + \text{diag} \left( \tilde{A}_{ei} \mathbf{1} \right),
\]
where all elements of the vector \( \mathbf{1} \) are equal to 1 and the operator \( \text{diag}(v) \) transforms the vector \( v \) in a diagonal matrix. Similarly, the reduced problem operator for zones is obtained with the selection of \( M_{Ei} = 0, M_{Ec} = 0 \), \( M_{EI} = 0 \), \( M_{Ec} = [M_{EV} \ 0] \) and
\[
M_{EE} = D_{EE} + \text{diag} \left( \left[ R_{E} \tilde{A} - M_{EV} R_{V} - D_{EE} R_{E} \right] \mathbf{1} \right),
\]
where \( R_{E} \in \mathbb{R}^{N_{E} \times N_{F}} \) and \( R_{V} \in \mathbb{R}^{N_{V} \times N_{F}} \) are the restriction operators onto the zonal-boundary and zonal-vertex unknowns, respectively (e.g. \( R_{E}\tilde{p} = \tilde{p}_{E}, R_{V}\tilde{p} = \tilde{p}_{V} \)). The block diagonal matrix \( D_{EE} \) can be written as
\[
D_{EE} = \bigoplus_{l=1}^{N_{B}} \left( R_{E_{l}} \tilde{A} R_{E_{l}}^{\top} \right),
\]
where \( R_{E_{l}} \) is the restriction operator onto zonal-edge unknowns associated to the zone \( \Omega_{B}^{l} \) and \( \bigoplus \) denotes the matrix direct sum. The matrix
\[
M_{EV} = R_{E} \left( \sum_{j=1}^{N_{B}} R_{E_{j}}^{\top} R_{E_{j}} \tilde{A} R_{V_{j}}^{\top} R_{V_{j}} \right) R_{V}^{\top},
\]
accounts for the influence of zonal-vertex unknowns on zonal-edge equations, where \( R_{V_{j}} \) is the restriction operator onto zonal-vertex unknowns associated to zone \( \Omega_{B}^{j} \). Note that in the absence of adjacent zones, \( D_{EE} = \tilde{A}_{EE} \) and \( M_{EV} = \tilde{A}_{EV} \). In addition, it should be remarked that the definition of \( M_{EE} \) also holds in a zone composed of only boundary CVs (following the previously introduced convention), for which \( M_{EE} \) represents a local problem with homogeneous Neumann boundary conditions.

The coarse-scale unknowns are determined by solving the coarse-scale problem (87) and hence, only one submatrix appears in the last row of \( M \), that is, the coarse-scale operator \( M_{cc} \) of the zMSFV method. Before specifying \( M_{cc} \), the solution of the upper triangular zMSFV system (94) (which can be obtained by a simple back-substitution) is expressed as
\[
y = M^{-1} r = \left( B M_{cc}^{-1} R_{c} + C \right) r
\]
where \( R_{c} \in \mathbb{R}^{N_{C} \times N_{F}} \) is the restriction operator onto the coarse-scale unknowns, i.e. \( R_{c} = [0 \ I_{cc}] \), and \( I_{cc} \in \mathbb{R}^{N_{C} \times N_{C}} \) is an identity matrix.
The prolongation operator \( B \in \mathbb{R}^{N_F \times N_C} \) prolongs the coarse-scale solution \( y_c = M_{cc}^{-1} r_c = M_{cc}^{-1} r_e \) to the fine-scale and contains extended zonal functions and basis functions, i.e. \( B = [\Psi_1, \ldots, \Psi_{N_B}, M_{NB}, \Phi_1, \ldots, \Phi_{N_V}] \), which is algebraically expressed as

\[
B = \begin{bmatrix}
-\tilde{A}_{ii}^{-1} \left( \tilde{A}_{ic} - \tilde{A}_{iIE} \tilde{M}_{EE}^{-1} \tilde{M}_{Ec} \right)
- M_{ee}^{-1} \left( \tilde{A}_{ec} - \tilde{A}_{eE} \tilde{M}_{EE}^{-1} \tilde{M}_{Ec} \right)
- \tilde{A}_{II}^{-1} \left( \tilde{A}_{Ic} - \tilde{A}_{IE} \tilde{M}_{EE}^{-1} \tilde{M}_{Ec} \right)
- M_{EE}^{-1} \tilde{M}_{Ec} \\
\end{bmatrix}.
\]

The matrix \( C \in \mathbb{R}^{N_F \times N_F} \) is given by

\[
C = \begin{bmatrix}
\tilde{A}_{ii}^{-1} & -\tilde{A}_{ii}^{-1} \tilde{A}_{ie} M_{ee}^{-1} & 0 & -\tilde{A}_{ii}^{-1} \left( \tilde{A}_{IE} - \tilde{A}_{iIE} \tilde{M}_{EE}^{-1} \tilde{M}_{Ec} \right) M_{EE}^{-1} & 0 \\
0 & M_{ee}^{-1} & 0 & - M_{ee}^{-1} \tilde{A}_{eE} M_{EE}^{-1} & 0 \\
0 & 0 & \tilde{A}_{II}^{-1} & - \tilde{A}_{II}^{-1} \tilde{A}_{IE} M_{EE}^{-1} & 0 \\
0 & 0 & 0 & M_{EE}^{-1} & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

and the term \( Cr \) in Eq. (100) is the algebraic representation of the correction function, which is now also defined within the zones. Equation (100) has exactly the same form as derived in [50] for the standard MSFV method and following the same ideas, it can be shown that the coarse-scale operator is given by

\[
M_{cc} = X \tilde{A} B,
\]

where the coarse-scale restriction operator \( X \in \mathbb{R}^{N_C \times N_F} \) is the algebraic analogon of the weighted integration performed in Eq. (87). The coarse-scale rhs \( r_c \) reads

\[
r_c = X \left( I - \tilde{A} C \right) \tilde{q}.
\]

In order to write the last equation it was implicitly assumed that

\[
r = [\tilde{q}, \tilde{q}_e, \tilde{q}_l, \tilde{q}_E r_e]^T,
\]

which is equivalent to neglecting the reduced problem modification (79) of the rhs in the computation of the correction function. The assumption only affects the zMSFV method solution, if gravity or capillary pressure is considered, in which case \( r_e \neq \tilde{q}_e \) and \( r_E \neq \tilde{q}_E \). Furthermore, the assumption has
no effect on the convergence behaviour of MSFV/zMSFV method based iterative schemes, since the modification only affects the rhs. The coarse-scale restriction operator $X$ can be specified as

$$X = B^T$$  \hspace{1cm} (106)

for the pure Galerkin type coarse-scale coupling introduced in Eq. (88) or as

$$X = \begin{bmatrix} H \\ \hat{B}^T \end{bmatrix}$$  \hspace{1cm} (107)

for the Petrov-Galerkin coupling (90), where the rows of the matrix $H \in \mathbb{R}^{N_P \times N_P}$ are the discrete version of $\mathcal{H}_i^P$ defined in Eq. (89) and $\hat{B} \in \mathbb{R}^{N_F \times (N_C - N_P)}$ is a matrix composed of a selection from $N_C - N_P$ column vectors of $B$.

Inserting Eqs. (104) and (105) in Eq. (100) yields

$$y = M^{-1}_{zms} \tilde{q} = \left[ BM^{-1}_{cc} X \left( I - \tilde{A} C \right) + C \right] \tilde{q}$$  \hspace{1cm} (108)

after some manipulation, where the operator $M^{-1}_{zms}$ represents the zMSFV preconditioner. The classical MSFV preconditioner [51, 63] has exactly the same form as in Eq. (108), but relies on a different definition of the coarse-space, i.e. on a different prolongation matrix $B$. MSFV method based iterative schemes have initially been used in combination with local solvers (smoothers) aiming at improving the localization condition directly via the correction function [26]. Later they were also used in combination with Krylov subspace methods [51, 69, 63]. As discussed in [69] and [63], the correction function itself can be regarded as a local solver step aiming at reducing high frequency error components and thus can be replaced by other local solvers. In the following numerical studies the preconditioned Richardson iteration

$$y^{\nu+1} = y^{\nu} + M^{-1}_{zms} \left( \tilde{q} - \tilde{A} y^{\nu} \right)$$  

$$= y^{\nu} + \left[ BM^{-1}_{cc} X \left( I - \tilde{A} M^{-1}_{local} \right) + M^{-1}_{local} \right] \left( \tilde{q} - \tilde{A} y^{\nu} \right)$$  \hspace{1cm} (109)

is considered, where an incomplete LU decomposition with zero fill-in (ILU(0)) replaces the correction function $C$ as the local preconditioner $M^{-1}_{local}$.

Note that the iterative procedure in Eq. (109) can equivalently be expressed as a two-stage procedure [69] with the "local step"

$$y^{\nu+\frac{1}{2}} = y^{\nu} + M^{-1}_{local} \left( \tilde{q} - \tilde{A} y^{\nu} \right),$$  \hspace{1cm} (110)
followed by the "multiscale step"

$$y^{r+\frac{1}{2}} = y^{r+\frac{1}{2}} + BM_{cc}^{-1} X \left( \tilde{q} - \tilde{A} y^{r+\frac{1}{2}} \right).$$  \hfill (111)

### 16.3 Selection of zones

In order to apply the algebraic formulation of the previous section, one has to define the permutation matrix $P$. Besides information about the underlying dual-grid, $P$ also contains information about the location of zones. It is straightforward to obtain the dual-grid in the case of structured fine-scale grids, while for the problems considered here the location of zones mainly depends on the local permeability values. If the locations of zones are not known a-priori, then an automatic selection of zones is required. Here, a simple algorithm guided by the diagonal elements $a_{ii}$ of the fine-scale system matrix $A$ is used. In particular, we mark all fine-scale unknowns, for which the corresponding diagonal element fulfils

$$\gamma_{\text{min}} < |a_{ii}| < \gamma_{\text{max}},$$  \hfill (112)

as zonal unknowns, where $\gamma_{\text{min}}$ and $\gamma_{\text{max}} > \gamma_{\text{min}}$ are user defined parameters. The selection of zones, i.e. the agglomeration of zonal unknowns into single zones, is then simply obtained by computing the connected components of the adjacency matrix $R_z A_0 R_z^T$, where $R_z \in \mathbb{R}^{N_z \times N_F}$ is the restriction operator onto the $N_z$ zonal unknowns, and $A_0 \in \mathbb{R}^{N_F \times N_F}$ is the adjacency matrix of the fine-scale grid, i.e. the matrix with the elements

$$a_{0,ij} = \begin{cases} 1 & \text{if } a_{ij} \neq 0, i \neq j \\ 0, & \text{otherwise} \end{cases}.$$  \hfill (113)

It should be remarked that the zone selection algorithm will not deliver optimal coarse-space sizes, since high-conductive and low-conductive regions completely embedded in dual CVs, so-called inclusions [22, 21], will eventually be defined as zones. However, inclusions do not negatively influence the convergence rate [21], since their effect is already included in the coarse-space via the standard basis functions. Thus, in order to obtain optimal coarse-space sizes, inclusions should be filtered out in the detection process. In the context of MSFE methods and related preconditioners [21], enriched coarse-spaces with optimal size are obtained using spectral information, i.e. by solving a set of generalized eigenvalue problems and by adding selected eigenvectors to the set of basis functions. An alternative is to select zones on
edges and faces (for 3D problems) of the dual CVs, similar to the procedure described for the GeMSFV method in § 10.4. Furthermore, by considering zones with only one single fine-scale CV, the i-GeMSFV method is recovered. In this part of the thesis, however, the focus is not on obtaining an optimal coarse-space size, and hence no filtering is applied to the zone selection algorithm.
17 Numerical results

In order to test the convergence properties of the method it is sufficient to consider the simple case of single-phase flow without gravity, which is equivalent to substituting $\Lambda$ in Eq. (91) with $K/\mu$ and considering a rhs with only well related source terms. From now on, constant viscosity ($\mu = 1$ [kg/ms]) is assumed. The convergence rates of the stationary preconditioned Richardson method and of the preconditioned generalized minimal residual method (GMRES) are investigated for the following three preconditioners:

- the MSFV method with Petrov-Galerkin (MSFV-PG) coarse-scale restriction,
- the MSFV method with Galerkin (MSFV-G) coarse-scale restriction, and
- the zMSFV method with Galerkin (zMSFV-G) coarse-scale restriction.

All preconditioners employ ILU(0) as local solver.

17.1 High-contrast media

The first test-case considered is the high-contrast permeability field shown in Fig. 28(a). The permeability takes values $K_{channels}$ within the channels and 1 otherwise. The pressure is fixed along the lower and upper boundary CVs and takes values of 1 and 2, respectively, while on the remaining boundaries no-flow boundary conditions are applied. The problem is discretized on an equidistant fine-scale grid with $100 \times 100$ CVs and $10 \times 10$ primary coarse CVs, resulting in $N_C = 100$ coarse-scale DoF for both MSFV-PG and MSFV-G preconditioners. For the zMSFV method 24 zones are introduced (one for each channel) and a zonal coarse-scale DoF is introduced after every 16th boundary CV, resulting in a coarse-space about twice as large as for the MSFV method ($N_C = 186$, of which $N_v = 89$ DoF are related to the dual CV vertices and $N_V = 97$ are zonal coarse-scale DoF). The zMSFV method grids
Figure 28: a) High-contrast permeability field with values $K_{\text{channels}}$ in the channels (red) and 1 otherwise. b) Dual coarse grid with zones for the zMSFV method.
17.1 High-contrast media

<table>
<thead>
<tr>
<th>$\log_{10}(K_{\text{channels}})$</th>
<th>MSFV-PG ($N_C = 100$)</th>
<th>MSFV-G ($N_C = 100$)</th>
<th>zMSFV-G ($N_C = 186$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-5</td>
<td>-</td>
<td>488</td>
<td>29</td>
</tr>
<tr>
<td>-4</td>
<td>-</td>
<td>475</td>
<td>29</td>
</tr>
<tr>
<td>-3</td>
<td>-</td>
<td>372</td>
<td>28</td>
</tr>
<tr>
<td>-2</td>
<td>141</td>
<td>118</td>
<td>28</td>
</tr>
<tr>
<td>-1</td>
<td>30</td>
<td>28</td>
<td>32</td>
</tr>
<tr>
<td>0</td>
<td>22</td>
<td>21</td>
<td>21</td>
</tr>
<tr>
<td>1</td>
<td>35</td>
<td>32</td>
<td>23</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>177</td>
<td>21</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>1461</td>
<td>22</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
<td>$&gt; 2000$ (8.66 $\cdot 10^{-4}$)</td>
<td>22</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>$&gt; 2000$ (4.04 $\cdot 10^{-3}$)</td>
<td>22</td>
</tr>
</tbody>
</table>

Table 1: Number of iterations required to reduce the $l^2$ norm of the residual to $10^{-8}$ with the stationary preconditioned Richardson method. If the scheme did not converge within 2000 iterations, the residual after the 2000th iteration is given in parenthesis, while (-) denotes diverging iterations. The total number $N_C$ of coarse-scale unknowns is reported in parenthesis. The tested permeability field is shown in Fig. 28(a).

are shown in Fig. 28(b). The number of iterations required to reduce the $l^2$ norm of the residual vector to $10^{-8}$ with the simple Richardson method are reported in Table 1 for different values of $K_{\text{channels}}$. Hereby, 5 local steps (110) were performed for each multiscale step (111). The spectra of the iteration matrices associated to the preconditioned Richardson scheme (109), i.e. with a single local step, are shown in Fig. 29 for the case $K_{\text{channels}} = 10^4$.

The results clearly show that the zMSFV preconditioner outperforms both MSFV-G and MSFV-PG preconditioners. Furthermore, the MSFV-PG based scheme is only conditionally stable, resulting in diverging solutions, except for very moderate contrast values. The MSFV-G preconditioner performs reasonably for moderate contrast values, but requires considerably more than 2000 MSFV iterations for $K_{\text{channels}} > 10^4$. Indeed, the spectral radius of the corresponding iteration matrix (with a single local step) is fairly close to unity ($\rho(G_{\text{MSFV-G}}) = 0.998$). On the contrary, the zMSFV-G based scheme converges within 30 iterations independently of the contrast considered and thus, it is up to two orders of magnitude faster than the classical MSFV-PG based solver.
Figure 29: Spectrum of the iteration matrix $G$ for to the preconditioned Richardson method (109) with $z$MSFV-G (a) MSFV-G (b) and MSFV-PG (c) preconditioners. The spectral radii are $\rho(G_{z\text{MSFV-G}}) = 0.8336$, $\rho(G_{\text{MSFV-G}}) = 0.9998$ and $\rho(G_{\text{MSFV-PG}}) = 413$. The permeability field is shown in Fig. 28(a), where $K_{\text{channels}} = 10^4$ was used.
A somewhat similar convergence behaviour is seen for the preconditioned GMRES method. Table 2 reports the number of iterations required for GMRES to reduce the relative error $\epsilon_{rel} = (p_{\text{zms}} - p_{\text{ref}})/p_{\text{ref}}$ to $10^{-8}$ measured in the $l^2$ norm, i.e. $||\epsilon_{rel}||_2 < 10^{-8}$, where $p_{\text{ref}}$ is the solution obtained by solving the linear system of equations (92) with a direct method. The zMSFV-G preconditioner delivers contrast independent convergence rates and is 6 to 7 times faster than MSFV-PG and MSFV-G preconditioners, which suffer a consistent loss of convergence speed as the contrast increases. The reason for this behaviour can be explained by considering the convergence histories shown in Fig. 30(b). Increasing the contrast in the medium leads to longer plateaus, i.e. to a stagnation of the GMRES method for more iterations if the MSFV-G preconditioner (circles and squares) is used. The plateaus are related to missing information in the coarse-scale operator or, in other words, due to the unresolved long-range effect of channels cutting the dual CV edges. On the other hand, the zMSFV method (solid line) directly resolves the high-conductive regions via zonal function and thus, includes the long-range information in the coarse-scale operator. Fig. 30(a) demonstrates the effect of the number of zonal DoF on the convergence behaviour. Using a single DoF per zone ($N = 24$ in Fig. 30(a)) only slightly improves the convergence rate since the zonal functions is constant within each zone and thus, does not allow for a variation of the solution. By adding more zonal unknowns, better convergence rates are achieved. Already adding a zonal DoF after every 30th zone-boundary CVs, for a total of 68 zonal DoF, results in an optimal convergence rate, which can’t be further improved even by adding DoF on every single boundary CV (1330 DoF).
### Table 2: Number of GMRES iterations required to achieve $||\epsilon_{rel}||_2 < 10^{-8}$ for the three preconditioners. The tested permeability field is shown in Fig. 28(a).

<table>
<thead>
<tr>
<th>$\log_{10}(K_{\text{channels}})$</th>
<th>MSFV-PG ($N_C = 100$)</th>
<th>MSFV-G ($N_C = 100$)</th>
<th>zMSFV-G ($N_C = 186$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-5$</td>
<td>104</td>
<td>84</td>
<td>35</td>
</tr>
<tr>
<td>$-4$</td>
<td>99</td>
<td>84</td>
<td>35</td>
</tr>
<tr>
<td>$-3$</td>
<td>94</td>
<td>82</td>
<td>33</td>
</tr>
<tr>
<td>$-2$</td>
<td>78</td>
<td>69</td>
<td>32</td>
</tr>
<tr>
<td>$-1$</td>
<td>43</td>
<td>39</td>
<td>31</td>
</tr>
<tr>
<td>0</td>
<td>31</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>1</td>
<td>40</td>
<td>35</td>
<td>29</td>
</tr>
<tr>
<td>2</td>
<td>86</td>
<td>71</td>
<td>28</td>
</tr>
<tr>
<td>3</td>
<td>128</td>
<td>113</td>
<td>27</td>
</tr>
<tr>
<td>4</td>
<td>156</td>
<td>136</td>
<td>27</td>
</tr>
<tr>
<td>5</td>
<td>184</td>
<td>159</td>
<td>25</td>
</tr>
</tbody>
</table>
Figure 30: a) Convergence histories of the preconditioned GMRES method with the zMSFV-G preconditioner for different numbers $N$ of zonal coarse-scale unknowns. The permeability field is shown in Fig. 28(a), where $K_{\text{channels}} = 10^4$ was used. b) Convergence histories of GMRES with MSFV-G preconditioner for $K_{\text{channels}} = 10^3$ (squares) and $K_{\text{channels}} = 10^4$ (crosses). The solid line corresponds to the convergence history of zMSFV-G with $N = 97$ in figure a).
17.2 SPE10

The second test-case is based on the permeability field of the SPE10 bottom layer [12] shown in Fig. 31(a). The fine-scale and coarse-scale grids have dimensions $220 \times 60$ and $20 \times 6$, respectively. The pressure is set on the left and right domain boundaries, while no-flow boundary conditions are applied at the top and bottom. Zones are created by applying the approach outlined in §16.3 with $\gamma_{\text{min}} = \gamma$ and $\gamma_{\text{max}}$ being arbitrarily large. The zMSFV method dual-grid and the zones detected for $\gamma \in [10^1, 10^2, 10^3, 10^4]$ are depicted in Fig. 31. Zonal DoF are placed after every 15th zonal-boundary CV independent of the selected value $\gamma$ and at least two DoF are placed in each zone. The numbers of zones and zonal unknowns are listed in Table 3. The convergence histories of the zMSFV-G preconditioned GMRES method are shown in Fig. 32. Moreover, the convergence histories of the MSFV-G preconditioned GMRES method for the same permeability field (red solid line) and for a homogeneous permeability field (green solid line) discretized on the same fine-scale and coarse-scale grids are reported. The latter can be seen as the optimal convergence rate which can be attained for a given coarse grid size. Clearly, the zMSFV-G preconditioner approaches the optimal convergence rate, if $\gamma = 10^3$ is used and, as expected, convergence is always faster than for the MSFV-G preconditioner, independent of the value of $\gamma$. The enhanced convergence rates are obtained at the cost of introducing a larger coarse-space. For the nearly optimal choice of $\gamma = 10^3$ the size of the coarse-space of the zMSFV-G method is about 3 times larger than for the MSFV-G method. We note however that the MSFV-G preconditioner already performs well in the case considered here, since the optimal convergence speed is only two times faster. The reason for the good performance is that the high-contrast channels present in the SPE10 bottom layer are already well resolved by the dual grid and thus the coarse-scale operator already contains most information about the underlying permeability field.
Figure 31: a) Permeability field of SPE10 bottom layer. b-e) Dual grid and zones of the zMSFV method for $\gamma = 10^1, 10^2, 10^3$ and $10^4$, respectively.
Table 3: Number of zones ($N_B$), dual CV related DoF ($N_v$), zonal DoF ($N_V$) and total number of coarse DoF ($N_C$) for different choices of $\gamma$. The related grids and zones are depicted in Fig. 31.

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>$N_B$</th>
<th>$N_v$</th>
<th>$N_V$</th>
<th>$N_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^1$</td>
<td>0</td>
<td>120</td>
<td>0</td>
<td>120</td>
</tr>
<tr>
<td>$10^2$</td>
<td>2</td>
<td>27</td>
<td>215</td>
<td>242</td>
</tr>
<tr>
<td>$10^3$</td>
<td>4</td>
<td>35</td>
<td>261</td>
<td>296</td>
</tr>
<tr>
<td>$10^4$</td>
<td>76</td>
<td>86</td>
<td>298</td>
<td>384</td>
</tr>
<tr>
<td></td>
<td>23</td>
<td>116</td>
<td>49</td>
<td>165</td>
</tr>
</tbody>
</table>

Figure 32: Convergence histories of GMRES with zMSFV-G preconditioner for different threshold values $\gamma_{\min}$. The underlying permeability field is displayed in Fig. 31(a). Also shown are the convergence histories for the MSFV-G preconditioner (red line) and for the MSFV-G preconditioner applied to a homogeneous permeability field with the same dimensions, boundary conditions and grid sizes as for the other runs.
In this section, the zonal MSFV framework for the numerical solution of coupled second order elliptic equations was presented. The framework allows for a flexible and specific treatment of special zones within the computational domain of interest. Special zones may arise due to physics, models or discretizations, which differ from the surrounding problem solved with the classical MSFV method. The notion of zonal functions spanning the solution-space within each zone was introduced, while the coupling of the zonal solutions with the rest of the domain was obtained via extended zonal functions, i.e. by computing local problems in all dual CVs in the direct neighbourhood of a given zone. The proposed framework is a generalization of previously developed extensions of the MSFV method, most noticeably those related to the treatment of complex wells, fractures and coarse-space enrichment strategies.

The zMSFV method in algebraic form was proposed as a special case of the framework and applied to the solution of high-contrast problems. Zones defined as either high or low conductive regions of the permeability field were introduced to obtain a preconditioner delivering convergence rates independent of the permeability contrast in the media.
Part V
Conclusion and Outlook
In this thesis, robust MSFV based iterative schemes for the solution of large linear systems of equations arising from the discretization of elliptic PDEs with highly heterogeneous coefficients were introduced. The proposed i-Ge-MSFV method exhibits higher convergence rates than the classical i-MSFV method, especially in the presence of high-contrast permeability fields. The method relies on the selective enrichment of the MSFV coarse-space, i.e. on the addition of functions incorporating missing fine-scale information to the set of functions spanning the initial coarse-space. Coarse-space enrichment is performed either a-priori or adaptively by introducing coarse-scale DoF on the dual CV boundaries and computing the corresponding local problems for all DoF involved. As a result, the i-Ge-MSFV coarse-space is spanned by proper partition of unity functions. The robustness of the method with respect to the heterogeneity of the underlying permeability fields, and changes of boundary and initial conditions, was demonstrated for very challenging test-cases. Furthermore, the i-Ge-MSFV method retains all features of previously developed MSFV based iterative schemes; most important: the capability of computing conservative fine-scale fields after any iteration.

Possible improvements of the efficiency of the i-Ge-MSFV method are mostly related to the enrichment step and to the resulting coarse-space size. The strategies adopted to enrich the coarse-space, i.e. the DoF location detection algorithms, are not guaranteed to be optimal with respect to the size of the resulting coarse-space. In other words, more coarse-scale DoF than required might be introduced. Hence, more sophisticated detection algorithm could be investigated in future works. More generally, in large-scale simulations the coarse-scale system will exceed the maximum size, which can be handled by direct methods, even without considering enrichment of the coarse-space. Recently, a multilevel approach for the classical MSFV method was proposed in [43]. An adaptation of the method for the more general case of the i-Ge-MSFV method would be worthwhile to be investigated.

The computational efficiency (in terms of pure CPU time) of the i-Ge-MSFV method was not compared to state-of-the-art linear solvers (e.g. AMG), since it would require the development of a highly optimized implementation of the method on huge distributed memory machines. Hence, a highly efficient implementation of the method would clearly help to demonstrate its efficiency. Furthermore, the overall efficiency of the i-Ge-MSFV method will also depend on the smoother, which is part of the solver framework. Here, only line-relaxation and ILU(0) based smoothers were considered. A careful investigation of the performance of the method in combination with different smoothers (e.g. block ILU, ILU(k), one-level DD methods) should be per-
formed in order to assess the optimal configuration.

In this work, the i-Ge-MSFV method was applied only for the solution of a specific elliptic problem. However, the proposed method can be applied for the numerical solution of any elliptic PDE and is particularly efficient, if only approximate conservative solutions are required. Furthermore, the application of the method to the solution of parabolic PDEs encountered in compressible flows [45] should be rather straightforward, especially if a formulation similar to [28] is adopted.

The zonal MSFV framework generalizes ideas and concepts introduced for the classical MSFV methods. In this thesis, the framework was used to derive a general algebraic formulation of enriched MSFV methods. The zMSFV method preconditioner was shown to deliver contrast independent convergence rates when used in combination with Krylov subspace methods. Similar results were observed for the simple Richardson method.

Here, only a single elliptic problem was considered in entire domain. The general formulation provided by the zMSFV framework, however, gives rise to the possibility of coupling additional mathematical models to the MSFV method in a straightforward manner. An interesting example (and of relevance for practical applications) is represented by pore-network models, which might be introduced in some parts of the domain to appropriately account for pore-scale effects (e.g. relative permeability). The zMSFV framework would allow for a two-way coupling between pore-scale computations and Darcy-scale MSFV computations, with the influence of the former being automatically included in the MSFV coarse-space via extended zonal functions. Similar considerations apply for the coupling of different governing equations. For example, this situation will arise, if incompressible and compressible flow models (governed by parabolic PDEs) are considered in distinct regions. Hence, the zonal MSFV framework can be seen as a first step towards a computationally efficient multiscale multi-physics modelling approach.

A property of the zMSFV framework, which could be further investigated, is the free choice of zonal functions. The zMSFV based preconditioner employs zonal functions, which are computed similar to basis and correction functions, i.e. by computing numerical solutions of the governing equations in each zone subject to reduced problem boundary conditions. However, other types of zonal functions could be used to approximate the solution within a zone (e.g. spectral methods).
An additional interesting application of the zMSFV framework is related to the grid problems discussed in § 12. As an example, the possibility to define an arbitrary large subset of the domain as a zone would allow to split the interaction region around a fault into multiple adjacent zones. The extended zonal functions couple such adjacent zones in a simple and automated way. The central advantage is that each zone has its own independent "coarse grid" and hence, there is no coarse grid matching condition to be fulfilled at the interface between two zones.


References


REFERENCES


REFERENCES


