Remeshed smoothed particle hydrodynamics for the simulation of compressible, viscous, heat conducting, reacting & interfacial flows

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Remeshed Smoothed Particle Hydrodynamics for the Simulation of Compressible, Viscous, Heat Conducting, Reacting & Interfacial Flows

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## Nomenclature

**Roman Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>interpolated function</td>
</tr>
<tr>
<td>A</td>
<td>amplitude the jet pulsing</td>
</tr>
<tr>
<td>B</td>
<td>slot width</td>
</tr>
<tr>
<td>$c_{p_s}$</td>
<td>specific heat at constant pressure</td>
</tr>
<tr>
<td>$c_v$</td>
<td>specific heat at constant volume</td>
</tr>
<tr>
<td>D</td>
<td>domain</td>
</tr>
<tr>
<td>$\frac{D}{Dt}$</td>
<td>material derivative</td>
</tr>
<tr>
<td>d</td>
<td>molecular diameter</td>
</tr>
<tr>
<td>$D_h$</td>
<td>slot hydraulic diameter</td>
</tr>
<tr>
<td>$D_{s,m}$</td>
<td>mixture average diffusion coefficient of species s</td>
</tr>
<tr>
<td>F</td>
<td>force</td>
</tr>
<tr>
<td>f</td>
<td>frequency</td>
</tr>
<tr>
<td>Fo</td>
<td>Fourier number.</td>
</tr>
<tr>
<td>Fr</td>
<td>Froude number</td>
</tr>
<tr>
<td>$g_i$</td>
<td>gravitational acceleration component</td>
</tr>
<tr>
<td>Gr</td>
<td>Grashof number</td>
</tr>
<tr>
<td>h</td>
<td>characteristic distance between the particles</td>
</tr>
<tr>
<td>H</td>
<td>nozzle-to-impingement surface spacing</td>
</tr>
<tr>
<td>h</td>
<td>heat transfer coefficient</td>
</tr>
<tr>
<td>k</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>L</td>
<td>length scale</td>
</tr>
<tr>
<td>L</td>
<td>impingement plate length</td>
</tr>
<tr>
<td>$L_{\infty}$</td>
<td>relative error</td>
</tr>
<tr>
<td>m</td>
<td>mass</td>
</tr>
<tr>
<td>M</td>
<td>Mach number</td>
</tr>
<tr>
<td>$M_5$</td>
<td>quartic spline</td>
</tr>
<tr>
<td>n</td>
<td>normal of the interface</td>
</tr>
<tr>
<td>$n_d$</td>
<td>normalization constant</td>
</tr>
<tr>
<td>Nu</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>p</td>
<td>pressure</td>
</tr>
<tr>
<td>Pe</td>
<td>Peclet number</td>
</tr>
<tr>
<td>Pr</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>q</td>
<td>heat flux vector</td>
</tr>
<tr>
<td>$\dot{Q}$</td>
<td>heat source rate</td>
</tr>
<tr>
<td>r</td>
<td>location vector</td>
</tr>
<tr>
<td>R</td>
<td>gas constant</td>
</tr>
</tbody>
</table>
Ra  Rayleigh number
Re  Reynolds number
$\dot{R}_s$  mass rate of production of species $s$
s  species index
ST  surface tension term
Str  Strouhal number
T  temperature
t  time
u  thermal energy per unit mass
$u_i$  velocity vector
$V_b$  volume of the particle $b$
$V_s$  diffusion velocity of species $s$
$v$  velocity
$\overline{v}$  average jet velocity
W  kernel function
We  Weber number
x  coordinate
$x_i$  position vector
$X_s$  mole fraction of species $s$
y  coordinate
$Y_s$  mass fraction of species $s$

**Greek Symbols**

$\alpha$  acceleration
$\gamma$  ratio of the specific heat capacities
$\Delta T$  characteristic variation of temperature
$\delta$  mean molecular spacing
$\delta$  Dirac delta function
$\epsilon$  specific Lennard-Jones parameters
$\kappa$  curvature of the interface
$\lambda$  mean free path
$\mu$  dynamic viscosity
$\rho$  density
$\sigma$  specific Lennard-Jones parameters
$\tau_{ij}$  viscous stresses
$\phi$  potential energy function
$\phi$  level set function
$\varphi$  phase angle between the two jets
$\omega$  vorticity
ω  angular velocity of the jet pulsing

Subscripts
0  reference value
A  particle a
Av average
b  particle b
ex exact solution
i  particle i
Max maximum
N  total number of particles
S  solid
SPH  SPH solution

Superscripts
*  dimensionless quantity

Abbreviations
ALE  arbitrary lagrangian eulerian
CFD  computational fluid dynamics
CSF  continuum surface force
DNS  direct numerical simulation
DSMC  direct simulation monte carlo
FD  finite difference
FEM  finite element methods
FV  finite volume
GFD  generalized finite difference method
LBM  lattice boltzmann method
LGA  lattice gas automata
LJ  lennard-jones
MAC  marker and cell
MD  molecular dynamics
MLPG  meshless local petrov-galerkin method
PDE  partial differential equations
PIC  particle-in-cell
RKPM  reproducing kernel particle method
RSPH  remeshed smooth particle hydrodynamics
SPH  smooth particle hydrodynamics
VOF  volume of fluid
Abstract

Numerical simulations are presented for low Mach number compressible, viscous, heat conducting, reacting and interfacial flows. The numerical method is based on the classical scheme of Smooth Particle Hydrodynamics (SPH). SPH is enhanced for handling accurately diffusion type processes. A novel feature of the SPH approach is the periodic re-initialization (remeshing) of the particles, which are distorted by the flow map. The robustness and accuracy of the proposed Remeshed SPH (RSPH) methodology is tested for a number of benchmark problems involving flow and energy transport. The accuracy of the developed RSPH method comes with a minimal additional computational cost, while maintaining the adaptive character of the method.

The method is used to simulate:

The effect of jet pulsation on the heat transfer and fluid dynamics characteristics of single and double jet impingement on a heated surface. The strong aerodynamic and thermal interaction between the gaseous jets and the impingement surface leads to non-linear system responses, with serious implications on the heat transfer. The characteristics of the dynamic behavior of this system are identified.

Moreover, RSPH methodology is applied for the simulation of chemically reacting flows using detailed chemical mechanism. The major conclusion is that the particle discretization of the basic equation describing reacting flows with complex chemistry is a flexible and excellent way to obtain numerical solutions.

The RSPH methodology can be extended for the simulation of interfacial flows in the presence of phase change. Within this context, RSPH methodology is applied in preliminary fashion to the simulation of interfacial and multiphase flows. The level set approach is coupled with the RSPH. The implemented Lagrangian level set is tested against basic interface tracking test cases and interface instabilities (e.g. Rayleigh-Taylor). The results indicate that the Lagrangian level set is a robust and accurate scheme, which is not suffering from time step limitations.

Zusammenfassung


Es werden folgende Vergleichsprozesse zur Bewertung herangezogen:

Darüber hinaus wird die RSPH-Methode zur Simulation chemisch reagierender Strömungen eingesetzt, wobei die chemischen Abläufe detailliert modelliert werden. Es wird deutlich, dass die Diskretisierung der massgeblichen Gesetze für eine chemisch komplex reagierende Strömung durch Partikel eine exzellente und flexible Vorgehensweise darstellt, um exakte numerische Simulationen zu erzielen.

Chapter 1
Overview of Meshfree and Particle Methods

1.1 Introduction

The computational solution of engineering problems involves several steps. Starting from a physical problem, we assume a mathematical model that governs the physical problem with a certain level of approximation. After choosing the mathematical model, one has to usually select a suitable discretization technique. The most common techniques are: finite difference (FD), finite volume (FV) and finite element methods (FEM). These methods have become popular and are widely used in engineering computations. The main common feature of these methods is that they partition a continuum into discrete elements (discretization). In FEM and generally in all other conventional computational methods (e.g. FD, FV), the individual elements are connected together by a topological map (mesh/grid). The finite element interpolation functions are then built upon the mesh. However, the physical phenomena of a continuum are not always compatible with the numerical capabilities of the numerical schemes, and finite element interpolation may not be beneficial. For example, in Lagrangian computations, one may experience mesh distortion, which can result in a deterioration of the accuracy and possibly the termination of the computations. Additionally, high gradients often require finer meshes and consequently adaptivity is necessary. Remedies such as regrinding introduce error the control of which is not always efficient.

In engineering science, several processes require modeling of problems with time dependent geometry or boundary conditions. Problems like impact/penetration, explosion/fragmentation and fluid-structure interaction have become common tasks, encountered in processes like metal forming and removing, internal combustion engines, and phase change. Conventional methods (e.g. FEM) can handle this type of problems using adaptive remeshing techniques. The difficulties involved are not only the remeshing technique but also most importantly the mapping of the state variables from the old to the new mesh. This mapping can introduce numerical errors, and frequent remeshing should be avoided. Special numerical techniques (e.g. Arbitrary Lagrangian Eulerian (ALE) method [161]) have been developed in order to move the mesh independently from the material in order to minimize the mesh distortion. Even with the ALE method, the convective transport effects can lead to severe numerical errors in the form of spurious oscillations. Consequently, it would be computationally useful to discretize the continuum by only a set of nodal points (particles), without any mesh constraints, which is the main feature of all modern meshfree methods [115].

The main advantages of meshfree particle methods can be summarized as follows:

- They can handle large deformations, since the connectivity among the nodes is generated during the computation and can change in time;
- Accuracy can be controlled easily, since nodes can be added in the regions where refinement is necessary;
- The particle discretization can provide accurate representation of complex geometries.
Based on physical principles, particle methods can be classified as deterministic and probabilistic. Based on the computational formulation and the approximation of the partial differential equations (PDEs), particle methods can be classified as strong and weak formulation of the PDE.

To approximate the strong formulation of a PDE using particle methods, the equation is usually discretized by a collocation technique. Representative methods based on the strong form include the Smooth Particle Hydrodynamics (SPH) [101, 171, 189, 191], Vortex Methods [64, 63, 151, 150, 70] and the Generalized Finite Difference Method [159]. The SPH and Vortex Method were initially probabilistic techniques; nowadays they are most frequently used as deterministic.

The majority of particle methods are based on probabilistic principles. The most important methods in this category include the Molecular Dynamics [5, 106, 232], the Monte Carlo methods [37, 35], the Lagrangian Probability Density Functions (PDF) methods [223], Lattice Gas Automata (LGA) or Lattice Gas Cellular Automata [237], and the (later derived) Lattice Boltzmann Method (LBM) [267].

Another class of particle methods is based on different Galerkin weak formulations (Meshfree Galerkin Methods). Prominent variants of these methods are: the Diffuse Element Method (DEM) [205], the Element Free Galerkin Method (EFGM) [29], the Reproducing Kernel Particle Method (RKPM) [166], the h-p Cloud Method [160], the Partition of Unity Method [176, 15] and the Meshless Local Petrov-Galerkin Method (MLPG) [10].

Some particle methods can be used in both strong and weak formulation. Particle-In-Cell (PIC) method [115] is such a case.

In various areas, like astrophysics, solid-state physics and biomedical research, the object under consideration is a set of “particles” (i.e. asteroids, electrons). Particle methods are then the natural choice for numerical simulation. Related examples are the dynamic interaction of molecules and the non-equilibrium movement of atoms in nano-scales. The current trend in computational methods is to use particle methods both as discretization tools, as well as physical models for continuum physics simulations. The Lattice Boltzmann method is the latest example for fluid mechanics applications.

In the following sections, we summarize the main meshfree methods.

### 1.1.1 Smooth Particle Hydrodynamics

Smooth Particle Hydrodynamics is the one of the oldest meshfree methods in modeling fluid dynamics. Early contributions have been summarized in several review articles [189, 191]. The technique was introduced in 1977 independently by Lucy [171] and Gingold with Monaghan [101]. They were interested in problems in astrophysics such as the formation of asteroids and the evolution of galaxies. The movement of particles in SPH is collective, similar to fluid flow (gas or liquid), and can be modeled by the classical Newtonian hydrodynamic equations. The fluid is represented by particles, which follow the fluid motion, preserving Galilean invariance and reducing the numerical diffusion (mainly due to the nonlinear convection terms) of the flow properties including momentum. The particles are nodes in space carrying some physical quantity. Each particle has mass, volume, Lagrangian position, velocity and internal energy. All the other quantities are derived by interpolation or from constitutive relations.

SPH has been used in a variety of astrophysical applications and it is considered today as a standard numerical tool in many astrophysical problems. Typical SPH applications include the
formation and collision of galaxies [196, 263, 112, 33, 34], coalescence of black holes [146, 147], star formation [58, 222], supernova evolution [118] and detonation in white dwarfs [96]. Due to the Lagrangian nature of SPH, the method has been widely adopted as an efficient technique for practical problems. The main advantages of the method are:

- There are no constraints imposed from the system geometry and the system may evolve far from the initial conditions;
- The particles map onto the mass density of the fluid, leading automatically to higher resolution in the high-density regions.

The fundamental idea of SPH methodology is different from traditional discretization methods (e.g. FD, FEM and FV), which discretize the system into a discrete algebraic system. In astrophysics, the physical system itself is discrete by nature, and the introduction of a localized kernel function works as a smoothing interpolation filter that generates a locally continuous field.

Starting from integral interpolants theory, a linear interpolation operator, can be written in the form

\[
\langle A(r) \rangle = \int_D A(r') W(r - r', h) dr'
\]

where \( r \) is a location vector, \( A(r) \) is the interpolated function, \( D \) is the domain, \( W \) is a kernel function, which is used to localize the partial differential equations through a convoluted integration and \( h \) is a scaling variable with dimensions of length. The symbol \( \langle \cdot \rangle \) denotes the approximated interpolation value. The scaling variable is referred to as the smoothing length, as it controls the degree to which the particle is spread in space. The function \( W \) is the key element of SPH and has the following properties:

\[
\int_D W(r - r', h) dr' = 1
\]

\[
\langle A(r) \rangle \rightarrow A(r), \quad h \rightarrow 0
\]

If the interpolation points are distributed in space, the operator \( \langle \cdot \rangle \) can be approximated numerically using quadrature:

\[
\langle A(r) \rangle \approx \sum_{b=1}^{N} A_b \frac{m_b}{\rho_b} W(r - r_b, h)
\]

where the field quantities at particle \( b \) are designated by subscript \( b \), and \( N \) is the total number of particles. The mass associated with particle \( b \) is \( m_b \) and its density \( \rho_b \). The quantity \( m_b/\rho_b \) is the inverse of the number density, and in a sense the volume of the particle.

It is possible to obtain an estimate of the gradient of the field \( A \) (provided \( W \) is differentiable) simply by differentiating the summation interpolant:

\[
\langle \nabla A(r) \rangle \approx \sum_{b=1}^{N} A_b \frac{m_b}{\rho_b} \nabla W(r - r_b, h)
\]

Under this consideration, SPH is always able to specify the interaction between individual particles, and the physical equations can be applied in their most basic intuitive form. The equations governing the evolution of the fluid become expressions for inter-particle (particle to particle) forces and fluxes. It is possible to formulate SPH approximations in a way that mass, momentum and energy
are algebraically conserved. The kernel representation is not only a technique to smoothly discretize partial differential equations, but also an advanced interpolation scheme on a set of moving particles.

SPH is an extremely versatile method; however, in certain applications, numerical errors can be substantially large (compared to errors using methods adapted for specific problems). Cases where the geometry is highly irregular or dynamic are quite readily solved by SPH. There are many applications where the Lagrangian nature of SPH can be applied without the requirement of complicated grids and refinement techniques.

The typical systems, for which SPH was first applied were characterized by very low dissipation. Representative examples are the Euler equations:

\[
\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{v} \tag{1-5}
\]

\[
\rho \frac{D\vec{v}}{Dt} = -\nabla p \tag{1-6}
\]

\[
\frac{du}{dt} = -\left(\frac{p}{\rho}\right) \nabla \cdot \vec{v} \tag{1-7}
\]

the Eqs. (1-5) - (1-7) are the mass, momentum and energy equations respectively. In these equations, the term \(\frac{D}{Dt}\) is the material derivative,

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla ,
\]

\(\rho\) is density, \(\vec{v}\) velocity, \(p\) pressure and \(u\) thermal energy per unit mass.

Later, an artificial viscosity was introduced to allow for the simulation of shocks [194, 197, 201]. Artificial viscosity was included as a means of dissipating macro-scale translational energy in the system into micro-scale energy of the molecules. In most astrophysical problems, the molecular viscosity of the gas is very small, and dissipation ideally occurs only in shocks.

Most astrophysical applications of SPH involve an isolated cloud of gas with no definite boundary; consequently, the contributions from the effective boundary of the fluid are usually neglected. There are other applications where the contribution from the boundary terms should not be neglected, in order to improve the accuracy of the simulations. This is the case, when a fluid with distinct boundary is modeled and boundary terms are necessary. There are several approaches, which include such contributions. The most conventional one is to include special boundary particles in the simulation, imposing the boundary contribution.

The application of SPH in a wide range of problems has lead to significant extensions and improvements of the original method. The method has been applied to solve both compressible [72] and incompressible flow problems [194, 200], multiple phase and surface tension problems [190, 272, 195, 200, 198], heat conduction problems [66], solid mechanics [217, 154, 231] and impact and penetration [124, 126, 18, 125]. A technique coupling SPH and FEM was developed in [13].

Several researchers have performed theoretical-numerical analysis of SPH [188, 175, 17, 199, 32]. Various improvements have been proposed through the years, aiming to improve pathologies or shortcomings in the numerical computation, such as implementation of boundary conditions [272,
1.1 Introduction

Tensile instability is the situation that particles become unstable under certain tensile (hydrostatic) stress state.)

Besides resolving the fundamental issues, as mentioned above, progress has been made in improving the performance of SPH. These attempts have focused on applications, as well as algorithmic efficiency.

Recently, SPH is reformulated by the formal convolution of the original hydrodynamics equations, in a new action principle, where the force acting on each particle is determined by solving the Riemann problem for each particle pair. The use of the Riemann solver strengthens the method, allowing the accurate study of phenomena with strong shocks.

1.1.2 Vortex Particle Methods

In computational fluid mechanics, most of the numerical algorithms for the solution of the Navier-Stokes equations are based on the velocity-pressure (v-p) formulation.

\[ \rho \frac{D\vec{v}}{Dt} = -\nabla p + \mu \nabla^2 \vec{v} \]  
(1-8)

\( \rho \) being the density, \( \vec{v} \) the velocity, \( p \) the pressure and \( \mu \) the dynamic viscosity.

An alternative technique is the vorticity-velocity (\( \omega-v \)) formulation. Here the governing equations can be written in Lagrangian form, and the velocity field can be obtained from the solution of a Poisson equation.

\[ \omega = \nabla \times \vec{v} \]  
(1-9)

\[ \rho \frac{D\omega}{Dt} = \rho \vec{v} \cdot \nabla \omega + \mu \nabla^2 \omega \]  
(1-10)

Vortex methods discretize the Lagrangian equation (1-10), based on a finite number of moving particles. The first numerical calculation of a flow using an approximation to the vorticity equation is due to Rosenhead [236], who studied the evolution of a vortex sheet, using the point (singular) vortex method. The introduction of modern vortex methods as a practical technique was initiated with the calculations of flow past a cylinder by Chorin [62], using the vortex blob method. Vortex blobs induced a bounded velocity field with finite kinetic energy and the diffusion of vorticity was calculated using the random walk imposed on the trajectories of vortex particles. A smoothing kernel function was used to eliminate singularities, so that the algorithm could be more stable. It may be noted that the idea of the vortex blob method is very similar to that of SPH.

Two versions of vortex methods were used in early implementations: Chorin’s random walk [62, 64] and Leonard’s core spreading technique [151, 150]. The vortex method was first used to simulate inviscid incompressible flow [7, 22], and later was applied to solve viscous flow problems [91, 90, 137, 138, 69, 218].

1.1.3 Molecular Dynamics

Molecular Dynamics (MD) is probably the most important and widely used family of particle methods. Introduced about half a century ago, it was initially applied to the simulation of condensed matter [3, 4]. If one is interested in macroscopic thermophysical properties, like heat capacity and viscosity, MD is the most understandable way of using a computer to generate a phase-space
1. Overview of Meshfree and Particle Methods

trajectory for an assembly of interacting atoms it amounts simply to the stepwise integration of Newton's equations of motion from a completely specified starting point (provided that the interaction potentials are known):

\[ F_i = m_i \alpha_i, \quad (1-11) \]

where \( F_i \) is the force exerted on particle \( i \), \( m_i \) is the mass of particle \( i \), and \( \alpha_i \) is the acceleration of particle \( i \).

If the system obeys the ergodic principle, which states that the time average over these phase-space trajectories is equivalent to the ensemble average, each macroscopic observation can be related to atomic motions through statistical mechanics. These include time dependent quantities such as transport coefficients, which explicitly involve the dynamical motion of the atoms and their correlation in time. MD can also be used to investigate relaxation towards equilibrium to explore the space configuration of a system and find the potential energy global minimum (the potential energy depends on the conformation of the molecules). The techniques of MD and the many algorithmic innovations are described in the books such as Allen and Tildesley [5], and Haile [106].

There are two types of molecular dynamics methods: the first principles or “ab initio” methods, and the semi-empirical methods. Both have been applied to traditional engineering areas such as mechanical, chemical, aerospace and electrical engineering.

As a particle method, “ab initio” molecular dynamics is used to study material properties at the atomic scale. It requires the computation of the wavefunctions of electrons as well as the motion of the nuclei. Sophisticated and accurate potentials have been derived for classes of material and applied to great effect, but the ubiquitous stumbling block has been the treatment of systems in which chemical bonding changes. While the effects of changes in bonding may be taken into account in an average way so that e. g. phase transitions may be approximately treated, it appeared impossible to circumvent the quantum mechanics when one is interested in molecular reactions on surfaces.

A major breakthrough came in the mid-80’s, when Car and Parrinello published their seminal work on a unified approach to electronic structure and MD [51]. The crucial ingredient, which makes the method "ab initio" or first-principles, is the density-functional theory, which is used to describe the quantum mechanical behavior of the valence electrons. The method is efficient enough to be used for large number of evaluations of energy and forces, which are needed for MD. In short, the MD technique can now be used to a certain extend even when chemical bonding is changing.

The ambitions and achievements of Car-Parrinello calculations have enjoyed a quite remarkable expansion over the last decade, fuelled by algorithmic developments and computer speedup, the latter providing a huge impetus through the advent of massively parallel machines. Car-Parrinello MD calculations on metals, semiconductors and insulators, surface reactions, carbon polymorphs and even biological systems are common. Computational molecular dynamics involves the simulation of particles under the influence of inter-particle forces. MD simulations are applicable in many areas, including the study of material properties at the microscopic scale and problems associated with DNA-protein molecular interactions. Parallel computers have spawned increased interest in MD simulations because both larger systems and longer time-scales can be simulated. However, these two benefits are realizable only when the MD algorithm is scalable to large numbers of processors and the computational load is uniformly distributed among the processors.
Due to the limitation in computer resources, at present, “ab initio” methods are restricted to simulations of several hundreds of atoms within a characteristic total time scale of a nanosecond. The simulation of larger system is beyond the current computational technology. Therefore, in order to study larger and more realistic systems with large number of atoms for longer time, a simpler model is desirable, which can represent most features at the atomic level.

With current computer resources, classical molecular dynamics (semi-empirical) are capable of simulating big systems (up to ten million atoms), as they do not require the calculation of electron distributions, but only the forces acting on each atom, which are determined by the gradient of the potential energy function $\phi$.

The potential energy function is determined from empirical knowledge or from “ab initio” simulation. The best known potential is the Lennard-Jones (LJ) potential [148, 149]:

$$
\phi^{LJ}(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right],
$$

where $\sigma$ and $\varepsilon$ are the specific Lennard-Jones parameters, different for different interacting particles.

The force between two molecules is given by

$$
F^{LJ}(r) = -24\varepsilon \left[ \left( \frac{\sigma^{12}}{r^{13}} \right) - \left( \frac{\sigma^{6}}{r^{7}} \right) \right]
$$

For simulation of anisotropic crystalline solids the LJ potential is not accurate any more, and more complex potential are needed. To remedy this inadequacy, the Embedded-Atom potential Method (EAM) has been used in simulations, in order to obtain information related to properties of solids (structure dynamics, phase transition, vibration, diffusion and segregation) [76]. The embedded-atom method [75, 19, 93, 20, 76] consists of two source terms, the embedding energy for each atom to be introduced to the system and the short range core-to-core repulsion between nucleus pairs.

The recent resurgence of MD (quantum and classical), is mostly due to the emergence of nano-technology. Many materials at the nano-scale demonstrate remarkable properties. For example, it is claimed that carbon nano-tubes are remarkably strong and have better heat conductivity and electrical conductance than cooper at room temperature [255].

**1.1.4 Monte Carlo Methods**

Haviland and Lavin [111, 143] introduced the first probabilistic simulation method, named “test particle Monte Carlo method”. A Monte Carlo method is derived from the Liouville equation (basic statistical mechanics equation for a gas, which expresses the conservation of N particle distribution in a 6N dimensional space). All Monte Carlo methods exploit the statistical nature of multiple collisions in microscopic systems. When particle densities are high enough that the system of particles can be considered continuous, the Navier-Stokes equations, or various subsets of them, usually describe the fluid motion. Because molecular dynamics is based on the most fundamentals set of equations, it is in principle valid over the entire range of non-dimensional critical flow parameters of gases (Knudsen...
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number $Kn = \frac{\lambda}{L}$ where $\lambda$ is the distance traveled by molecules between collisions (mean free path), and L characteristic length dimension). Based on physical reasoning, MD can be used for all ranges of densities and system sizes, thus it may be impracticable computationally in many cases.

The alternative to the above “test particle Monte Carlo” approach is to introduce time as a variable and simultaneously follow the trajectories of a very large number of simulated molecules. The method is called Direct Simulation Monte Carlo (DSMC). The DSMC method was first applied to the homogenous gas relaxation problem [36]. A DSMC simulation, like a continuum computational fluid dynamics (CFD) calculation, proceeds from a set of prescribed initial conditions. The particle positions, velocities, collision cross sections, and boundary conditions determine the subsequent evolution of the system. As in a continuum solution or an experiment, the solution that evolves may be very sensitive to the particular choice of initial and boundary conditions. In the past 20 years, DSMC has been used primarily for problems in rarefied atmospheric dynamics. The many comparisons of calculations with experiments have been vital in gaining widespread acceptance of DSMC. These comparisons have both validated and advanced DSMC methodology and experiment design. As in standard finite-difference or finite-volume methods, the original DSMC method used a rectilinear, orthogonal, Cartesian grid. This is the simplest, most cost-effective grid. Statistical accuracy requires enough simulated particles in a computational cell, setting a lower limit on cell size. However, as in the case of continuum problems, there are situations with curved or time-changing obstacles and boundaries for which a different grid is necessary. Thus, advances in grid generation were applied to DSMC. A number of DSMC efforts use unstructured grids (e.g. with triangular, tetrahedral, and other shapes) as well as sophisticated gridding methods for flows around complex bodies. In principle, any size or shape of computational cell may be used for DSMC. The only requirements are that particle locations in space can be computed, the correspondence between particles and cells identified, and the cell areas and volumes calculated.

The need to model a variety of transition-regime gas flows (transition-regime flow is considered a flow that the mean free path, $\lambda$, is neither very small nor very large in comparison with a typical linear dimension) quantitatively has significantly advanced DSMC methodology. New advances considered are Lagrangian DSMC, the optimization of the computation on parallel computers, and advances of hybrid algorithms for computations in mixed-flow regimes. Growth in DSMC capabilities has, in many respects, paralleled and gained from developments in continuum techniques.

For Navier-Stokes simulations, the time step may be even further limited by the stability and accuracy conditions for computing the effects of processes such as thermal conduction, momentum transfer, molecular diffusion, and especially fast chemical reactions. However, DSMC is not subject to the same stability conditions that apply to reactive-flow Navier-Stokes simulations. None of the above time step limitations inherent to reactive Navier-Stokes computations occur in determining the time step for a DSMC computation. Many of the input conditions for Navier-Stokes codes, such as chemical reaction rates and diffusion coefficients, imply unrealistic rates of information transfer when the computational cell is beyond a certain size. This problem is not encountered in DSMC. In addition, none of the problems of numerical stability associated with continuum methods occur in DSMC. If it were feasible to use DSMC throughout its physically realistic range (Knusden number),
the applicability and generality of the solution to transitional flow problems would be substantially greater. However, computational costs of DSMC are high, even in regimes where it is being used now, and much of the potential range of the method is beyond current computational capabilities. DSMC has already given quantitative answers to a broad range of questions that otherwise could not have been answered with sufficient accuracy. The simplicity and flexibility of the implementation and the stability of the solution make it an attractive tool for solving physics and engineering problems.

Summarizing, DSMC is computationally much more efficient than MD, because one of the basic assumptions of DSMC is that the movement of the particles can be decoupled from their interaction. Note that the most time consuming part of a MD simulation is the calculation of the forces between the particles. DSMC method has been used successfully in the study of rarefied gas flows form many years, and recently found applications in chemistry and physics [209].

1.1.5 Other Methods

1.1.5.1 Generalized Finite Difference Method

One of the early contributions of strong form collocation meshfree methods, besides SPH, is the Generalized Finite Difference Method (GFD), proposed by Liszka and Orkisz [159]. GFD extends classical concepts of finite differences to irregular sets of points, without any need for mesh, by deriving finite difference schemes for non-uniform, non-rectangular and unstructured grids, and is suitable for irregular geometries. It is possible to use finer mesh near critical flow conditions and coarser mesh where flow change is less drastic. This leads to considerable reduction of grid points and CPU savings. The GFD computational model has been used in applications involving heat transfer, deformation of membranes and flow in deformable tubes [203, 281, 274].

1.1.5.2 Lagrangian PDF Methods

The Lagrangian PDF methods [223, 224, 79, 81, 225] have arisen as a combination between the PDF methods and stochastic Lagrangian methods, similar to those that have been used for a long time to study turbulent dispersion. These numerical methods are developed to integrate the stochastic differential equations that arise in a particle method for modeling turbulent flows. The Lagrangian PDF methods provide a computationally good way of calculating the statistics of inhomogeneous turbulent flows, and are particularly attractive if chemical reactions are involved [213, 174, 292, 123]. The computational implementation of these methods is simple and natural, as the flow at a given time is represented by a large number of particles with specific properties. These properties evolve in time according to stochastic equations.

1.1.5.3 Mesh-free Galerkin Methods

Meshfree Galerkin methods are relative young compared to SPH. Several research groups in early 1990s were looking for either meshless interpolants to reduce the heavy computational load of the structured mesh generation, which is required from the finite element refinement process, or interpolants having multiple scale computational capability [169, 204, 205, 165, 206]. Nayroles et al. [205] derived the diffuse element method from the moving least square interpolant and Liu et al.
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[166] the reproducing kernel particle method (RKPM) as an attempt to construct a corrective SPH interpolant. The RKPM was used to solve structural mechanics problems [166, 168, 127].

Belytschko et al in 1994 [29] used the moving least squares interpolant in the Galerkin procedure, by forming a variational formulation to accommodate for the interpolant. This consists the Element Free Galerkin Method, which is used to solve elastic problems [26, 30, 31]. The Partition of Unity method is an extension of the FEM, for problems where the classical FEM fail or is prohibitively expensive [176, 15, 16].

The Meshless Local Petrov-Galerkin method (MLPG) [10, 11, 12, 156, 104, 105, 157, 9, 170] has been successfully used on both potential and elasticity problems to obtain accurate results. The MLPG method is based on a local weak form and a moving least squares (MLS) approximation. This method does not need any “element” or “mesh”, but uses a distributed set of nodes for both field interpolation and background integration. Although the MLPG method is attractive, the method is computationally more expensive than the FEM, and it is not as mature and comprehensive as the FEM. There is a great interest in combining different numerical methods, because such coupling could exploit the potential of each method while avoiding their deficiencies.

The h-p cloud method [82, 160, 95, 177] is a generalization of previously developed meshless techniques for the analysis of elliptic boundary-value problems. In the h-p cloud method, the domain of interest is covered by a collection of open sets (the clouds) over which a partition of unity is built. These functions are then used to generate h-p cloud approximations using spectral or specially customized functions. The sizes of the clouds are represented by the parameter h and the polynomial order associated with them by the parameter p.

Meshfree Galerkin methods were initially used to simulate critical phenomena in fracture mechanics (e.g. crack growth) [26]. Special techniques have been developed in modeling discontinuous fields [28, 140]. The big advantage of the meshfree Galerkin methods over FEM is the ability to handle large deformations (for example in metal forming [59], and rubber materials [60]). Meshfree Galerkin methods have been applied extensively in simulations of strain localization problems [152].

The meshfree interpolants have been used for multiple scale computations [169] and applied in areas such as acoustics and wave propagation [162, 284], fluid dynamics [167, 164, 163] and large eddy simulation [286].

1.1.5.4 Particle-in-cell method

The particle in cell method is a hybrid (Eulerian Lagrangian) method. The main idea is to trace the motion of a set of material points, which carry information of the state variables, in a Lagrangian way, while the spatial discretization, and consequently the displacement interpolation is made in an Eulerian frame [42, 41, 48, 210].

1.1.5.5 Lattice gas cellular automata

The first lattice gas cellular automata model was introduced in the 70’s by Hardy, de Pazzis and Pomeau [108], and was applied to study ergodicity-related problems. The efficiency of the lattice gas cellular automata method is even higher than that of the Direct Simulation Monte Carlo method, but
this is achieved at the expense of physical reality. In fact, lattice gas cellular automata models can be described as providing gas analogues rather than gas models.

The lattice gas takes its name from the regular array of points or nodes into which physical space is discretized. The nodes can be occupied by fluid particles. Thus space is discretized, and in practice it is also finite. Proper (periodic or other) boundary conditions can be implemented. Interactions between particles are simple: they may only take place on nodes with several particles, taking the form of local instantaneous collisions. The collision rules are chosen in order to conserve both mass and momentum. In this model there is no additional conservation law associated to energy, since energy is directly proportional to mass; it is thus trivially conserved.

These systems being entirely discrete, have the advantage of allowing straightforward implementation on computers, and allow the performance of simulations with much more particles than "realistic" models in which one has to take into account the continuous values of positions, velocities and interaction potentials with a finite precision. More details can be found in [40].

1.1.5.6 Lattice Boltzmann method

The Lattice Boltzmann Method (LBM) is a derivative of the lattice gas automata method [61, 230]. Nowadays, the method is applied to a number of engineering flow problems. The LBM method is a powerful technique for the computational modeling of a wide variety of complex fluid flow problems, including single and multiphase flow in complex geometries. In recent years, the (LBM) has emerged as a promising numerical method for simulation of fluid flows [229, 273, 61, 89, 180]. Unlike conventional methods, which solve the discretized macroscopic Navier-Stokes equations, the LBM is based on microscopic particle models and mesoscopic kinetic equations. It is a discrete computational method based upon the Boltzmann equation. A simple derivation of the Boltzmann is provided by [37]. For monatomic gas molecules in binary gas collisions the integro differential equation reads

$$\frac{\partial (n_f)}{\partial t} + \xi_j \frac{\partial (n_f)}{\partial x_j} + F_j \frac{\partial (n_f)}{\partial \xi_j} = J(f, f^*)((1-15))$$

where $n_f$ is the product of the number density, $x_j$ the coordinate vector and $\xi_j$ the speeds of a molecule, $F_j$ the external force, and $J(f, f^*)$ the nonlinear collision integral. The Boltzmann equation considers a typical volume element of fluid to be composed of a collection of particles that are represented by a particle velocity distribution function for each fluid component at each grid point. The time is counted in discrete time steps, and the fluid particles can collide with each other as they move, possibly under applied forces. The rules governing the collisions are designed so that the time-average motion of the particles is consistent with the Navier-Stokes equations. The method naturally accommodates a variety of boundary conditions such as the pressure drop across the interface between two fluids and wetting effects at a fluid-solid interface. It is an approach that bridges microscopic phenomena with the continuum macroscopic equations. Further, it can model the time evolution of systems. The LBM is especially useful for modeling interfacial dynamics, flows over porous media, and multi-phase flows. Furthermore, the LBM algorithm tends to be very simple, allowing parallelism in a straightforward manner.
The underlying lattice gas (or mesh) is a rectangle (or hexagon) in two dimensions or a cube (or a shape with perfect geometric symmetry) in three dimensions, equivalent to the regular Cartesian grid (equidistant) used by conventional Navier-Stokes solvers. As a result, solution domains with inclined or curved boundaries are approximated by staircase-like steps. This restriction severely limits the applicability of LBM as most industrial and practical flows are characterized by complex flow geometries. For this reason, recent efforts have aimed in extension the LBM to irregular grids [130].

1.1.6 Summary

Most of the methods discussed above do not require a mesh structure. Meshfree methods can be applied to deformable geometries; additionally adaptive refinement and parallelization can be most of the times easily implemented. Many problems that cannot be solved with the conventional methods are tractable by meshfree methods. Although much has been achieved over the last decade, they are still many challenges for the meshfree methods.

The applicability of the methods described in the previous sections is most of the times limited. Some information for gases is recast in quantitative form in Figure 1, which shows the regimes of validity of the methods. These regimes are expressed as function of an important characteristic length $L$ and the density ratio. The density scale is related to the mean molecular spacing $\delta$. For fixed molecular diameter $d$, as the mean spacing between the molecules decreases, the density increases. This corresponds to the horizontal axis of Figure 1. Molecular Dynamics is based on the most fundamental set of equations, it is in principle valid throughout the entire range of parameters; there no physical reasons that prevent the applicability of MD for all range of densities and system sizes, even though it is impractical computationally.

![Figure 1](image-url) Regimes of a gas as functions of density $\rho$ (relative to air at STP $\rho_0$) and length scale $L$, where $\delta$ is the mean molecular spacing, $d$ is the molecular diameter, $\lambda$ is the mean free path. Adapted from [37].

On the other hand, all other methods (deterministic, or probabilistic) have restrictions and cannot be applied for the entire range of the parameter space. According to the Knudsen number, the
flow regimes can be divided into various sub regions, such as the continuum, slip, transition, and free-
molecular. In Figure 1 the Knudsen number scales with the inverse of density and length scale.

The continuum-based flow models rely on the Navier-Stokes equations. The Euler equations correspond to the inviscid continuum limit, which shows a singular limit since the fluid is assumed to be inviscid and non-conducting, and they correspond to $Kn=0.0$. For Knudsen number larger than 0.1 the Navier-Stokes equations break down. In contrast, the discrete particle or molecular based models, are based on the Liouville equation. The Liouville equation is an integro-differential equation and the solution of this equation is limited to few cases. For this reason, a way of solving high Knudsen number flows is through molecular based direct simulation techniques like the Direct Simulation Monte Carlo method.

As a consequence, the Direct Simulation Monte Carlo (DSMC) has been a popular technique for the simulation of high Knudsen number gas flows, where the conventional Navier-Stokes Eqs. are inaccurate. The DSMC may be used very efficiently in the transition regime $O(0.1)<Kn<O(10)$. The DSMC remains valid for much lower values of the Knudsen number but it is computationally extremely expensive. DSMC has emerged because of the rebirth of importance and applicability of high Knudsen number flows in nanotechnology. It is obvious that after molecular dynamics, DSMC is the second more applicable technique for simulations.

All other methods described in this chapter have smaller range of applicability. The deterministic methods are limited to the upper triangle of Figure 1. Meshless methods (mostly the deterministic ones) still require considerable improvement before they equal the prominence of FEM and FD in computer science and engineering. SPH for example is robust and versatile and mainly applied in astrophysical applications. SPH carries the advantages of automatically adapting to the solution; however, it is not considered accurate enough for engineering problems where viscous forces are important. Vortex methods have today reached a level of development, offering an interesting alternative to finite difference and spectral methods for high-resolution numerical solutions of the Navier-Stokes equations [71] but are not yet widely applied widely in engineering science and are time intensive.

The Lattice Boltzmann Method (LBM) appears to be a method with great potential. LBM is based on microscopic particle models and mesoscopic kinetic equations. For this reason it can be applied to higher Knudsen number flows where the other methods based on continuum approach fail. It is especially useful for modeling interfacial dynamics, flows over porous media, and multi-phase flows. However, the applicability of LBM is still limited.

The greatest challenge appears to be in developing hybrid techniques by combining the advantages of different methods (e.g., particle and grid based methods, particle methods and molecular dynamics). This seems to be a very promising way to include multiple scales in the numerical methods and consequently unexplored physics.

1.2 Motivation and objectives of the present study

The goal of the present work was to attack a complex jet flow / wall interaction problem involving complex phenomena, such as multiphase flow, heat diffusion and convection, reaction, and phase change. The simulation of such coupled phenomena is difficult with convectional methods.
Overview of Meshfree and Particle Methods

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(FEM, FD, FV), and advanced numerical implementations must be applied (overlapping grids, interface capturing etc.). A meshfree method can avoid by its Lagrangian nature some of the elementary difficulties (e.g. complicated geometry) of the process and was selected as the preferred approach.

Complex phenomena usually include more than one of the following components

- Fluid dynamic
  - Viscous Flow
  - Multiphase Flow and Free-Surface Modeling

- Energy - Heat Transfer
  - Conduction
  - Convection
  - Conjugate heat transfer
  - Combustion
  - Radiation

- Mass Transfer
  - Reactions
  - Mass Diffusion
  - Phase Change

The process of interest is shown in its entirety in Figure 2. This process is based on the interaction of a jet (for example high-density pure oxygen) with a hot surface. Liquid oxygen is injected against a hot surface and evaporates. The gas oxygen impinges on the surface. Simultaneously oxygen is absorbed from the surface, diffuses inside the liquid layer and reaction takes place. The released heat is convected to the gas phase and is conducted inside the liquid phase. Phase change and oxidation occurs in the solid and liquid phase. The present work deals with a host of aspects of this process employing simplified scenarios. The first significant step the development of a Lagrangian computational method based on the classical scheme of smooth particle hydrodynamics. One major assumption of the Eulerian approach is that the fluid is homogeneous. Any fluid that is not homogeneous, for example one with multiple phases, requires additional complex internal mathematical modeling to represent these phases. Eulerian models are grid based. Smoothed Particle Hydrodynamics (SPH) is a grid free Lagrangian based method in which the fluid flow is represented by fluid pseudo-particles. The use of Lagrangian based methods effectively eliminates the homogeneous fluid assumption of the Eulerian methods. The result is that in the areas where Eulerian methods struggle, Lagrangian methods can effectively model multiple phases naturally, even with greatly differing densities. These qualities make it very well suited to multiple phase Mechanical Engineering applications such as: fluid jets, tank sloshing, metal casting and extrusion, multiple phase pipe flow, fluid impacts and cavitation. The Lagrangian approach of SPH extends to complex three-dimensional geometry extremely well. SPH has several advantages, two and three-dimensional complex geometries are handle easily, momentum dominated flows are handled well, complex free surfaces are modeled naturally, and complicated physics such as multiphase, realistic equations of state, compressibility, radiation and solidification can be added easily.
In the present study, SPH is extended for first time to handle accurately diffusion-type processes, and is used for the numerical simulation of compressible, viscous, heat conducting, reacting and interfacial flows. A novel feature of the proposed SPH approach is the periodic re-initialization (remeshing) of the particles, which are distorted by the flow map. Remeshing schemes have been used in the past beneficially in the context of vortex methods [135, 70], where the remeshing procedure allows a progressive inclusion of particles in the computation that are activated by diffusion processes, while maintaining a minimal level of resolution during all stages of the computation. A concern in using SPH, is the accurate implementation of realistic (instead of artificial) viscous effects [288] when the particle map is distorted. Use of the remeshing procedure in SPH, enables a more accurate representation of viscous, and more generally diffusion processes.

The remeshed SPH (which from now on will be called RSPH) [55] methodology is presented and validated with simulations of compressible viscous flows, with and without heat conduction (Chapter 2), situations involving aspects of the complex physics of the process in Figure 2.

After demonstrating its credibility the proposed RSPH method is then used to simulate:

- The effect of jet pulsation on the heat transfer and fluid dynamics characteristics of single- and double-jet impingement on a heated surface (Chapter 3). The simulation of jet impingement focuses on the quantitative description of the flow field and the energy exchange between jet and surface [54, 57, 56]. The strong aerodynamic and thermal interaction that exists between the gaseous jet and the impingement surface greatly enhances the local heat transfer in the stagnation and wall jet regions as well as the average heat transfer over the surface.

- Laminar chemically reactive flows, using elemental chemical kinetics and detailed transport at low Mach number (Chapter 4). The combustion process is usually
characterized by the presence of multiple time and length scales, as well as flow speeds at a wide variation of Mach number. The range of chemical time scales is large and the numerical solution is affected by the species that have the fastest reaction rates. The simulation of reacting systems is a difficult test for numerical schemes, since the chemical reaction rates are nonlinear and widely disparate in general, and may cause the non-linear equations to be “stiff”, leading to non-convergent numerical solutions. The RSPH computational results are compared with simulation results from a spectral element method. It should be noted that it is the first time that SPH is used for simulation of reactive flows [53].

- Interfacial flow. The level set method is implemented in the RSPH methodology. The capturing capability of the Lagrangian level set implementation has been used for cases like translation, rotation, and stretching and finally applied to simulate instabilities of an interface (e.g. Rayleigh-Taylor) (Chapter 5). It should be noted that this is the first time that level set method is applied in a Lagrangian scheme. This is directly related to the material removal aspect of the process of Figure 2. This chapter presents a formulation and preliminary results and is meant to be a first step towards future work.

The accuracy of the proposed SPH methodology is tested for a number of relevant applications involving flow, energy and mass transport. The results indicate that the new methodology is capable for Direct Numerical Simulation (DNS) quality simulations while maintaining robustness and adaptivity. In Chapter 6 some general conclusions and summary for the RSPH methodology are presented.
Chapter 2
Remeshed Smoothed Particle Hydrodynamics for the Simulation of Viscous and Heat Conducting Flows

2.1 Background

The Smooth Particle Hydrodynamics (SPH) is a Lagrangian numerical method introduced by Gingold and Monaghan [101], in order to model problems in continuum physics while circumventing some of the limitations of grid-based methods. SPH is a robust numerical technique that has been applied to a wide range of problems, from compressible fluid mechanics to astrophysics and flow structure interactions [101, 194, 190, 195, 200, 66]. Although the method enjoys the properties of Lagrangian schemes, such as automatic adaptivity and numerical stability, the extension of the method to handle diffusion-type effects has been limited. One of the key difficulties is the approximation of diffusion-type operators on the Lagrangian mesh, which is usually distorted by the flow map. A methodology to overcome these difficulties is presented in this chapter.

The development of the classical SPH methodology for compressible flow fields is described in detail by Monaghan [191]. The computational elements are particles whose location is following the flow map in a Lagrangian fashion. The initial flow field quantities are interpolated on the particle locations, and all the flow quantities can be reconstructed by a linear superposition of the flow quantities carried by the particles weighted by a smooth interpolation kernel [247, 246]. The discrete equations are obtained from the continuum equations by expressing the flow quantities as a linear superposition of the physical quantities that are being carried by the particles.

SPH belongs to a class of Lagrangian methods called particle methods. The key advantage of all Lagrangian particle methods is to avoid the explicit discretization of the non-linear convection term while maintaining an automatic adaptivity for the computational elements. However particle methods are faced with difficulties when dealing with the approximation of viscous effects. The approximation of diffusion operators in the context of particle methods is a subject that has been extensively addressed in the context of vortex methods in the last decade [70]. Several options have been identified such as the derivation of conservative schemes based on the approximation of the diffusion operator by an integral operator [77, 78], the differentiation of the smoothing kernel [90], and the approximation of the diffusion operator on the distorted Lagrangian grid using some averaging procedure [240].

In this chapter we present a numerical scheme to account for diffusion effects in the context of Smooth Particle Hydrodynamics by incorporating a remeshing strategy for the particle locations along with an efficient calculation of the diffusion operators in the distorted particle locations.

The fact that viscosity plays an important role in many physical phenomena of engineering interest, underlines the need to improve the modeling of viscous forces while maintaining the adaptivity and robustness of SPH. A commonly employed methodology to account for diffusion effects in SPH is the introduction of artificial viscosity so that conservation of momentum is ensured.
However, this scheme usually yields inaccurate results, because the separation of shear and bulk viscosity is not allowed [191, 288].

An alternative approach to remedy this situation is based on a Taylor series expansion of the field quantities in the neighborhood of each particle and combines the standard first-order SPH derivatives with the finite difference method [46]. The method of Brookshaw [46] is computationally efficient, since only the first derivative of the kernel is required and conserves the linear momentum, while the angular momentum is approximately conserved. This approximation for the diffusion term has been implemented successfully to simulate heat conduction problems [46, 66], and incompressible viscous flows [200] with solid boundaries, but it may lead to inaccurate results when the velocity or the density field is noisy [288].

Another approximation of viscous effects in SPH involves the nested application of the difference approximation thus calculating second derivatives from first derivatives [92, 288]. This method can calculate any second derivative in such a way, that the formulas are symmetric and conserve linear and angular momentum. However, this method is not computationally efficient as it would require repeated calculations involving all particles, and may yield inaccurate results when the density is noisy [288].

Finally, an alternative approximation of the diffusion terms is based on the direct computation of the second derivative of the kernel [90, 272]. However, this method is considered to be very sensitive to disordered particle locations, particularly for low-order kernels [46]. Moreover, it depends strongly on the number of neighbors around each particle. In order to achieve accurate results, a minimum number of neighboring particles is necessary. At the same time, as the computational cost is proportional to the number of neighboring particles, it is desirable to keep this number low. In order to circumvent this difficulty, most of the SPH implementations are using variable smoothing length (h), which allows for an efficient balancing of the number of neighboring particles near the lower limit.

In the work presented in this chapter, the direct differentiation of the kernel function is used to compute second order derivatives. In order to remedy the drawbacks of the method associated with the particle disorder, the particle locations are periodically reinitialized (remeshed) onto a uniform grid. This remeshing process constitutes the key novel feature of the computational scheme presented herein. With this feature it is possible to construct a computational algorithm based on the direct differentiation of the kernel (first and second derivatives) to solve a system of differential equations describing flow and heat transport in a Lagrangian frame, while accurately accounting for viscous and heat diffusion effects.

The process of remeshing has been introduced in incompressible flow simulations using Vortex Methods [135] in order to eliminate spurious vortical structures resulting from non-overlapping smooth vortex particles. Earlier relevant studies have addressed in detail issues such as efficient rezoning of particles and particle number control in the particle in cell (PIC) method [142], as well as convergence problems of vortex particle methods using random rezoning [45].

In the present SPH implementation, the remeshing process maintains the particle resolution while ensuring that the computation of the viscous terms involves a constant number of neighboring particles.
The capabilities of the remeshed SPH (RSPH) methodology developed herein is tested against finite difference calculations for a number of benchmark problems demonstrating the capabilities of the present SPH methodology as a tool for accurate and robust numerical simulations.

This chapter is organized as follows: In Section 2.2 we outline the governing compressible Navier-Stokes equations for viscous and heat conducting flows. In Section 2.3 we present the discretization of the governing equations, and in Section 2.4 the validation of the proposed methodology.

2.2 Governing equations

The fundamental system of differential equations governing the motion of a two-dimensional viscous, heat conducting, compressible medium describe the conservation of mass, momentum and energy. The conservation equations for a caloriically perfect gas without an energy source are:

\[
\frac{D\rho}{Dt} = -\rho \frac{\partial u_i}{\partial x_i} \tag{2-1}
\]

\[
\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \tag{2-2}
\]

\[
\rho c_v \frac{DT}{Dt} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) - p \frac{\partial u_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} \tag{2-3}
\]

where

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right)
\]

where index notation with Einstein’s summation convection is used for vectors and tensors in Cartesian coordinates \((i, j, k = 1, 2)\) and \(x_i\) are the components of the position vector, \(u_i\) the velocity vector components, \(\rho\) is the density, \(p\) the pressure, \(g_i\) the gravitational acceleration component, \(\tau_{ij}\) the viscous stresses, \(T\) the temperature, \(\mu\) the viscosity, \(k\) the thermal conductivity, and \(c_v\) the specific heat at constant volume.

We employ Sutherland’s law to determine the dependence of the viscosity \(\mu\) on the temperature as \(\mu = T^{-\frac{2}{3}} \frac{1+S_1}{T+S_1}\) (where \(S_1\) is a material dependent constant).

The system of the differential equations (2-1), (2-2) and (2-3) is closed with the equation of state for an ideal gas.

\[
p = \rho R T \tag{2-4}
\]

where \(R\) is the gas constant.

The non-dimensional variables are obtained from the physical variables as follows:
2. RSPH for the Simulation of Viscous and Heat Conducting Flow

\[ x^* = \frac{x}{L_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad t^* = \frac{tU_0}{L_0}, \quad u^*_i = \frac{u_i}{U_0}, \quad T^* = \frac{T}{T_0}, \]

\[ p^* = \frac{p}{\rho_0 RT_0}, \quad \mu^* = \frac{\mu}{\mu_0}, \quad g^*_i = \frac{g_i}{g_0}, \quad k^* = \frac{k}{k_0}, \quad c_v^* = \frac{c_v}{c_{v_0}} \]

where the superscript * and the subscript 0 indicate the non-dimensional and the reference quantities. The quantities \( L_0, \rho_0, U_0, T_0, \mu_0, g_0, k_0 \) and \( c_{v0} \) denote the characteristic length, density, velocity, temperature, dynamic viscosity, gravity, thermal conductivity and specific heat at constant volume, respectively. The dimensionless numbers that appear in the equations are:

\[ Re = \frac{\rho_0 U_0 L_0}{\mu_0}, \quad M^2 = \frac{U_0^2}{\gamma RT_0}, \quad Pr = \frac{\mu_0 c_p}{k_0}, \quad Fr = \frac{U_0}{\sqrt{g_0 L_0}}, \]

where \( \gamma \) is the ratio of the specific heat capacities. Re denotes the Reynolds number, M the Mach number, Pr the Prandtl number, and Fr the Froude number. Other dimensionless numbers can be defined as a function of the reference quantities and these dimensionless numbers.

\[ Ra = \frac{g_0 L_0^3 \rho_0^2 c_p \Delta T}{\mu_0 k_0 T_0} = \frac{Re^2 Pr \Delta T}{Fr^2 T_0}, \quad Gr = \frac{Ra}{Pr} = \frac{Re^2 \Delta T}{Fr^2 T_0}, \]

where \( \Delta T \) is a characteristic variation of temperature of the flow, and Ra denotes the Rayleigh number, and Gr the Grashof number.

Finally, the non-dimensional system of governing equations can be written:

\[ \frac{D\rho^*}{Dt^*} = -\rho^* \frac{\partial u^*_i}{\partial x^*_i} \]

\[ \rho^* \frac{Du^*_i}{Dt^*} = -\frac{1}{M^2} \frac{\partial p^*}{\partial x^*_i} + \frac{1}{Re} \frac{\partial \tau^*_y}{\partial x^*_j} + \frac{1}{Fr^2 \rho^*} g^*_i \]

with

\[ \rho^* c_v^* \frac{DT^*}{Dt^*} = \gamma \frac{\partial}{\partial x^*_i} \left( k^* \frac{\partial T^*}{\partial x^*_i} \right) - (\gamma - 1) \rho^* \frac{\partial u^*_i}{\partial x^*_i} + \frac{M^2 \gamma (\gamma - 1)}{Re} \rho^* \frac{\partial u^*_i}{\partial x^*_j} \]

\[ p^* = \rho^* T^* \]

\[ \tau^*_y = \mu^* \left( \frac{\partial u^*_i}{\partial x^*_j} + \frac{\partial u^*_j}{\partial x^*_i} - \frac{2}{3} \delta^*_y \frac{\partial u^*_k}{\partial x^*_k} \right) \]

The information, which is necessary for the initial and boundary conditions, is imposed with the system of differential equations in order to obtain a well-posed problem. The initial conditions are usually prescribed functions that describe the velocity field and the two of the three scalar intensive properties (density, temperature and pressure) of the flow.
2.3 The SPH Method

The method is based on the Lagrangian formulation of the governing equations. The flow quantities are discretized into particles. Each particle \( \alpha \) is associated with a mass \( m_\alpha \), density \( \rho_\alpha \), velocity \( u_\alpha \), viscosity \( \mu_\alpha \), pressure \( p_\alpha \), and position \( r_\alpha \). The initial flow field quantities are interpolated on the particle locations and all the flow quantities can be reconstructed by a linear superposition of the flow quantities carried by the particles weighted by a smooth interpolation kernel. This interpolation is based on the theory of integral interpolants [247, 246], and the interpolated value of any function \( A \) at position \( r \) is expressed as

\[
A(r) = \int A(r') W(r - r', h) dr',
\]

where the integration is over the computational domain, \( W(r,h) \) is an interpolation function, and \( h \) a characteristic distance between the particles which is closely related to the domain of influence of the kernel (smoothing length). The choice of the interpolation kernel is the core of the method. Most SPH simulations use splines kernel (cubic, quartic or quintic) [200, 288, 66]. In our implementation we employ the quartic spline [247, 246]. The quartic spline is constructed from three B-splines requiring kernel and its first, second and third derivative be continuous. The kernel is defined as:

\[
W(r,h) = M_s(r,h) = n_d \begin{cases} 
\frac{s^4}{4} - \frac{5s^2}{8} + \frac{115}{192} & 0 \leq s < \frac{1}{2}, \\
-\frac{s^4}{6} + \frac{5s^3}{6} - \frac{5s^2}{4} + \frac{5s}{24} + \frac{55}{96} & \frac{1}{2} \leq s < \frac{3}{2}, \\
\frac{25 - 5s}{24} & \frac{3}{2} \leq s < \frac{5}{2}, \\
0 & s \geq \frac{5}{2}.
\end{cases}
\]

where \( n_d \) is a normalization constant that depends on the dimensionality of the problem and it is function of the smoothing length \( h \) [247, 246, 189, 186, 191]. The quartic spline has compact support involving 21 neighboring particles contributing to the interpolation (in 2D). The compact support ensures that the number of neighboring particles is finite, thus minimizing the computational cost. The quintic spline interpolant has the same properties with the quartic spline and additionally continuous fourth derivative, but causes an increase in the computational cost (in 2D, 29 neighboring particles contribute in the interpolation). Both kernels are second order accurate.

Numerically, the integral is approximated by a quadrature at the \( N \) particle locations:

\[
A(r) = \sum_b A_b \ V_b \ W(r - r_b, h),
\]

where the summation index \( b \) denotes a particle label and \( V_b \) is the volume of the particle \( b \left( V_b = \frac{m_b}{\rho_b} \right) \).

The particles move in a Lagrangian fashion according to the formula:

\[
\frac{d\vec{x}}{dt} = \ddot{u}
\]

(2-15)
In the context of the scheme proposed by Fishelov [90], if the kernel is differentiable, it is possible to calculate the derivative of any function $A$ at position $r$ as:

$$\frac{\partial A(r)}{\partial x_i} = \sum_b A_b V B \frac{\partial W(r - r_b, h)}{\partial x_i}$$  \hspace{1cm} (2-16)

The equation (2-16) is not in symmetric form but it is possible to rewrite it in symmetric form, when the differentiation is centered on a particle location $\left(\frac{\partial A(r_a)}{\partial x_i} = (\nabla A)_a\right)$, by using the operator:

$$\nabla A = \nabla (FA) - A \nabla F$$  \hspace{1cm} (2-17)

where $F$ is unity. Combining the equations (2-16) and (2-17) the gradient operator at the location of the $\alpha$ particle reads:

$$(\nabla A)_a = \sum_b V_b (A_b - A_a) \nabla W(r_a - r_b, h)$$  \hspace{1cm} (2-18)

An approximation of the second order derivatives, which describe the diffusion terms, is based on the direct computation of the second derivative of the kernel [90, 272].

$$\frac{\partial^2 A(r)}{\partial x_i x_j} = \sum_b A_b \frac{m_b}{\rho_b} \frac{\partial^2 W(r - r_b, h)}{\partial x_i \partial x_j}$$  \hspace{1cm} (2-19)

It is possible to rewrite the second derivative (equation (2-19)) in symmetric form by using the operator

$$\frac{\partial^2 A}{\partial x_i x_j} = \frac{\partial^2 A}{\partial x_i x_j} - A \frac{\partial^1 1}{\partial x_i x_j}$$  \hspace{1cm} (2-20)

and the second order derivative for the location of the $\alpha$ particle can be written:

$$\left(\frac{\partial^2 A}{\partial x_i x_j}\right)_a = \sum_b A_b V B \frac{\partial^2 W(r_a - r_b, h)}{\partial x_i x_j} - A_a \sum_b V_b \frac{\partial^2 W(r_a - r_b, h)}{\partial x_i x_j}$$

$$= \sum_b V_b (A_b - A_a) \frac{\partial^2 W(r_a - r_b, h)}{\partial x_i x_j}$$  \hspace{1cm} (2-21)

The use of symmetric differentiation formulas is important as it leads to simulations where the total momentum is conserved exactly [187].

2.3.1 SPH formulation of the governing equations

2.3.1.1 The Continuity Equation

The continuity equation can be discretized by defining the fluid density via an interpolation of the individual masses carried by the particles [189]

$$\rho_a (r) = \sum_b m_b W(r_a - r_b, h)$$  \hspace{1cm} (2-22)

Alternatively the continuity equation (2-1) may be expressed as:
2.3 The SPH Method

\[
\frac{DP_a}{Dt} = -\rho_a \sum_b V_b \bar{u}_b \cdot \nabla_a W(r_a - r_b, h) \quad (2-23)
\]

where \( V_b \) is the volume of the particle \( b \) \( \left( \nu_b = \frac{m_b}{\rho_b} \right) \). Equation (2-23) is not in symmetric form, but it is possible to rewrite it in symmetric form by using the concept of the Eqn. (2-18), yielding

\[
\frac{DP_a}{Dt} = -\rho_a \sum_b V_b (\bar{u}_b - \bar{u}_a) \cdot \nabla_a W(r_a - r_b, h) \quad (2-24)
\]

Equation (2-24) has now a symmetric form resulting in more accurate simulations than when equation (2-23) is implemented. This equation has the form of the continuity equation proposed by Monaghan [191]

\[
\frac{DP_a}{Dt} = -\sum_b m_b (\bar{u}_b - \bar{u}_a) \cdot \nabla_a W(r_a - r_b, h) \quad (2-25)
\]

An important difference is that in equation (2-24), when remeshing at each time step, the volume of the particles remains practically constant. Hence in our case the weight is the volume of the particles and not the mass. Equation (2-24) is used for the simulations as it has a computational advantage compared to equation (2-22) since the rate of change for all the physical variables can be computed simultaneously. This implies that all equations can be computed simultaneously for all particles. On the other hand, the drawback of this formulation is that the mass conservation is not algebraically guaranteed.

2.3.1.2 The Momentum Equation

The momentum equation (2-2) for a two dimensional flow without the gravitational force can be written for each particle \( \alpha \) as:

\[
\begin{align*}
\left\langle \rho \frac{Du}{Dt} \right\rangle_a &= -\left\langle \frac{\partial p}{\partial x} \right\rangle_a + 4 \left\langle \frac{\partial}{\partial x} \mu \frac{\partial u}{\partial x} \right\rangle_a - 2 \left\langle \frac{\partial}{\partial x} \mu \frac{\partial v}{\partial y} \right\rangle_a \\
&\quad + \left\langle \frac{\partial}{\partial y} \mu \frac{\partial u}{\partial y} \right\rangle_a + \left\langle \frac{\partial}{\partial y} \mu \frac{\partial v}{\partial x} \right\rangle_a \quad (2-26)
\end{align*}
\]

\[
\begin{align*}
\left\langle \rho \frac{Dv}{Dt} \right\rangle_a &= -\left\langle \frac{\partial p}{\partial y} \right\rangle_a + 4 \left\langle \frac{\partial}{\partial y} \mu \frac{\partial v}{\partial y} \right\rangle_a - 2 \left\langle \frac{\partial}{\partial y} \mu \frac{\partial u}{\partial x} \right\rangle_a \\
&\quad + \left\langle \frac{\partial}{\partial x} \mu \frac{\partial u}{\partial x} \right\rangle_a + \left\langle \frac{\partial}{\partial x} \mu \frac{\partial v}{\partial y} \right\rangle_a \quad (2-27)
\end{align*}
\]

where \( \bar{u} = (u, v) \). The symbol \( \left\langle \right\rangle_a \) denotes the discretized quantity for the particle \( \alpha \).

Using the standard SPH formulation [191] and the ideas outlined in previous section, the pressure gradient of the equations (2-26), (2-27) for particle \( \alpha \) can be written as:

\[
\left\langle \frac{\partial p}{\partial x} \right\rangle_a = \sum_b V_b (p_b - p_a) \cdot \frac{\partial}{\partial x} W(r_a - r_b, h) \quad (2-28)
\]
\[
\left\langle \frac{\partial p}{\partial y} \right\rangle_a = \sum_b V_b (p_b - p_a) \cdot \frac{\partial}{\partial y} W(r_a - r_b, h) \quad (2-29)
\]

A general formulation is adopted for the derivation of the viscous terms of the equations (2-26), (2-27) which accounts for variable viscosity \( \mu \) (the viscosity is a function of temperature). The viscous terms can be obtained with the help of the chain rule of differentiation:

\[
\left\langle \frac{\partial}{\partial x^i} \mu \frac{\partial u_k}{\partial x_j} \right\rangle_a = \left\langle \frac{\partial \mu}{\partial x^i} \right\rangle_a \left\langle \frac{\partial u_k}{\partial x_j} \right\rangle_a + \left\langle \mu \frac{\partial^2 u_k}{\partial x^i x_j} \right\rangle_a
\]

\[
\left( \sum_b V_b (\mu_b - \mu_a) \cdot \frac{\partial}{\partial x^i} W(r_a - r_b, h) \right) \left( \sum_b V_b (u_{k,b} - u_{k,a}) \cdot \frac{\partial}{\partial x^j} W(r_a - r_b, h) \right) + \mu_a \sum_b V_b (u_{k,b} - u_{k,a}) \cdot \frac{\partial^2}{\partial x^i x_j} W(r_a - r_b, h)
\]

The last term in equation (2-30) is constructed by using the same idea as for equations (2-19) - (2-21). If the viscosity is constant, the first term in the RHS of the above equation is zero. In this case, the final formulation for the momentum equation is symmetric and it conserves linear and angular momentum. The SPH formulation of the momentum equation terms (equations (2-26) and (2-27)) is obtained in a straightforward manner by combining equations (2-26)-(2-30) as needed. Note that equation (2-30) delivers all derivatives of the viscous terms (where \( i, j, k = 1,2 \) and \( x_1 = x, x_2 = y, u_1 = u, u_2 = v \)).

### 2.3.1.3 The Thermal Energy Equation

The two-dimensional version of the energy equation (2-3) reads

\[
\rho c_v \frac{DT}{Dt} = \left\langle \frac{\partial}{\partial x} k \frac{\partial T}{\partial x} \right\rangle_a + \left\langle \frac{\partial}{\partial y} k \frac{\partial T}{\partial y} \right\rangle_a - \left\langle p \left( \frac{\partial \mu}{\partial x} + \frac{\partial \nu}{\partial y} \right) \right\rangle_a + \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \left\langle \mu \left( \frac{\partial \nu}{\partial x} - \frac{\partial u}{\partial y} \right)^2 \right\rangle_a
\]

(2-31)

The derivation of the SPH formulation of the heat diffusion term, allowing for a temperature-dependent thermal conductivity, is similar to that of the viscous terms of the momentum equation described in the previous section. The final result reads

\[
\left\langle \frac{\partial}{\partial x^i} \left( k \frac{\partial T}{\partial x^j} \right) \right\rangle_a = \left\langle \frac{\partial k}{\partial x^i} \right\rangle_a \left\langle \frac{\partial T}{\partial x^j} \right\rangle_a + \left\langle k \frac{\partial^2 T}{\partial x^i x^j} \right\rangle_a
\]

\[
\left( \sum_b V_b (k_b - k_a) \cdot \frac{\partial}{\partial x^i} W(r_a - r_b, h) \right) \left( \sum_b V_b (T_b - T_a) \cdot \frac{\partial}{\partial x^j} W(r_a - r_b, h) \right) + k_a \sum_b V_b (T_b - T_a) \cdot \frac{\partial^2}{\partial x^i x^j} W(r_a - r_b, h)
\]

(2-32)
The compressibility and the viscous dissipation term in the energy equation can be easily discretized by using the general formula of equation (2-18). The energy by compression can be positive or negative, depending upon whether the fluid is expanding or contracting.

2.3.2 Particle Remeshing

Lagrangian numerical methods enjoy the advantage of automatic adaptivity for their computational elements. However, the flow strain can cluster particles in some regions of the flow field and spread them apart in another. When this occurs, equation (2-19) is not accurately representing diffusion effects resulting in inaccurate simulations. To circumvent this problem, the position of the particles is periodically re-initialized on a uniform grid and the properties of the old particles are interpolated onto the new particle locations. This kind of interpolation has been implemented in a number of calculations involving particle methods [70, 115, 135, 189], but to the best of our knowledge it has not been reported before, in the context of SPH in conjunction with the approximation of the diffusion operator.

For the remeshing procedure two types of interpolation are implemented: a second-order ordinary interpolation, and a third-order smoothing interpolation; these are further discussed in the following sections.

2.3.2.1 Ordinary Interpolation

The second-order ordinary interpolation formula [115, 70] is conserving the interpolated quantity (zero-order moment) as well as its first (impulse) and second moment (angular impulse). This interpolation \( \Lambda_2 \), which is used for the vortex particle simulations [136], can is expressed in one dimension as:

\[
\Lambda_2(x, h) = \begin{cases} 
1 - s^2 & 0 \leq s < \frac{1}{2}, \\
\frac{(1-s)(2-s)}{2} & 0 \leq s < \frac{3}{2}, \\
0 & s \geq \frac{3}{2}.
\end{cases} \tag{2-33}
\]

Then, as shown in Figure 3 (a), the contributions of the jth old particle with property \( Q_j \) located at \( x_j \) contributes in the new ith particle at \( \tilde{x}_i \), the interpolating quantity \( \Delta \tilde{Q}_i \):

\[
\Delta \tilde{Q}_i(\tilde{x}_i) = Q_j(x_j) \Lambda_2(\tilde{x}_i - x_j, h) \tag{2-34}
\]

The interpolation in higher dimensions is obtained using tensorial products in each coordinate direction, using 3, 9 and 27 points, in one, two or three dimensions, respectively. For example in two dimensions:

\[
\Delta \tilde{Q}_i(\tilde{x}_i, \tilde{y}_i) = Q_j(x_j, y_j) \Lambda_2(\tilde{x}_i - x_j, h) \Lambda_2(\tilde{y}_i - y_j, h) \tag{2-35}
\]

The interpolated quantity \( Q_i \) must be an extensive property of the particle that is conserved.
where \( m_j \) is the mass of the particle, \( m_j u_j \) and \( m_j v_j \) are the \( u \) and \( v \) momentum of the particle, and \( E_j \) the total energy of the particle. Note that the interpolation function \( \Lambda_2 \) is discontinuous at the interpolating node locations. This implies that the larger the fluctuations of the interpolating quantity, the larger the interpolation errors are.

\[
Q_j = \begin{pmatrix}
    m_j \\
    m_j u_j \\
    m_j v_j \\
    E_j
\end{pmatrix}, \quad (2-36)
\]

\( Figure 3 \) Detail of remeshing. The shaded cells are affected by the \( j^{th} \) particle. (a) Unbounded domain, (b) Bounded domain.

### 2.3.2.2 Smoothing Interpolation

The smoothing interpolation formulas attempt to minimize the error that the ordinary interpolation might produce providing us with moment-conserving \([115, 70]\) interpolation, which is continuous everywhere inside the interpolation stencil.

\[
M_s(x, h) = \begin{cases}
    1 - \frac{5s^2}{2} + \frac{3s^3}{2} & 0 \leq s < 1, \quad s = \frac{|x|}{h} \\
    \frac{(1-s)(2-s)^2}{2} & 1 \leq s < 2, \\
    0 & s \geq 2.
\end{cases} \quad (2-37)
\]

The interpolation function and its first and second derivative are continuous and reproduce second order polynomials. It uses 4, 16, and 64 points in one, two and three dimensions, respectively.

This interpolation is used in the present SPH implementation in the main computational domain, away from solid boundaries. For further details on the accuracy and the properties of the interpolating functions the reader is referred to \([70]\).
2.3 The SPH Method

2.3.2.3 Interpolation near solid boundaries

Near solid boundaries the remeshing procedure with ordinary or smoothing interpolating formulas cannot be used. The interpolating stencil may extend to the interior of the solid, by introducing spurious computational elements. Hence, in regions near boundaries we are using a biased ordinary interpolation [70] (Figure 3 (b)), which is again second order and conserves the same quantities as ordinary interpolation (conserves the first 2 moments and the quantity $Q_j$):

$$\Lambda(x, h) = \begin{cases} 
1 - \frac{3}{2} s + \frac{1}{2} s^2 & \text{for 1st cell away from the wall}, \quad s = \frac{|x|}{h} \\
\frac{s(2-s)}{s(s-2)} & \text{for 2nd cell away from the wall}, \\
\frac{1}{2} & \text{for 3rd cell away from the wall}, \\
0 & \text{otherwise.}
\end{cases}$$

(2-38)

2.3.3 Numerical implementation

2.3.3.1 Boundary Conditions

All boundary conditions are modeled by boundary particles, which have similar physical properties to those of the particles that represent the flow field. These boundary particles interact with the interior particles in such a way that the necessary boundary conditions are satisfied. (More detailed information for the implementation of boundary conditions can be found in [66, 272]).

For compressible flows the following boundary conditions can be applied, depending on the particular application:

- Inflow boundaries: Prescribed velocity, temperature and pressure,
- Solid surface: No-slip conditions for the velocity and prescribed temperature or heat flux,
- Outflow surface: Prescribed pressure and prescribed gradient of velocity and temperature,
- Symmetry plane: zero gradient normal to the boundary for all scalar quantities and the velocity component parallel to the surface and zero velocity for the component that is normal to the symmetry plane,
- Periodic plane: the computational domain is replicated in space.

2.3.3.2 Time Integration

We implemented second- and third-order Runge-Kutta schemes for the time integration. Higher-order schemes (fourth-order Runge-Kutta) can also be used. However, due to their larger stability limit, they allow integration using larger time steps. This may be detrimental to the overall accuracy of the simulation (as remeshing is performed only after each full time step), leading to additional errors caused by particle disorder in the last stage of the integration (particularly for flows with a large strain rate).
2.3.3.3 Remeshing

Particles are remeshed with a frequency that depend on the strain of the flow field. The number of time steps can vary from one to ten depending upon the flow field and the size of the time step. If the flow field is uniform without recirculation or stagnation regions, the remeshing can be performed after ten or more iterations as particles maintain their uniform distribution. However, for a flow with recirculation (e.g. shear layer), the remeshing procedure is performed every time step. The additional computational cost of the remeshing is less than 10% of the total computational cost even when applied every time step.

The additional computation time resulting from remeshing is a small penalty to pay compared to the significant advantage of ensuring that the particles are always almost equidistant, thus resulting in an accurate approximation of the viscous terms. This is a key aspect of the present work compared to ordinary SPH simulations where the distance between the particles can exhibit large variations.

Additionally, the remeshing procedure resolves one computational problem that usually occurs in SPH simulations. The pressure force in the momentum equation is proportional to the derivative of the kernel, which normally, for B-Splines, reduces to zero when the distance between two particles is small (Figure 4). As a consequence, in such cases the pressure force is attractive and this can introduce large errors in the simulations. The remeshing procedure does not allow the particles to get very close to each other. On the other hand, remeshing introduces numerical errors, which may be viewed as aliasing errors due to the implementation of remeshing kernels with finite support. The extra diffusion that the remeshing procedure introduces can be quite large (with remeshing at every time step). This is indeed a cause of concern. In contrast, it should be pointed out that the added dissipation induced by remeshing is proportional to the gradients of the flow field, which are induced by particle-distance distortion. These gradients remain very small when remeshing is performed at each time step.

![Figure 4](image-url)  
*Figure 4. The Quartic spline (-) and its first (--) and second (--) derivatives as a function of dimensionless distances.*
Using an anti-diffusive process is feasible (e.g. remeshing using Beale’s method [23]). However, there is no clear way to precisely control the error introduced by remeshing since this is strongly coupled with the particular flow map under consideration. Finally, as discussed in [68, 135], the overall effect of remeshing is to act as a subgrid-scale model which has been shown to have a negligible effect on the overall accuracy of the simulations [135].

2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

We examine the validity of our proposed methodology on a series of benchmark one and two-dimensional problems. These problems are:

- Shock Tube problem,
- Taylor-Green flow,
- Double shear layer,
- Lid-driven flow in a cavity,
- Natural convection in a differentially heated cavity and
- Mixed convection in a lid-driven cavity.

2.4.1 One-Dimensional Shock Tube problem

The first test for the SPH method is the shock tube problem. The shock-tube problem is a very interesting test case because the exact time-dependent solution is known and can be compared with the solution computed applying numerical discretization. The initial condition consists of two uniform states separated by a discontinuity located at the origin. This particular initial value problem is known as Riemann Problem. The initial left and right uniform states are usually introduced by specifying density, pressure and velocity. This initial set models a tube where the left and the right regions are separated by a diaphragm, and filled by the same gas in two different physical states. If all the viscous effects are negligible along the tube walls and the tube is infinitely long so as to avoid reflections at the tube ends, the exact solution of the full Euler equations can be obtained on the basis of a simple wave analysis. At the bursting of the diaphragm, the discontinuity between the two initial states breaks into leftward and rightward moving waves, which are separated by a contact surface. Each wave pattern is composed by a contact discontinuity in the middle, and a shock or a rarefaction wave at the left and the right sides separating uniform state solution. The shock-tube problem provides a good test of the ability of a compressible code to capture shocks and contact discontinuities with a small number of zones and to produce the correct density profile in a rarefaction. It also tests the ability to satisfy the Rankine-Hugoniot shock jump conditions.

The example considered here is known as Sod's Problem [256]. The initial data are:

\[
\begin{align*}
\rho &= 1.0 \\
u &= 0.0 \\
p &= 1.0
\end{align*}
\quad \& \quad 
\begin{align*}
\rho &= 0.25 \\
u &= 0.0 \\
p &= 0.1795
\end{align*}
\]

The ratio of specific heats \(\gamma\) is chosen to be 1.4 on both sides of the interface, with the pressure in the left region being greater than in the right one, the pressure discontinuity results in a shock wave,
propagating to the right. In addition, the central contact discontinuity propagates to the right, while a rarefaction wave propagates to the left of the origin.

*Figure 5* shows the numerical results at time $t=0.15$. The classical SPH [194] and the remeshed SPH (using 400 particles and $-0.5 < x < 0.5$) are compared with the exact solution. The overall behavior of RSPH is slightly better than the original SPH. It is obvious that the remeshing is not smoothing the discontinuities more than the original SPH.

*Figure 5* Sod’s shock-tube problem: (-) SPH with remeshing (RSPH), (--) classical SPH (without remeshing), (---) exact solution

### 2.4.2 Two-Dimensional Taylor-Green flow

As a test of the viscous SPH calculations we perform a simulation of the Taylor-Green flow. Taylor-Green flow consists of a periodic decaying array of vortices in the $x$-$y$ plane (*Figure 6*) specified in non-dimensional form by:

\[
\begin{align*}
    u(x, y, t) &= -U e^{bt} \cos(2\pi x) \sin(2\pi y) \\
    v(x, y, t) &= U e^{bt} \sin(2\pi x) \cos(2\pi y) \\
    p(x, y, t) &= p_{ref} - \frac{U^2}{4} e^{bt} \left( \cos(4\pi x) + \cos(4\pi y) \right)
\end{align*}
\] (2-39) (2-40) (2-41)

where $b = \frac{-8\pi^2}{\text{Re}}$ and $p_{ref} = \frac{1}{\gamma M^2}$. The reference Mach number $M$ is set to 0.5, the velocity $U$ is taken as 0.04 and the computational domain was the unit square $[0,1] \times [0,1]$. The simulations are performed for a wide range of the Reynolds number (0.1-1000) to test the accuracy of the method in cases where the viscous effects are either dominant (small Re), comparable (intermediate Re), or minimal (large Re) with respect to the inertial forces. The boundary conditions are periodic in all directions. A third-order Runge-Kutta scheme with constant time step is employed in all the
2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

Simulations. The smoothing interpolation formula $M'_4$ (equation (2-37)) was used at every time step for the remeshing. The time-dependent behavior of the maximum velocity of the flow for $Re=1$ calculated from RSPH (with 15625 particles, corresponding to 125 particles in each direction) is presented in Figure 7, and is compared to the analytical solution for an incompressible fluid and with numerical results from a compressible finite difference code.

![Streamlines of the Taylor-Green flow.](image)

*Figure 6* Streamlines of the Taylor-Green flow.

![Decay of maximum velocity for Re=1. Comparison of the RSPH solution with 15625 particles (-) with the exact incompressible solution (●) and with a high-order finite differences solution (+) [233].](image)

*Figure 7* Decay of maximum velocity for $Re=1$. Comparison of the RSPH solution with 15625 particles (-) with the exact incompressible solution (●) and with a high-order finite differences solution (+) [233].

The finite difference code is a Navier-Stokes solver in conservative form that uses 5th and 6th order compact Padé scheme for the convective and viscous terms, respectively and 3rd order Runge-Kutta for time integration [233]. The compressibility ($M=0.5$) effects have negligible influence in the Taylor-Green flow so that the incompressible analytical solution can be compared to the computational results. For the error analysis of the RSPH simulations the relative error ($L_\infty$) is used:

$$L_\infty = \max_{t=0}^{T_{max}} \left| \frac{u'_{ex} - u'_{SPH}}{u'_{ex}} \right|.$$
where $u_{ex}^t$ denotes the maximum velocity of the exact incompressible solution at time $t$, and $u_{SPH}^t$ the maximum velocity of the RSPH simulation at time $t$, and $T_{\text{max}}$ is the time where $u_{ex}^{T_{\text{max}}} = \frac{U}{50}$. The relative error ($L_\infty$) of the SPH calculations is less than 5% for Re=1 and decreases as the number of particles is increased (Figure 8).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure8.png}
\caption{$L_\infty$ error of RSPH simulations of the Taylor-Green flow for different particle resolutions (Re=1).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure9.png}
\caption{$L_\infty$ error of RSPH simulations of the Taylor-Green flow for different Reynolds number. (-) Simulation with 15625 particles and (--) with 40000 particles.}
\end{figure}

The RSPH simulation with 15625 particles remains accurate ($L_\infty < 4\%$) and particle resolution independent until Re=100 but it is necessary to increase the particle resolution for larger Reynolds numbers (Re=1000) (Figure 9).
2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

2.4.3 Two-Dimensional Double Shear layer

The second test for the RSPH calculations is the double shear layer (Figure 10), where the initial flow field consists of a horizontal shear layer of finite thickness, perturbed by a small amplitude vertical velocity.

\[ u(x, y) = U_o + (1 - U_o) e^{-((10y)^4)} \]  
\[ v(x, y) = \delta \sin(2\pi x) \cos(2\pi y) \]

where \( U_0 = -1 \) and \( \delta = 0.01 \). For the initial temperature the Crocco-Busemann relation is employed, which yields a general relation for the dependence of temperature on velocity, with the assumption of a Prandtl number of unity \[243\].

\[ T(x, y) = M^2 \frac{Y - 1}{2} \left[ u(x, y)(1 + U_0) - u(x, y)^2 - U_0 \right] + T_0 \frac{1 - u(x, y)}{(1 - U_0)} + \frac{u(x, y) - U_0}{(1 - U_0)} \]

where \( T_0 = 0.5 \) and \( M \) is the Mach number. For the simulation the following case was considered:

\[ M = 0.5 \quad \text{Re} = 1000 \quad \text{Pr} = 0.72 \]

and the computational domain was set to \([-0.5,0.5] \times [-0.5,0.5]\). For validation of the SPH calculations, the same high-order compressible finite difference code \[233\] as in example 2.4.2 above was employed. Both RSPH and finite difference simulations must be comparable from a common initial condition that satisfies the Navier-Stokes and the energy equations. The RSPH simulation is initialized from the finite difference solution at time \( t=0.3 \) by using a 7th order polynomial interpolation. From the comparison of density snapshots (Figure 11), one may observe that the two methods produce similar results. It is also clear that RSPH is smoothing the values of the physical quantities.

This is more apparent in the vorticity contours (Figure 12 and Figure 13). The time histories at two locations \((x,y)=(-0.25,-0.25)\) and \((x,y)=(0,0)\) in the domain show that the RSPH and finite difference solution exhibit the same behavior. RSPH seems able to capture almost all the details of the flow at these points with some smoothing of the amplitude (Figure 14 and Figure 15).
The double shear layer is a demanding benchmark problem as many numerical methods exhibit the generation of spurious structures at the thin shear layers [181]. The present RSPH methodology does not encounter this difficulty, although the results exhibit more dissipation compared to a high order finite difference scheme.

Figure 11 Density contour for smooth shear layer: Left RSPH solution with 90000 particles, right finite difference solution on a 150x200 grid [233].

Figure 12 Vorticity contours at time $t=3.0$: RSPH solution for 40000, 90000 and 160000 particles and finite difference solution on a 150x200 grid [233].
2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

Figure 13 Vorticity contours at time $t=5.0$: RSPH solution for 40000, 90000 and 160000 particles and finite difference solution on a 150x200 grid [233].

Figure 14 Time history of density, temperature, u and v velocity at point $x=-0.25$, $y=-0.25$: (-) RSPH simulation with 160000 particles, (-o-) finite differences simulation [233].
2. RSPH for the Simulation of Viscous and Heat Conducting Flow

![Time history of density, temperature, u and v velocity at point x=0, y=0: (-) RSPH simulation with 160000 particles, (-o-) finite differences simulation [233].](image)

**Figure 15** Time history of density, temperature, u and v velocity at point x=0, y=0: (-) RSPH simulation with 160000 particles, (-o-) finite differences simulation [233].

2.4.4 Lid-driven Flow in a Square Cavity

The driven cavity problem has been used to validate the RSPH in the presence of walls. For this simulation the characteristic numbers are taken as:

\[ M = 0.1, \quad Re = 100, \quad Pr = 0.72. \]

Because the Mach number is set to 0.1, the flow is considered practically incompressible. It is possible to set the Mach number smaller than this value but the time step of the calculations will be (unnecessarily) small, since it is proportional to the square of the Mach number (equation (2-9)). In the RSPH simulation 62500 particles are used (corresponding to a grid of \( [250 \times 250] \) nodes). Time integration is performed with a two-stage Runge-Kutta scheme, and the field is reinitialized every time step by using the smoothing interpolation formula in the main field and the ordinary and the one-side interpolation near the boundaries. For validation of the computations, the benchmark solution of Ghia et al. [98] is employed. The comparison of RSPH with the numerical results of Ghia et al. shows very good agreement for the vorticity along the moving boundary and the boundary layers in the stationary and moving walls (Figure 16 and Figure 17). The central and the secondary recirculation zones are predicted accurately (Figure 18) (compared to the benchmark solution [98], page 404, figure 4).
2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

*Figure 16* Vorticity along the moving boundary, and v velocity along horizontal line through geometric center of the cavity for Re=100. (-) RSPH simulation, (●) Ghia et al. [98]

*Figure 17* Horizontal u velocity along the vertical line through the geometric center of the cavity for Reynolds 100. (-) RSPH simulation, (●) Ghia et al. [98]

*Figure 18* Vorticity contours for flow in a driven cavity (Re=100).
2.4.5 Natural convection in a differentially heated cavity

Here, the RSPH implementation is tested for the problem of buoyant laminar flow in a closed cavity with side walls remaining at constant but different temperature, and with insulated bottom and top walls. In order to take into account the buoyancy forces, the gravitational force is included in the momentum equation (2-2), and the hydrodynamic pressure in the equation of state (2-4). The characteristic dimensionless numbers of the simulation are:

\[ M = 0.1, \quad Ra = 10^3 \& 10^4, \quad Pr = 0.71. \]

For the RSPH simulation 63000 particles are used, and the solution is compared to the benchmark solution of de Vahl Davis [74] (Table 1). The relative error is less than 8% for all quantities shown in Table 1, demonstrating good agreement with the benchmark solution.

Table 1 Comparison of the SPH simulation with the benchmark solution of Vahl Davis [74].

<table>
<thead>
<tr>
<th>Ra</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10^3</td>
<td></td>
<td>10^4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Benchmark</td>
<td>SPH</td>
<td>error %</td>
<td>Benchmark</td>
</tr>
<tr>
<td>U_{max}</td>
<td>3.649</td>
<td>3.431</td>
<td>5.97</td>
<td>16.178</td>
</tr>
<tr>
<td>Y</td>
<td>0.813</td>
<td>0.812</td>
<td>0.12</td>
<td>0.823</td>
</tr>
<tr>
<td>V_{max}</td>
<td>3.697</td>
<td>3.511</td>
<td>5.03</td>
<td>19.617</td>
</tr>
<tr>
<td>X</td>
<td>0.178</td>
<td>0.176</td>
<td>1.12</td>
<td>0.178</td>
</tr>
<tr>
<td>N_{u_{ave}}</td>
<td>1.118</td>
<td>1.037</td>
<td>7.25</td>
<td>2.243</td>
</tr>
<tr>
<td>N_{u_{1/2}}</td>
<td>1.118</td>
<td>1.039</td>
<td>7.07</td>
<td>2.243</td>
</tr>
<tr>
<td>N_{u_{0}}</td>
<td>1.117</td>
<td>1.033</td>
<td>7.35</td>
<td>2.238</td>
</tr>
<tr>
<td>N_{u_{max}}</td>
<td>1.505</td>
<td>1.392</td>
<td>7.51</td>
<td>3.528</td>
</tr>
<tr>
<td>Y</td>
<td>0.092</td>
<td>0.098</td>
<td>6.52</td>
<td>0.143</td>
</tr>
<tr>
<td>N_{u_{min}}</td>
<td>0.692</td>
<td>0.705</td>
<td>1.88</td>
<td>0.586</td>
</tr>
<tr>
<td>Y</td>
<td>1.000</td>
<td>1.000</td>
<td>0.00</td>
<td>1.000</td>
</tr>
</tbody>
</table>

**U_{max}** maximum horizontal velocity on the vertical mid-plane of the cavity and its y position;

**V_{max}** maximum vertical velocity on the horizontal mid-plane of the cavity and its x position;

**N_{u_{ave}}** the average Nusselt number throughout the cavity;

**N_{u_{1/2}}** the average Nusselt number on the vertical midplane

**N_{u_{0}}** the average Nusselt number on the vertical boundary of the cavity at x=0;

**N_{u_{max}}** the maximum value of the local Nusselt number on the vertical boundary of the cavity at x=0 and its position;

**N_{u_{min}}** the minimum value of the local Nusselt number on the vertical boundary of the cavity at x=0 and its position;

**error** relative error between the benchmark and SPH solution.

Similar accuracy is observed for the flow velocity and temperature fields (**Figure 19**) (compared to the benchmark solution [74], page 257, figure 4 (a) and (b) and page 259, figure 7 (a) and (b)).
2.4 Validation of RSPH methodology, for Isothermal and non-Isothermal Viscous flows

2.4.6 Mixed convection in a driven cavity

The last test for the RSPH implementation is the problem of mixed convection in a driven cavity. The top wall of a lid driven cavity moves with constant speed and it is at a constant temperature (hot). The other three walls are stationary. The side walls are adiabatic, and the bottom wall is isothermal (cold). The non-dimensional numbers of the simulation are:

$\text{Ma} = 0.1, \text{Re} = 400, \text{Pr} = 0.71, \text{Gr} = 10^2,$

and 63000 particles are used. The RSPH solution is compared with the numerical results of Iwatsu et al [120].

![Figure 19 Contours of temperature T for (a) Ra=10^3, (c) Ra=10^4, and vorticity for (b) Ra=10^3, (d) Ra=10^4 of the RSPH simulation with 63000 particles.](image1)

Figure 19 Contours of temperature T for (a) Ra=10^3, (c) Ra=10^4, and vorticity for (b) Ra=10^3, (d) Ra=10^4 of the RSPH simulation with 63000 particles.

![Figure 20 Temperature along the vertical line through the geometric center of the cavity for Re=400 and Gr= 10^2. (-) RSPH simulation with 63000 particles, (●) Iwatsu et al. [120].](image2)

Figure 20 Temperature along the vertical line through the geometric center of the cavity for Re=400 and Gr= 10^2. (-) RSPH simulation with 63000 particles, (●) Iwatsu et al. [120].
A schematic representation of the temperature profile along the vertical line through the geometric center of the cavity is presented in Figure 20, showing good agreement near the cold wall. The small difference of the temperature near the hot wall has minimal effect on the heat transfer coefficient (local Nusselt number) (Figure 21).

![Figure 21](image)

Figure 21: Local Nusselt profile at the top wall of the cavity for Re=400 and Gr=10^2. (-) RSPH simulation with 63000 particles, (●) Iwatsu et al.[120]

2.5 Summary

The present results indicate that Smooth Particle Hydrodynamics coupled with remeshing is an accurate numerical method to simulate low Mach number compressible viscous and heat conductive flows. The accuracy of the developed RSPH method comes with a minimal additional computational cost, while maintaining the adaptive character of the method. The implementation of high order remeshing schemes improves the accuracy of SPH and additionally increases the computational efficiency of the algorithm. The existence of high-frequency acoustic waves, which are resolved in the simulations, places a severe restriction on time-stepping increments. In the present study it is assumed that a Mach number less than 0.3 corresponds to a practically incompressible flow, which is a reasonable assumption [290].

The SPH implementation as a compressible flow algorithm can compute natural convection flows with large temperature differences thus providing us with a computational tool which exceeds the validity and therefore capability of Boussinesq-type models.

The remeshing scheme, due to its tensorial character, can be easily extended to 3-D allowing the proposed RSPH methodology to be employed for the simulation of 3-D flows.
Chapter 3

Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of single and double jet impingement on a heated surface, using Remeshed Smoothed Particle Hydrodynamics

3.1 Background

Jet impingement is a technique for enhancing heat transfer that is employed in a variety of applications ranging from drying of textiles and films, to metal sheet manufacturing and to gas turbine and electronic equipment cooling. Due to its importance, jet impingement heat transfer has been the topic of numerous investigations in recent years (see for example [173, 220, 285, 155]). Most of the previous studies have focused on optimizing transport process associated with steady jet impingement. Configurations that have received attention include impingement of axisymmetric (circular) and slot (two dimensional) jets, with different spacing between the jet(s) and the impingement surface, or different inlet velocity profiles (flat, developed, or inclined), and with or without confinement [173, 220, 285, 97, 80, 178, 261, 241, 116].

More recently, researchers started pursuing experimentally and numerically heat transfer enhancement via flow pulsation [131, 85, 296, 14, 185, 252, 183, 184, 242, 253, 182]. Some investigations involving jet pulsation show no enhancement or even deterioration of heat transfer due to pulsation [14, 252], because the pulsation energy in these studies affects mainly the large scales of the flow and not the small structures which can enhance the mixing. Others reported a marginal beneficial effect of pulsation [107]. There are also some studies which reported significant enhancement [85, 184, 242, 297], due to either the interaction of large scale structures with the boundary layer (periodic formation of vortical structures which impinge upon the heat transfer surface), or due to the secondary flow structures (vortex rings), or even due to chaotic mixing which mimics the beneficial effects of turbulence [183, 184, 182].

This chapter is presenting a basic research work that considers air jets, impinging on a heated solid wall at constant temperature or heat flux. This jet impingement arrangement is attractive due to its simplicity and to the high convective heat transfers coefficients it yields, corresponding to low wall temperatures. Most of the studies of jet impingement with pulsation presented until now focus on single jet configurations (Figure 22 (a)).

An early investigation of two-dimensional jet array impingement on an isothermal plate [97] showed heat transfer reduction but improved heat flux uniformity compared to the single jet geometry. Recently, Sheriff & Zumbrunnen in [253] investigated experimentally the effect of flow pulsation on the cooling performance of jet arrays and reported improved heat transfer uniformity as well as presence of coherent structures, but no significant enhancement, with respect to the heat transfer characteristics.

The focus of the present chapter is the investigation of a single and pair of pulsed slot jet impingement, in an absolute sense, as well as in comparison with single pulsed jet impingement at the same flow rate (Figure 22 (b)). More specific, in section 3.3.1 results of pulsating single jet
impingement on isothermal surface are presented. In section 3.3.2 results of single and pair pulsating jet impingement on a heated surface (constant heat flux) are shown and the dynamic analysis of system responses are also presented. In section 3.3.3 a quantitative analysis of a conjugate heat transfer problem is shown.

![Figure 22](image.png)

*Figure 22* Schematic representation of: (a) A single slot jet impingement on a heated surface, (b) a pair of planar air jets impingement on a heated surface.

### 3.2 Governing Equations and SPH Methodology

#### 3.2.1 Basic equations

The fundamental system of differential equations governing the motion of a viscous, heat conducting, compressible medium consists of the continuity, momentum and energy equations. The conservation equations for a calorically perfect gas without an energy source in non-dimensional form are explained in section 2.2 (equations (2-1) - (2-11)).

#### 3.2.2 Numerical Method

The RSPH method (Section 2.3) is used in the present study for the discretization and numerical solution of the governing equations. All the boundary conditions are modeled by boundary particles (imaginary particles), which have similar physical properties with the particles that represent the flow field. The boundary particles interact with the interior particles in such a way that the boundary conditions are satisfied. More detailed information for the implementation of boundary conditions in the SPH method can be found in [272, 200].
3.3 Results and Discussion

3.3.1 Jet impingement on isothermal surface

3.3.1.1 Single jet impingement normally on isothermal surface

The present work considers an air jet, exiting from a slot and impinging on an isothermal target solid. Such air jets can be easily obtained using a large aspect ratio of rectangular channel or a slot. The jet impingement arrangement is attractive due to its simplicity and to the high convective heat transfer coefficients it yields, corresponding to high heat fluxes. This study represents the first step toward the modeling of applied engineering process using the RSPH methodology.

The flow field of the impinging jet can be subdivided into three characteristic regions: the free jet region, the stagnation flow region and the wall jet region.

- The free jet region is characterized by the viscous interaction of the exiting jet with the ambient air. The global effects in this region include the development of a non-uniform velocity profile within the jet, expansion of the jet, and modification of the jet temperature before it impinges upon the surface.
- The stagnation region is characterized by the turning of the jet.
- The wall jet region is characterized by a bulk flow in the outward direction.

The computational domain is shown in Figure 23, where B is the slot width, H the nozzle-to-impingement surface spacing and L the impingement plate length. The Reynolds number is defined as:

\[
\text{Re}_B = \frac{V_{\text{jet}} \rho B}{\mu}
\]

(3-1)

Figure 23 Computational domain

Unless otherwise noted, the typical ratios H/B=5 and L/B=20 are fixed in all our computational experiments. Due to the small value of the ratio H/B and the low value of Re_B (100<Re_B<400), preliminary computational simulations for the entire domain have shown that the flow remains symmetric about the y-axis and therefore only half of the domain is considered in the computations. The correct implementation of the initial and boundary conditions for RSPH simulations sometimes
requires substantial care. The direct coupling between momentum and energy implies that the initial conditions must satisfy the equations. More specifically, in the present study, the inflow boundary condition region I in Figure 23 needs special treatment to ensure that it does not introduce noise in the numerical experiments. For this reason, it is necessary to derive a relation between temperature and velocity at the inlet region I.

The procedure, described in White [290], is to search for a solution of temperature as a function of velocity. With the assumption of a Prandtl number of unity [243], the steady two-dimensional momentum and energy equations for fully developed channel flow (or for boundary layer flow) for of a compressible perfect gas can be combined to obtain:

\[
\frac{d^2 T}{dv^2} = -M^2 (y - 1) \tag{3-2}
\]

which can be integrated twice to yield an algebraic relation between temperature and velocity. For this integration two initial conditions are used

\[
v = 0 \Rightarrow T = T_0
\]

\[
v = V_{jet} \Rightarrow T = T_{jet} \tag{3-3}
\]

where \(V_{jet}\) denotes the jet mean velocity, and where \(T_0\) and \(T_{jet}\) are the ambient and the jet mean temperature, respectively. The inflow boundary conditions then read:

\[
u = 0 \quad v = V_{jet} (1 + A \sin(\omega t))
\]

\[
T = T(v) \quad \rho = \frac{1}{T}
\tag{3-4}
\]

where \(A\) and \(\omega\) denote the amplitude and the frequency of the jet pulsing.

The confinement plate, region II in Figure 23, is defined as an adiabatic wall (no-slip, \(dT/dy = 0\)), the outflow is defined as a zero gradient (\(du/dx = dv/dx = 0\)) and ambient pressure boundary, the impingement plate is defined as a solid isothermal wall (no-slip, \(T = T_w\)) and the axis of symmetry as a zero gradient boundary (\(u = dv/dx = dT/dx = d\rho/dx = 0\)).

The four-stage Runge-Kutta time integration method is used in the RSPH implementation. The Runge-Kutta schemes are well suited for the integration of the particle trajectories after remeshing, since they do not need information from the previous time step. Remeshing is applied over a finite number of time steps. The number of time-steps can vary from one to ten depending upon the flow field and the time step size. In the present study, remeshing is evaluated at every time step. This procedure introduces numerical dissipation, which is, however, minimal and of negligible influence to the computational results [135].

The local heat transfer can be expressed as

\[
h = -\frac{1}{T_w - T_{jet}} k \frac{dT}{dy} \bigg|_{w}
\tag{3-5}
\]

and it is function of the position along the impingement plate. Accordingly, the local and stagnation Nusselt numbers can be evaluated respectively as,

\[
Nu = \frac{h L}{k} \tag{3-6}
\]
3.3 Results and Discussion

and

$$\text{Nu}_{av} = \frac{h_{x=0} \cdot L}{k} \quad (3-7)$$

The average heat transfer coefficient and the average Nusselt number on the isothermal impingement plate in this study are evaluated as

$$h_{av} = \frac{1}{L} \int_{0}^{L} h \, dx \quad (3-8)$$

$$\text{Nu}_{av} = \frac{h_{av} \cdot L}{k} \quad (3-9)$$

Simulations are performed for $100 < \text{Re}_{B} < 400$ which corresponds to fully laminar jets. The Prandtl is 0.72 and the Mach number is 0.1. It is assumed that a Mach number less than 0.3 correspond to a practically incompressible flow. For the RSPH simulations, 67000 particles are used and produced a fully resolved solution (as shown in Section 2.4). The results are compared with experimental and numerical results of other investigators [97, 261, 6, 158]. Figure 24 presents the variation of the local Nusselt number along the isothermal impingement plate.

**Figure 24** Nusselt number variations along the plate. RSPH (-) $\text{Re}_{B}=200$, $H/B=4$ with uniform jet profile, RSPH (- -) $\text{Re}_{B}=200$, $H/B=5$ with uniform jet profile, Al-Sanea [6] (o) $\text{Re}_{B}=200$, $H/B=4$ with uniform jet profile, Sparrow & Wong [261] (●) $\text{Re}_{B}=150$, $H/B=5$ with parabolic jet profile.

The comparison shows good agreement with the results of earlier investigators for incompressible flows at similar conditions. Table 2 presents the stagnation and average Nusselt number, computed with RSPH (present study) and compares it with the values of an experimental correlation of Lin et, al. [158] of error margin 14.6% and numerical results of Al-Sanea [6]. The relative difference is always smaller than the maximum deviation of the correlation. Overall, the performance of the SPH method is deemed as indeed satisfactory.
Table 2 Comparison of stagnation and average Nusselt number for an unpulsed jet between RSPH and the correlations from Lin et al. [158] and Al-Sanea [6].

<table>
<thead>
<tr>
<th>Re_B</th>
<th>Nu_s SPH</th>
<th>Lin et al. [158]</th>
<th>Nu_s SPH</th>
<th>Al-Sanea [6]</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>101.7</td>
<td>91.1</td>
<td>28.4</td>
<td>31.1</td>
</tr>
<tr>
<td>200</td>
<td>138.9</td>
<td>128.8</td>
<td>43.8</td>
<td>48.8</td>
</tr>
<tr>
<td>400</td>
<td>183.6</td>
<td>182.2</td>
<td>66.9</td>
<td>74.6</td>
</tr>
</tbody>
</table>

Numerical simulations are performed with a sinusoidal pulsed jet (equation (3-4)). The range of the parametric values is indicated in Table 3. To compare the heat transfer coefficients, we introduce a normalization based on the coefficients of the steady state simulations presented in Table 2:

\[ \frac{N_u^{\text{s}}}{N_u^{\text{ss}}} = \frac{N_u^{\text{av}}}{N_u^{\text{av ss}}} \quad (3-10) \]

The time-averaged Nusselt number is based on the time-averaged heat transfer coefficient

\[ N_u^{\text{av}} = \frac{h_{av,T} L}{k} \quad (3-11) \]

where

\[ h_{av,T} = \frac{1}{T_{\text{pulse}}} \int_{t=t_{1}}^{t_{1}+T_{\text{pulse}}} h_{av} dt \quad (3-12) \]

and \( T_{\text{pulse}} \) is the period of the pulsing.

Table 3 Parametric range of simulations with sinusoidal pulse.

<table>
<thead>
<tr>
<th>Re_B</th>
<th>A</th>
<th>Str_B</th>
<th>Case</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.5</td>
<td>0.04</td>
<td>A</td>
</tr>
<tr>
<td>200</td>
<td>0.5</td>
<td>0.008</td>
<td>B</td>
</tr>
<tr>
<td>200</td>
<td>0.5</td>
<td>0.02</td>
<td>C</td>
</tr>
<tr>
<td>200</td>
<td>0.5</td>
<td>0.04</td>
<td>D</td>
</tr>
<tr>
<td>200</td>
<td>0.5</td>
<td>0.08</td>
<td>E</td>
</tr>
<tr>
<td>200</td>
<td>1.0</td>
<td>0.04</td>
<td>F</td>
</tr>
<tr>
<td>400</td>
<td>0.5</td>
<td>0.04</td>
<td>G</td>
</tr>
</tbody>
</table>

In the present section, we focus on the influence of frequency, amplitude and Reynolds number on the heat transfer coefficients. In Figure 25, the influence of the frequency on the normalized averaged Nusselt number is presented as a function of the phase angle. The different cases are defined in Table 3. Each curve corresponds to a different Strouhal number (different frequency of the pulse) for the same Reynolds number (Re_B=200) and amplitude (A=0.5). Starting from the lower Strouhal number (case B) the averaged Nusselt number shows an increase (albeit very small) compared to the unpulsed case (Table 2). This case (case B) yields an increase of 0.12% in the time-averaged Nusselt number calculated from equations (3-11) and (3-12) (Table 4). Increasing the Strouhal number...
(case C) the fluctuation amplitude of the normalized average Nusselt number values rises significantly, but the increase in the time averaged Nusselt number is only 1.53%.

Figure 25 Normalized average Nusselt number as a function of phase angle for different Strouhal numbers: Case B (- - -), case C (- -), case D (-), case E (- -).

Table 4 Percentage increase of time averaged Nusselt number for different Strouhal numbers

<table>
<thead>
<tr>
<th>Case</th>
<th>Strouhal</th>
<th>$\left( Nu_{av,r} - Nu_{av,s} \right)/Nu_{av,s}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.008</td>
<td>0.12</td>
</tr>
<tr>
<td>C</td>
<td>0.02</td>
<td>1.53</td>
</tr>
<tr>
<td>D</td>
<td>0.04</td>
<td>3.41</td>
</tr>
<tr>
<td>E</td>
<td>0.08</td>
<td>1.92</td>
</tr>
</tbody>
</table>

Upon a further doubling of the Strouhal number (case D), the fluctuation amplitude of the normalized average Nusselt number decrease but the overall heat transfer enhancement is 3.41% (Table 4). For an even higher Strouhal number (case E), the fluctuations and the time average heat transfer decrease observably, approaching the unpulsed jet limit. In summary, for the parametric domain of Figure 25, the influence of the frequency on the time- and length-averaged Nusselt number is non monotonic and overall very weak, although the effect of frequency on the length averaged Nusselt number is marked. This was also observed in experiments of planar [184] and round jets [14]. The effect of frequency on the heat transfer can be explained from the velocity field during one pulse period near the stagnation region (Figure 26). The results show a periodic generation of vortices near the nozzle (Figure 26(a)).

These vortices can enhance the mixing between the cold and the hot regions in some cases and increase the heat transfer (Figure 26 (c), (d)). It is interesting that in the steady-jet (unpulsed) situation there is neither traveling nor co-existence of vortices but only one vortex core. The distance between these vortices is dependent on the frequency of the pulse represented by the Strouhal number.
For higher Strouhal numbers the vortices can cancel each other out due to viscosity. For smaller Strouhal numbers the vortices exist, but are not ideally spaced or located within the domain and the enhancement of heat transfer is smaller. It appears that an optimum frequency must exist for heat transfer enhancement. As will be discussed later, the amount of enhancement is amplitude dependent; for the amplitude of Figure 25 this effect was marginal.

![Figure 26 Snapshots of velocity vectors for the case D during one pulse period.](image)

The amplitude of the pulse has a significant influence on heat transfer (Figure 27). The major effect of the amplitude is reported in [184] where an increase as high as 80% in time-averaged Nusselt number is measured above the steady-jet (unpulsed) results. In the present simulations, the time-averaged Nusselt number increase is 14%. The flow field shows (not shown here for brevity) that when the amplitude of the pulse increases, the generated vortices penetrate more in the wall jet region and boost the heat transfer.

The Reynolds number in the range (100-400) has a weak effect on the Nusselt number (Figure 28); in this range of fully laminar flow the flow characteristic do not change significantly, resulting in a corresponding marginal change in the heat transfer.

### 3.3.1.2 Conclusions

Heat transfer from a laminar pulsed jet has been studied numerically using the remeshed smooth particle hydrodynamics (RSPH) methodology. The numerical results indicate that within the investigated parametric domain, the amplitude of the jet oscillation had a marked effect on the overall heat transfer, while the frequency effect was marginal. Also marginal was the effect of the Reynolds number within the laminar regime. The pulsation generates periodic vortices near the nozzle, which travel toward the plate and enhance the mixing between the cold and the hot regions.
3.3 Results and Discussion

Figure 27 Normalized average Nusselt number as a function of phase angle for different jet amplitudes: Case D (-), case F (---).

Figure 28 Normalized average Nusselt number as a function of phase angle for different Reynolds numbers: Case A (---), case D (-), case G (---).

3.3.2 Jet impingement on a heated surface with constant heat flux

3.3.2.1 Pair jet impingement on a heated surface

The work presented in this section focuses on the effect of jet pulsation on the heat transfer and fluid dynamics characteristics of single and double jet impingement on a constant heat flux heated surface. In principle, a particular flow problem may be solved by integrating the mass, momentum and energy equations, which are described in section (Chapter 2), together with the equation of state. The initial conditions and/or boundary are prescribed functions that describe the velocity field and the two of the three scalar intensive properties (density, temperature and pressure) of the flow.

The computational domains used in the present section are shown in Figure 22 (a)-(b). The inflow conditions are parabolic velocity profile at constant (ambient) temperature.
3. Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of jet impingement using RSPH

**Single Jet:**

\[
\begin{align*}
  u &= 0, \\
  v &= v_{\text{max}} \left( 1 - \frac{x^2}{B^2} \right), \\
  T_{\text{inlet}} &= 1
\end{align*}
\] (3-13)

where \( v_{\text{max}} \) is the time dependent maximum velocity of the jet (at the centerline)

\[
v_{\text{max}} = V_{\text{max}} \left( 1 + A \sin(\omega t) \right)
\] (3-14)

**Pair of Jets:**

\[
\begin{align*}
  u &= 0, \\
  v &= v_{\text{max}} \left( 1 - \frac{\left( \frac{x - L_T}{2} \right)^2}{\left( \frac{B}{2} \right)^2} \right), \\
  T_{\text{inlet}} &= 1
\end{align*}
\] (3-15)

As in the case of a single jet,

\[
v_{\text{max}} = V_{\text{max}} \left( 1 + A \sin \left( \omega t \pm \frac{\phi}{2} \right) \right)
\] (3-16)

where \( A \) and \( \omega \) denote the amplitude and the frequency of the jet pulse, \( V_{\text{max}} \) denotes the jet time-averaged maximum velocity (at the centerline), and \( \phi \) denotes the phase angle between the two jets.

The average jet velocity \( \langle V \rangle \) of the parabolic profile is

\[
\langle V \rangle = \frac{2 V_{\text{max}}}{3}
\] (3-17)

The Reynolds number is defined as

\[
Re = \frac{\langle V \rangle \rho D_h}{\mu}
\] (3-18)

where \( D_h \) is the slot hydraulic diameter; \( D_h = 4B \) for the single jet and \( D_h = 2B \) for the jet-pair configurations, respectively.

The top plate is defined as an adiabatic wall (no-slip, no penetration, \( \frac{dT}{dy} = 0 \)), the side outflow conditions are those of zero gradient (\( \frac{dV}{dx} = \frac{dV}{dx} = \frac{dT}{dx} = 0 \)) and ambient pressure boundary. The impingement plate is defined as a solid wall (no-slip, no penetration) heated with constant heat flux. In dimensionless form of this heat flux reads:

\[
Q = -\frac{q''_{\text{wall}} L_0}{k_0 T_0}
\] (3-19)

In order to be able to compare the heat transfer performance between the single jet and the jet-pair configurations Figure 22 we need an equivalency criterion. The criterion is that the same flow rate is issued from the two configurations. As a result, and based on the definitions above, the cooling performance of the single jet configuration for a certain Reynolds number will be compared to the cooling performance of the jet pair configuration, for a Reynolds number half as large.

A commonly examined configuration, [97], i.e. \( H/B = 5 \), \( L_T/B = 5 \) and \( L/B = 20 \) and \( Q = 2 \) (the value of \( Q \) allows for a visible rise in the temperature but at the same time the buoyancy effects are negligible) is adopted in all computations unless otherwise noted.
Additionally, a numerical simulation of compressible flow requires an accurate control of wave reflections from the computational domain. For accurate predictions, it is necessary to eliminate the acoustic waves by a mechanism as non-reflecting or absorbing boundary conditions \([276, 219]\). Moreover all thermodynamic and transport properties depend on temperature \([133, 132]\) and for the time integration, the ordinary differential equation integrator VODEPK \([49, 47]\) is used, which can handle stiff and non-stiff systems accurately and with optimum computational cost.

The local heat transfer coefficient can be expressed as

\[
h = \frac{1}{T_{\text{wall}} - T_{\text{inlet}}} q_{\text{wall}}'
\]  

(3-20)

where \(T_{\text{inlet}}\) is the jet inlet temperature and \(T_{\text{wall}}\) is the wall temperature. The unknown in the above equation is the wall temperature. The corresponding local Nusselt number reads,

\[
Nu = \frac{h L}{k}
\]  

(3-21)

It is clear from equations (3-20) and (3-21) that the maximum wall temperature corresponds to a minimum Nusselt number. Additionally, the maximum temperature is a critical design parameter for a cooling process, exemplified by the reliable performance of electronic equipment. For this reason, the maximum wall temperature will be the basic monitoring quantity in our investigation.

Simulations are performed for \(66.6<\text{Re}<533.3\) for the single jet case, which corresponds to fully laminar jets. The Prandtl number is 0.72 and the Mach number is 0.1. A Mach number less than 0.3 corresponds to a practically incompressible flow \([215]\). For the SPH simulations, 10000-80000 particles are used, depending on the Reynolds number, resulting in resolved solutions for all the cases.

Out of the extensive set of cases that have been simulated, we have selected a representative group that we shall utilize for quantitative comparisons. In Figure 29 the maximum temperature of the surface is shown as a function of time for the single and pair jets with steady forcing. It is clear that the jet pair configuration always features higher maximum temperature when compared to a single jet of an equivalent (twice as large) Reynolds number.

![Figure 29](image)

*Figure 29* Maximum surface temperature as a function of time (non-dimensional). (■) Single jet Re=133.3, (•) Single jet Re=266.6, (-----) Single jet Re=533.3, (–) Pair jet Re=66.6, (- -) Pair jet Re=133.3, (––) Pair jet Re=266.6.
This difference in the maximum temperature between the single jet and the jet pair can be explained from the variation of the temperature along the plate (Figure 30). The convection in the middle of the plate is very weak for the jet pair configuration (Figure 30(b)) in contrast to the single jet (Figure 30(a)) where it is in this region that the maximum convective heat transfer occurs. On the other hand, the temperature variation along the surface is smaller for the jets pair configuration (Figure 30). It is also of interest to note that the maximum temperature difference between equivalent Reynolds numbers for single- and double-jet configurations is increasing, with the increase of the Reynolds number. This means that the relative efficiency of the double-jet configuration is decreasing, when compared with the single-jet one, as the Reynolds number increases. The flow field is shown in Figure 31, where it is obvious that two recirculation zones close to the middle of the plate (for the jet pair case) cause reduction of the heat transfer in that region. It is clear that the two vortices (near the middle of the plate) oppose each other and the convective effect is small in that region.

In Figure 32 the maximum temperature is shown as a function of time for different phase angle differences of the pulsating jet pair. This figure shows that the pulsation of the two jets with amplitude A=0.5 and angular velocity $\omega = 2$ in phase ($\phi = 0$), increases the maximum temperature by 0.4% (negligibly). Increasing the phase difference between the two jets, for example to $\phi = 1\text{rad}$, the maximum temperature decreases by 2% compared to the steady jet pair case but it is still higher than that of the single steady jet.
Figure 31 Velocity vectors for single jet impingement (top) and array jet impingement (bottom)

For an even larger phase angle difference ($\phi = 2 \text{ rad}$) the temperature is reduced more (5% compared with the steady jet pair) and it is comparable to the single steady jet. For the maximum possible phase angle difference ($\phi = 3.14 \text{ rad}$) the temperature is reduced even more (6% compared with the steady pair) and is now smaller than that of the single steady jet.

Figure 32 Maximum surface temperature as a function of time (non-dimensional). (---) Steady single jet for Re=266.6, (---) Steady pair jet for Re=133.3, (---) Pulsating pair jet $A=0.5$, $\omega = 2$, $\phi = 0$ for Re=133.3, (---) Pulsating pair jet $A=0.5$, $\omega = 2$, $\phi = 1 \text{ rad}$ for Re=133.3, (---) Pulsating pair jet $A=0.5$, $\omega = 2$, $\phi = 2 \text{ rad}$ for Re=133.3, (---) Pulsating pair jet $A=0.5$, $\omega = 2$, $\phi = 3.14 \text{ rad}$ for Re=133.3.
Figure 33 Maximum surface temperature as a function of time (non-dimensional). (●) Steady single jet for Re=266.6, (--) Steady pair jets for Re=133.3, (●--) Pulsating pair jets A=0.5, ω = 1, φ = 3.14 rad for Re=133.3, (--•--) Pulsating pair jets A=0.5, ω = 2, φ = 3.14 rad for Re=133.3, (○--) Pulsating pair jets A=0.5, ω = 4, φ = 3.14 rad for Re=133.3.

The effect of the frequency (or angular velocity) for the jet pair and a comparison to a single jet is shown in Figure 33. Interestingly, the maximum temperature is not a monotonic function of the frequency, which is also experimentally observed [252]. It is also shown that when the frequency is low, the maximum temperature is higher than the one reached in the steady state case. This is obviously the effect of the prevalence of lower air velocities for a relatively long period of time. Figure 34 shows the effect of the frequency variation on the maximum temperature for the case of single jet impingement. The pulsation increases the maximum temperature compared to the steady case (a not beneficial effect for the stand point of temperature control).

Figure 34 Maximum surface temperature as function of time (non-dimensional). (●) Steady single jet for Re=266.6, (--•--) Steady pair jets for Re=133.3, (●--) Pulsating single jets A=0.5, ω = 1 for Re=133.3, (--•--) Pulsating single jets A=0.5, ω = 2 for Re=133.3, (○--) Pulsating single jets A=0.5, ω = 4 for Re=133.3.
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Figure 35 Maximum surface temperature as function of time (non-dimensional). (●—) Steady single jet for $\text{Re}=266.6$, (—) Steady pair jets for $\text{Re}=133.3$, (●—) Pulsating pair jets $A=0.5$, $\omega = 2$, $\phi = 3.14 \text{ rad}$ for $\text{Re}=133.3$, (●—) Pulsating pair jets $A=1.0$, $\omega = 2$, $\phi = 3.14 \text{ rad}$ for $\text{Re}=133.3$.

One crucial parameter for heat transfer enhancement is the amplitude of the pulse. In Figure 35, the maximum surface temperature is shown as a function of time for two different amplitudes, compared always with the steady single jet and jet pair cases. An important thermal design finding is that a marked decrease of the maximum temperature can be achieved by varying the amplitude: For $A=1.0$, an 11% decrease in maximum temperature is found compared to the steady jet-pair case, and a decrease of about 6% compared to the steady single jet.

The importance of the effect of the amplitude is reported in [185] where a major increase of the heat transfer characteristics is found compared with the steady-jet results. As the amplitude of the pulse increases, the generated vortices penetrate more in the wall jet region and boost the heat transfer.

For $\text{Re}=133$, a portion of the velocity and temperature time series is shown in Figure 36 (a), (b), where the unit of “n” represents 5 time steps of the computation. The velocity and temperature sampling location in this and subsequent figures is designated with a circle in Figure 22 (b). This location is arbitrarily selected, but we have verified that the nature of the results presents is not affected by this selection. The power spectrum of the signals obtained from longer time series is shown in Figure 36 (c), where the peak in $f_0 = 0.31831$ corresponds to the frequency imposed from the pulsation. (The frequency $f_0$ is related to the angular velocity of the pulse $\omega$, $f_0 = \frac{\omega}{2\pi} = \frac{2\ rad}{2\pi}$).

The two-dimensional time delay reconstruction [129] of the velocity signal is shown in Figure 36 (c) where the time delay used is about one tenth of the period. It is obvious that the system is characterized by a limit cycle behavior, obeying the forcing frequency of the two jets.

In Figure 37 the maximum temperature of the surface is shown as a function of time. The increase of the pulsation amplitude decreases the maximum plate temperature, for Reynolds number 533.3 (Re_{single} = 533.3, Re_{pair} = 266.6), an observation similar to that of Figure 35. The difference between the steady single jet and the steady jet pair is smaller for smaller Reynolds numbers
3. Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of jet impingement using RSPH

\[ \text{Re}_{\text{single}} = 266.6, \quad \text{Re}_{\text{pair}} = 133.3 \]. For the maximum amplitude of the pulsation \( A=1.0 \), the maximum temperature decrease is approximately 12%, compared to the steady jet pair.

Figure 36 Pulsating pair jets \( A=1.0, \quad \omega = 2, \quad \phi = 3.14 \text{rad} \) for \( \text{Re}=133.3 \). (a) Velocity time series, (b) Temperature time series, (c) Frequency (–) of the velocity and (—) temperature, (d) 2-dimensional time delay reconstruction of the phase space.

Figure 37 Maximum surface temperature as a function of time (non-dimensional). (●) Steady single jet for \( \text{Re}=533.3 \), (—) Steady pair jets for \( \text{Re}=266.6 \), (●●) Pulsating pair jets \( A=0.5, \quad \omega = 2, \quad \phi = 3.14 \text{rad} \) for \( \text{Re}=266.6 \), (●○●) Pulsating pair jets \( A=0.75, \quad \omega = 2, \quad \phi = 3.14 \text{rad} \) for \( \text{Re}=266.6 \), (●●○●) Pulsating pair jets \( A=1.0, \quad \omega = 2, \quad \phi = 3.14 \text{rad} \) for \( \text{Re}=266.6 \).

For the Reynolds number \( \text{Re}=266.6 \) the signal is not periodic any more (Figure 38 (a)). In the frequency spectra of the velocity signal many sub-harmonics appear, Figure 38 (b). The two-dimensional time delay reconstruction of the signal is presented in Figure 38 (c) where the time delay used is about one tenth of the period. The calculated maximum Lyapunov exponent is \( \lambda = 0.0075 \text{ bits/orbit} \) which is an evidence of a weakly chaotic signal [129]. The small value of the
computed Lyapunov exponent is however within the numerical error margin, for this Reynolds number, and thus non-conclusive. The frequency spectrum and the emergence of subharmonics, on the other hand, hint towards a rich dynamical behavior and the possibility of a period doubling scenario [88]. This observation guides us in exploring the evolution of the system as the parameter (i.e. Reynolds number) increases from 133.3 (Figure 36) to 266.6 (Figure 38).

![Figure 38 Pulsating pair jets](image)

In Figure 39 (a), a part of the velocity signal for Re=218.6 is shown (Figure 39 (b) depicts a similar time series for temperature). The emergence of a second frequency, 1/2 of the main forcing frequency of the system, is observed (Figure 39 (c)). The attractor (Figure 39 (d)), shows also that the period of the velocity signal is twice the period of the pulse. The delay is again about one tenth of the period and the embedding dimension is again two.

An exhaustive set of simulations has been conducted, in order to pinpoint the exact Reynolds number that this first period-doubling bifurcation takes place. It was found that this occurs at Re ≈ 208, between the two cases presented in Figure 36 and Figure 39, with accuracy better than 1 in the Reynolds number scale. Further increasing the Reynolds number leads to an increase of the amplitude of the first sub-harmonic, \( f = f_0/2 \). At the same time, the trajectories in the time delay reconstruction start to separate in two cycles as shown in Figure 39 (d) [88, 153, 228].

As the Reynolds number increases further, the amplitude of the sub-harmonic frequency \( f = f_0/2 \) becomes dominant and in the attractor the two cycles become unequal. Further increase of the Reynolds number (Re = 258.6) leads to an even smaller sub-harmonic (Figure 40 (b)), which has frequency \( f = f_0/8 \). The attractor (Figure 40 (c) and Figure 40 (d)) shows likewise the existence of that sub-harmonic, as the smaller cycle of the attractor Figure 39 (d) splits into four trajectories Figure 40 (d).
3. Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of jet impingement using RSPH

**Figure 39** Pulsating pair jets $A=1.0$, $\omega = 2$, $\varphi = 3.14\, rad$ for $Re=218.6$, (a) Velocity time series, (b) Temperature time series, (c) Frequency (---) of the velocity and (---) temperature, (d) 2 dimensional time delay reconstruction of the phase space.

**Figure 40** Pulsating pair jets $A=1.0$, $\omega = 2$, $\varphi = 3.14\, rad$ for $Re=258.6$, (a) Velocity time series, (b) Frequency spectrum of the velocity, (c) 2 dimensional time delay reconstruction of the phase space, (d) Focus of the 2 dimensional time delay reconstruction of the phase space.

The minimal sufficient embedding dimension is $m = 3$ (all attractor depictions in the present work are two-dimensional, however wherever quantitative phase-space computations are performed, like in the case of Lyapunov exponents, higher embedding dimensions are utilized as necessary). It is
clear that the system is not following the usual period doubling bifurcation (period-2 \(\Rightarrow\) period-4 \(\Rightarrow\) period-8 \(\Rightarrow\) etc) [228]. Such incomplete sequences have been observed in fluid dynamic systems (usually coupled with heat transfer) [275, 8, 294].

For higher Reynolds numbers the same behavior of the system is observed and the trajectories of the attractor draw away from each other (Figure 41). The smaller sub-harmonic is still \(f = f_0/8\).

For even higher Reynolds numbers, (\(Re=533.3\)), the signal is fully non-periodic, as hinted by the time series in Figure 42 (a) and by the filling up of the spectrum in Figure 42 (b). The calculated maximum Lyapunov exponent is, in this case, \(\lambda = 0.37 \pm 0.01 \text{ bits/}\text{orbit}\), which allows for a confident characterization of this case as fully chaotic.

![Figure 41](image)

\textit{Figure 41} 2-dimensional time delay reconstruction of the phase space: (a) \(Re=261.3\), (b) \(Re=262.6\), (c) \(Re=264\), (d) \(Re=265.3\).

The existence of intermittent intervals of periodicity, within the overall chaotic time series, can be made from Figure 42 (a) [221] (the same behavior is evident in the temperature time series also). We can verify that the apparently periodic portions of the signal in Figure 42 (a) are indeed periodic, by examining the relative segments of the time series, Figure 42 (d) and the corresponding frequency domain signatures, Figure 42 (e). This switching from fully aperiodic to periodic behavior, for this Reynolds number, has implications in the observed maximum temperatures: for the aperiodic intervals, the maximum temperature presents us with significantly larger values and a much more intense oscillatory behavior than those observed during the periodic intervals (Figure 43 (a)). There is a predictable relationship between the operating temperature of electronic parts and reliability. Materials employed in the manufacture of electronic devices have finite temperature limits; when these limits are exceeded, the physical properties are altered and the device ceases to perform its intended function. Failure also can occur gradually as a result of sustained operation at intermediate temperatures, producing slow but persistent deterioration of materials and finally ending in failure of the device. The performance of such components is affected by high temperatures for “finite time” (Figure 43 (b)) and not just instantaneous single picks.
Figure 42 Pulsating pair jets $A=1.0$, $\omega = 2$, $\varphi = 3.14 \text{ rad}$ for $Re=533.3$, (a) Velocity time series, (b) Frequency spectra of the velocity signal (a) (c) Phase space reconstruction of (a) with time delay about one fifth of the period. (d) Portion of (a), (e) Frequency spectra of the velocity signal (b)

Figure 43 Pulsating pair jets $A=1.0$, $\omega = 2$, $\varphi = 3.14 \text{ rad}$ for $Re=533.3$, (a) Maximum temperature, (b) Maximum temperature using a low pass filter (1-period)
The prevalence of a period doubling bifurcation scenario, (see Figure 39 and Figure 40 and discussion for transition from $f_0/2$ to $f_0/8$), which moreover presents us with intermittent behavior for particular values of the Reynolds number, dictates a scrutinized investigation of the parameter space of interest, guided by engineering design considerations: Dynamical systems theory, when applied to systems of the nature described herewith, introduces universal behavior laws, where bifurcation and state diagrams are concerned. More specifically, as can be observed from a typical bifurcation diagram for period-doubling systems, Error! Reference source not found., the possibility for “discontinuous” behavior for parameter intervals, embedded within the chaotic regime is possible. After the accumulation of bifurcations has occurred (Feigenbaum [88]), and the transition to chaotic states has been realized, the possibility exists that a further increase in the Reynolds number may lead to periodic or quasiperiodic behavior, the famous windows of periodicity in bifurcation theory. By investigating the temporal behavior of the system for a series of states within the chaotic regime, we identify a region of non-monotonic behavior.

\[\text{Figure 44 Bifurcation diagram for period-doubling systems, depicting a periodic window.}\]

\[\text{Figure 45 shows that from Reynolds number 273.33 until Reynolds number 346.66, the system presents us with a significant drop in maximum temperature, and a accompanying decrease in the temperature fluctuation, signatures of periodic behavior, as we have seen from Figure 43. A much more pronounced drop in temperature can be observed if we focus at our control point (shown in Figure 22 (b)) in the flow field, (Figure 46). Dynamical systems theory predictions are indeed confirmed, if we investigate dynamic behavior for the four Reynolds numbers identified in Figure 46 as a), b), c), and d).}\]
3. Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of jet impingement using RSPH

Figure 45 Maximum temperature of the plate as a function of Reynolds number: (—) Average temperature of the maximum temperature time series signal on the plate, (⋯⋯) Maximum temperature of the maximum temperature time series signal on the plate, (----) Minimum temperature of the maximum temperature time series signal on the plate.

Figure 46 Temperature of a control point as a function of Reynolds number: (—) Average of the temperature time series signal for a control point, (⋯⋯) Maximum of the temperature time series signal for a control point, (----) Minimum of the temperature time series signal for a control point.
3.3 Results and Discussion

Figure 47 Dynamic behavior for the four states identified in Figure 45 and Figure 46. First column: Velocity time series, Second column: Frequency spectrum of the velocity, Third column: 2-dimensional time delay reconstruction of the phase space.

Figure 47 shows time histories, frequency spectra and attractors for the last chaotic state (Re=273.33, a), the first periodic state of the identified window (Re=280.0, b), the last periodic state of the identified window (Re=333.33, c) and the first chaotic state of the new chaotic regime (Re=346.66, d), after the window in periodicity has been surpassed.
The condition represented by state c), has an apparently complex attractor shape Figure 47 (c), but examination of the corresponding frequency spectrum reveals a series of distinct peaks, and not the fuller broad spectrum, characteristic of chaos, that we see for example for states a) and d), Figure 47 (a), (d).

A Lyapunov exponent computation for this case c) gives a value that fluctuates around zero, confirming our observations. What this set of observations tell us is that there exists an optimal Reynolds number (which corresponds to Figure 46 (c)), where the flow rate is the maximum allowing periodic behavior along with the corresponding desirable decrease for the maximum temperature. From a design point of view, this last condition would correspond to a very favorable operating point for the configuration, since it combines the controlled behavior of periodic flow, (that allows for avoidance of sustained maximum temperature peaks), with the highest flow rate that such a periodic state is possible. We must note that dynamical systems theory provides for the existence of additional periodic windows, further down the parameter scale, however these windows are of significantly smaller width in the Reynolds number scale, and for the system under investigation, non-exploitable practically.

3.3.2.2 Conclusions

A detailed set of two-dimensional resolved simulations for the flow and heat transfer characteristics of single and pair slot pulsating jets impinging on a hot, constant heat flux surface, has been conducted. We have investigated the performance of these configurations, using the maximum temperature of the impingement surface as the principal design criterion. By varying systematically the pulsation characteristics (frequency, amplitude and phase angle) as well as the Reynolds number, we have identified optimum operating regimes. For the case of Re=133.33, A=1.0, $\omega = 2$ and $\phi = 3.14\text{ rad}$, we have found an improvement of 6% when compared to the single non-pulsating jet. Enhancement in performance is observed when the jets are pulsating out of phase. Moreover, guided by dynamical systems theory, we have identified both intermittent behavior of the system (periodic/chaotic) for particular Reynolds numbers, and more importantly, windows of pure periodicity at post-chaotic values of the Reynolds number. This latter observation can assist in the selection of particularly favorable design regimes, since it allows for all the beneficial features of periodic behavior (i.e. quiescent behavior of the maximum temperature with lower average values as well), at higher than intuitively accessible flow rates.

3.3.3 Conjugate heat transfer jet impingement

In many engineering problems, the domain of interest consists of liquid and solid regions. The thermal energy transport occurs additionally across the solid liquid interface. The heat fluxes on the side of solid and liquid must match at the interface.

Conjugate heat transfer requires that the energy equation is solved for different materials simultaneously. The study of the coupled forms of heat transfer between forced convection flows and conduction in surfaces is very important due to the existence of these simultaneous effects in practical heat transfer processes. The calculation of separate solutions for solid and liquid regions would require an involved iterative procedure for matching the interface conditions.
The fundamental system of differential equations governing the fluid motion of a viscous, heat conducting, compressible medium consists of the continuity, momentum and energy equations. The conservation equations for a calorically perfect gas without an energy source in non-dimensional form are explained in Section 2.2 (equations \((2-1)-(2-11))

For the solid region an additional differential equation for energy is required:

\[
\rho_s \ c_{p_s} \ \frac{DT}{Dt} = \frac{\partial}{\partial x_i} \left( k_s \ \frac{\partial T}{\partial x_i} \right), \tag{3-22}
\]

where \(\rho_s\) is the density, \(c_{p_s}\) the specific heat at constant pressure and \(k_s\) the thermal conductivity of the solid.

The non-dimensional variables are obtained (in the same way as in Section 2.2) from the physical variables and the new variables follows:

\[
\rho_s^* = \frac{\rho_s}{\rho_0}, \quad k_s^* = \frac{k_s}{k_0}, \quad c_{p_s}^* = \frac{c_{p_s}}{c_{p_0}} = \frac{c_{p_s}}{\gamma c_{v_0}}, \tag{3-23}
\]

where the superscript \(^*\) and the subscript \(0\) indicate the non-dimensional and the reference quantities.

A dimensionless number that appear in the Eqn. (3-22):

\[
Fo = \frac{k_0 \ t_0}{\rho_0 \ L_0 \ c_{p_0}}, \tag{3-24}
\]

where \(\gamma\) is the ratio of the specific heat capacities. and \(Fo\) denotes the Fourier number. Finally the non-dimensional form of Eqn. (3-22) can be written as:

\[
\rho_s^* \ c_{p_s}^* \ \frac{DT^*}{Dt^*} = Fo \ \frac{\partial}{\partial x_i^*} \left( k_s^* \ \frac{\partial T^*}{\partial x_i^*} \right), \tag{3-25}
\]

The heat conduction equation in the solid can be discretized using the concept of the RSPH methodology (as discussed in Section 2.3.1.3), where new particles are introduced in the computational domain to represent the solid [66]. The solid particles can exchange only heat fluxes (momentum and mass fluxes are imposed to zero), with the surrounding particles.

The RSPH implementation is used to simulate the conjugate heat transfer phenomenon coupled with jet impingement (Figure 48). The examined configuration, i.e. \(H/B = 5, \ H/B = 0.5, \ Lq/B = 1.5, \ L/B = 20\), and \(Q = 25\) (the value of \(Q\) defined by Eqn. (3-19)) allows for a large rise in the temperature and the buoyancy effects are significant). Additionally after finite period of time the jet is pulsating (Eqn. (3-14)). The coupling between fluid and solid is performed using the Patankar implementation [216].
3. Study of the effect of jet pulsation on the heat transfer and fluid flow characteristics of jet impingement using RSPH

**Figure 48** Schematic representation of conjugate heat transfer simulation.

**Figure 49** Snapshots of temperature contour (gray scale) and particle trajectories for the conjugate heat transfer simulation.

In *Figure 49* a qualitative simulation of the pulsed jet impingement with conjugate heat transfer for Reynolds number $Re=400$ is shown. The heat is conducted inside the solid and then convection
transfers the heat inside the fluid. The buoyancy effect, as expected, elevates a significant amount of particle near the confinement plate.

Moreover, in Figure 50 the effect of the thermal conductivity of the solid is shown. We employed simulations for three cases. The results indicate that the material with the higher conductivity (Figure 50 (c)) is conducting the heat faster, and consequently the gradients are also higher.

3.4 Summary

The present study is a fundamental step in the evaluation of the RSPH methodology in jet flows with strong coupling between flow and the temperature field. The performance of the RSPH is deemed as clearly satisfactory, which encourages its future implementation to the modeling of the impinging jet flow in the presence of more complex phenomena. Moreover the latter phenomena are fundamental for the numerical simulation of complex processes that include the fluid structure interaction as shown in Figure 2.
Figure 50. Snapshots of temperature contour inside the solid and in the near fluid region. \( k_s = 37.5 \text{W/mK}, k_b = 75 \text{W/mK}, \) and \( k_c = 150 \text{W/mK}, \) for non-dimensional times \( t^* = 50, 100, 150, 200. \)
Chapter 4
Remeshed Smoothed Particle Hydrodynamics for the simulation of Laminar Chemically Reactive flows

4.1 Background

The mathematical description of combustion processes is, therefore, quite complicated involving not only the complexities associated with multi-phase, multi-component flows of compressible gases, but also the coupled effects of chemical kinetics and physical transport. One way to gain fundamental understanding into the complex phenomena occurring in combustion is through mathematical modeling.

The combustion process is usually characterized by the presence of multiple, very different time and length scales, as well as by flow speeds at a wide range of Mach numbers. The chemical time scales are widely spread. Stiff nonlinear coupling characterizes the system of differential equations for the species, which govern the combustion process. Moreover, the analysis of flow in the presence of chemical reactions depends on the stability and accuracy of the numerical scheme that is used to couple chemistry and fluid dynamics. Of particular importance is the robustness of the numerical algorithm used for the solution of the governing differential equations, and the detailed chemical mechanism that is used for describing the chemical kinetics. The simulation of reacting systems is a tough test for numerical schemes, since the chemical reaction rates are nonlinear and widely disparate in general, and may cause the non-linear equations to be stiff, leading to non-converging numerical solutions. Therefore the numerical simulation of reacting problems is an additional challenge to overcome for our RSPH implementation.

The simulation of reacting flows using detailed modeling is a unique approach for understanding flames and for devising combustion models for turbulent combustion. Regarding the numerical techniques, grid-based approaches (e.g. finite element, finite difference, finite volume and spectral methods) [65] have reached a level of maturity and are used extensively for the simulation of reacting flows. Substantial efforts have been made concerning the extension of Lagrangian particle methods for the treatment of reacting flows. From the purely mathematical point of view, the Lagrangian representation of the transport equations that describe a chemically reacting flow is not complicated. On the other hand, the development of an appropriate solution procedure capable of solving these transport equations within the Lagrangian frame is not trivial. Vortex methods were applied successfully in the simulation of incompressible flows, but the extension to reacting flows is a serious task. There are two general ways by which the effect of chemical reaction is taken into account in vortex methods:

− interface methods and
− direct lagrangian methods.

In interface methods, chemical reactions assumed to occur within a narrow zone. The thickness of the reaction zone is small compared to the characteristic size of the flow. These approaches are best suited for simulating unsteady premixed flames. The chemical reaction effect is included in the vortex
methods by adding a thermal expansion and baroclinic torque term in the continuity and vorticity transport equations, respectively [99, 100].

The direct Lagrangian methods were developed as an extension of the transport element method [139, 257] for the simulation of unsteady reacting flows. These techniques are able to capture the effects of flames without restrictive assumptions regarding the flame structure. Chemistry is imposing an additional strength adjustment, which is solved in a fractional step manner (like convection, diffusion and stretching) [259]. No assumptions are made with respect to the structure and topology of the reaction zone, however these models are considered still primeval [102] at least not ready for applied combustion research (compared to the conventional combustion modeling techniques). The method has been applied successfully in fundamental theoretical aspects of reacting flows (e.g. reacting mixing layer simulations), mainly with a single-step reaction with finite or infinite rate. Direct lagrangian methods can be extended to systems with more species, but are restricted to equal diffusivities of the species [258].

The coupling errors that are caused by the combination of convection and other physical processes in reacting vortex methods are not well understood, and may lead to wrong solutions [103]. Certainly the big advantage of lagrangian methods is in flows dealing with convective transport (e.g. turbulent flows), where the major contribution of the non-linear convection term can be computed more accurately. The direct lagrangian methods are regarded more often as large eddy simulation technique [102] using modeling mechanism to account for small-scale transport [99, 100, 139, 21, 257, 259, 258, 260].

Another particle method that has been successfully applied in the simulation of systems with reaction is the particle-in-cell (PIC) [210, 44]. Convective transport is solved using particles, while the other processes are solved on a grid. However, PIC with reaction is computationally expensive compared to same order grid-based methods [142].

To the best of our knowledge, SPH has never been applied in simulating reacting flows. Our effort is to include in the implementation presented in Chapter 2 the additional equations and necessary terms that represent the reaction process. For the solution, all the transport equations and terms are solved in a lagrangian fashion simultaneously (without linearization or background grid based differentiation).

The present chapter is organized as follows: in section 4.2 the governing equations and their particle discretization are presented. Section 4.3 presents’ simulation results for an H2/Air opposed-jet burner with detailed chemistry and transport. One reason for this choice (classical burner geometry) was the availability of results with other methods for comparison. A second reason is that it contains essential features of the basic configuration of Figure 2 (jet flow, stagnation region). The parametric study is considering the effect of particle number (resolution), compressibility (Mach number) and outflow boundary condition (length of the domain). The RSPH computational results are compared with other numerical results produced by a spectral element implicit scheme and by a one-dimensional code. The major conclusion is that the particle discretization of the basic equation describing reacting flows is a flexible and excellent way for the numerical solution of chemically reacting flows.
4.2 Governing Equations and RSPH Methodology

4.2.1 Governing equations

The motion of a viscous, heat conducting, reacting, and compressible medium is described by the continuity, momentum, energy, and species concentration equations. For a calorically perfect gas with an energy source for multi-component reaction system the conservation equations are [291]:

\[
\frac{D\rho}{Dt} = -\rho \frac{\partial u_i}{\partial x_i} \tag{4-1}
\]

\[
\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{4-2}
\]

\[
\rho \frac{c_s}{c_s} \frac{D T}{D t} = -p \frac{\partial u_i}{\partial x_i} + \tau_{ij} \frac{\partial u_j}{\partial x_j} + \dot{Q} - \nabla \cdot q \tag{4-3}
\]

\[
\frac{D \rho Y_s}{D t} = -\rho Y_s \frac{\partial u_i}{\partial x_i} - \nabla \cdot (\rho Y_s V_s) + \dot{R}_s \tag{4-4}
\]

where

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \tag{4-5}
\]

\[
q = -k \frac{\partial T}{\partial x_i} + \rho \sum_{s=1}^{\text{Species}} c_p, T Y_s V_s \tag{4-6}
\]

where index notation with Einstein’s summation convection is used for vectors and tensors in Cartesian coordinates (i, j, k=1,2) and \(x_i\) are the components of the position vector, \(u_i\) the velocity vector components, \(\rho\) is the density, \(p\) the pressure, \(T\) the temperature, \(\mu\) the viscosity, \(k\) the thermal conductivity, \(c_v\) the specific heat at constant volume, \(\dot{Q}\) is the heat source rate, \(s\) is the species index, \(c_p\) the specific heat at constant pressure of species \(s\), \(Y_s\) the mass fraction of species \(s\), \(\dot{R}_s\) is the mass rate of production of species \(s\) and \(V_s\) is the diffusion velocity of species \(s\). The heat flux vector \(q\) (Eq.( 4-6 )) consist of the heat conduction and the thermal diffusion effect ( or “Soret effect”). The Dufour effect is usually of minor importance and will be neglected. Also radiation is neglected. The diffusion velocities \(V_s\) are written in the classical Fickian form:

\[
V_s = v_s^C + v_s^T + V_s, \tag{4-7}
\]

where \(v_s^C\) is the ordinary diffusion velocity written in the Curtiss-Hirschfelder [113] approximation as

\[
v_s^C = -\frac{1}{X_s} D_{m,n} \nabla X_s, \tag{4-8}
\]

\(v_s^T\) the thermal diffusion velocity (necessary only for low molecular weight species)
4. RSPH for the simulation of Laminar Chemically Reactive flows

\[ v_s^r = - \frac{D_{s,m} \Theta_s}{X_s} \frac{1}{T} \nabla T, \quad (4-9) \]

where \( X_s \) is the mole fraction and \( D_{s,m} \) is the mixture average diffusion coefficient, given explicitly in terms of the binary diffusion coefficient \( D_{s,k} \) and \( \Theta_s \) is the thermal diffusion ratio. Mixture-average diffusion coefficients are approximations \([132, 133]\), and do not guarantee that the net species diffusion flux is zero (i.e. \( \sum_{s=1}^{\text{Species}} Y_s v_s^r = 0 \)) that will result in loss of mass conservation (i.e. \( \sum_{s=1}^{\text{Species}} Y_s \neq 1 \)). One approach to correct this is to use a constant correction factor \( V_c \) \([67]\), which is independent of species, but spatially varying. It is defined as:

\[ V_c = - \sum_{s=1}^{\text{Species}} Y_s \left( v_s^c + v_s^r \right). \quad (4-10) \]

Note that all thermodynamic and transport properties depend on temperature only \([172, 132]\).

The system of differential equations (4-1) - (4-4) is closed with the equation of state for an ideal gas

\[ p = \rho RT, \quad (4-11) \]

where \( R \) is the gas constant.

The non-dimensional variables are obtained from the physical variables as follows:

\[ x_i^* = \frac{x_i}{L_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad t^* = \frac{t}{L_0 \overline{U}_0}, \quad u_i^* = \frac{u_i}{\overline{U}_0}, \quad T^* = \frac{T}{T_0}, \]

\[ p^* = \frac{p}{\rho_0 RT_0}, \quad \mu^* = \frac{\mu}{\mu_0}, \quad k^* = \frac{k}{k_0}, \quad c_s^* = \frac{c_s}{c_{s,0}}, \quad c_{p,s}^* = \frac{c_{p,s}}{c_{v,0} \gamma} \quad (4-12) \]

\[ \dot{Q}^* = \frac{\dot{Q}}{\rho_0 c_{v,0} T_0 \overline{U}_0 L_0}, \quad D_{s,m}^* = \frac{D_{s,m}}{D_0}, \quad \dot{R}^* = \frac{\dot{R}}{\rho_0 \overline{U}_0 L_0} \]

where the superscript * and the subscript 0 indicate the non-dimensional and the reference quantities, respectively. The quantities \( L_0, \rho_0, U_0, T_0, \mu_0, k_0, D_0 \) and \( c_{v,0} \) denote the characteristic length, density, velocity, temperature, viscosity, thermal conductivity, diffusion coefficient, and specific heat at constant volume, respectively. The dimensionless numbers that appear in the equations are:

\[ \text{Re} = \frac{D_0 U_0 L_0}{\mu_0}, \quad M^2 = \frac{U_0^2}{\gamma RT_0}, \quad \text{Pr} = \frac{\mu_0 \gamma c_{v,0}}{k_0}, \quad \text{Pe} = \frac{U_0 L_0}{D_0} \quad (4-13) \]

where \( \gamma \) is the ratio of the specific heat capacities. The symbol Re denotes the Reynolds number, M the Mach number, Pr the Prandtl number and Pe the Peclet number.

In non-dimensional form, the system of governing equations (the Soret effect is neglected Eq. (4-9)) can be written:
4.2 Governing Equations and RSPH Methodology

\[ \frac{D\rho^*}{Dt^*} = -\rho^* \frac{\partial u^*_i}{\partial x_i^*} \]  \hspace{1cm} (4-14)

\[ \rho^* \frac{Du^*_i}{Dt^*} = -\frac{1}{M^2 \gamma} \frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re} \frac{\partial \tau_{ij}^*}{\partial x_j^*} \]  \hspace{1cm} (4-15)

with

\[ \rho^* c_v^* \frac{DT^*}{Dt} = -(\gamma - 1) \rho^* \frac{\partial u^*_i}{\partial x_i^*} + \frac{M^2 \gamma (\gamma - 1)}{Re} \frac{\partial u^*_i}{\partial x_j^*} + \frac{\partial}{\partial x_i^*} \left( \frac{k^*}{Re} \frac{\partial T^*}{\partial x_i^*} \right) \]  \hspace{1cm} (4-16)

\[ \frac{D\rho^* Y_s}{Dt} = -\rho^* Y_s \frac{\partial u^*_i}{\partial x_i^*} + \frac{1}{Pe} \frac{\partial}{\partial x_i^*} \left( \rho^* Y_s \frac{D_{s,m}^*}{X_{s,m}} \frac{\partial X_{s,m}}{\partial x_i^*} \right) \]  \hspace{1cm} (4-17)

\[ p^* = \rho^* \mu \left( \frac{\partial u^*_i}{\partial x_i^*} + \frac{\partial u^*_j}{\partial x_j^*} - \frac{2}{3} \delta_{ij} \frac{\partial u^*_k}{\partial x_k^*} \right) \]  \hspace{1cm} (4-18)

\[ \tau_{ij}^* = \mu \left( \frac{\partial u^*_i}{\partial x_j^*} + \frac{\partial u^*_j}{\partial x_i^*} - \frac{2}{3} \delta_{ij} \frac{\partial u^*_k}{\partial x_k^*} \right) \]  \hspace{1cm} (4-19)

The set of equations presented above include acoustic interactions and compressibility effects, as well as heat effect due to viscous dissipation. Body forces (e.g. gravitational) and thermal radiation effects are neglected.

4.2.2 Numerical Method

The RSPH (Section 2.3) is used for the discretization and numerical solution of the governing equations. They are repeated here for completeness.

The continuity and the momentum equation for a 2-D flow are discretized in exactly the same way as in Chapter 2

\[ \frac{D\rho_a}{Dt} = -\rho_a \sum_b V_b (\bar{u}_b - \bar{u}_a) \cdot \nabla_a W(r_a - r_b, h) \]  \hspace{1cm} (4-20)

\[ \left( \frac{D\mu}{Dt} \right)_a = -\left( \frac{\partial \mu}{\partial x} \right)_a + \frac{4}{3} \left( \frac{\partial \mu}{\partial x} \frac{\partial u}{\partial x} \right)_a - \frac{2}{3} \left( \frac{\partial \mu}{\partial y} \frac{\partial u}{\partial y} \right)_a \]  \hspace{1cm} (4-21)
\[
\left( \rho \frac{Dv}{Dt} \right)_a = -\left( \frac{\partial p}{\partial y} \right)_a + \frac{4}{3} \left( \frac{\partial}{\partial y} \mu \frac{\partial v}{\partial y} \right)_a - \frac{2}{3} \left( \frac{\partial}{\partial y} \mu \frac{\partial u}{\partial x} \right)_a + \left( \frac{\partial}{\partial y} \mu \frac{\partial u}{\partial x} \right)_a + \left( \frac{\partial}{\partial x} \mu \frac{\partial v}{\partial x} \right)_a + \left( \frac{\partial}{\partial x} \mu \frac{\partial v}{\partial x} \right)_a
\]  
(4-22)

with

\[
\left( \frac{\partial p}{\partial x} \right)_a = \sum_b V_b \left( p_b - p_a \right) \frac{\partial}{\partial x} W(r_a - r_b, h)
\]  
(4-23)

\[
\left( \frac{\partial p}{\partial y} \right)_a = \sum_b V_b \left( p_b - p_a \right) \frac{\partial}{\partial y} W(r_a - r_b, h)
\]  
(4-24)

A general formulation is adopted for the derivation of the viscous terms of the equations \((4-21), (4-22)\) which accounts for variable viscosity \(\mu\) (the viscosity being only a function of temperature). The viscous terms are written out with the help of the chain rule of differentiation and the SPH formulation for the viscous terms reads:

\[
\left( \frac{\partial}{\partial x_j} \mu \frac{\partial u_k}{\partial x_j} \right)_a = \left( \frac{\partial}{\partial x_j} \mu \frac{\partial u_k}{\partial x_j} \right)_a + \left( \mu \frac{\partial^2 u_k}{\partial x_j^2} \right)_a
\]

\[
\left( \sum_b V_b \left( \mu_b - \mu_a \right) \frac{\partial}{\partial x_j} W(r_a - r_b, h) \right) + \left( \sum_b V_b \left( u_{k,b} - u_{k,a} \right) \frac{\partial}{\partial x_j} W(r_a - r_b, h) \right)
\]

\[
+ \mu_a \sum_b V_b \left( u_{k,b} - u_{k,a} \right) \frac{\partial^2}{\partial x_j x_j} W(r_a - r_b, h)
\]

(4-25)

The SPH formulation of the momentum equation terms (equations \((4-21)\) and \((4-22)\)) is obtained in a straightforward manner by combining equations \((4-23)-(4-25)\) as needed. Note that equation \((4-25)\) delivers all derivatives of the viscous terms (where \(i, j, k=1,2\) and \(x_1=x, x_2=y\), \(u_1=u, u_2=v\)).

The two-dimensional version of the energy equation \((4-3)\) reads

\[
\left( \rho \frac{c_v DT}{Dt} \right)_a = -\left( \rho \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right)_a + \left( \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right)_a
\]

\[
+ \left( \frac{\partial}{\partial x} \left( \rho c_v k \frac{\partial T}{\partial x} \right)_a + \left( \frac{\partial}{\partial y} k \frac{\partial T}{\partial y} \right)_a + \left( \frac{\partial}{\partial x} k \frac{\partial T}{\partial x} \right)_a \right)
\]

(4-26)

The compressibility and the viscous dissipation term in the energy equation can be easily discretized by using the general formula of Eq. \((2-18)\). The energy by compression can be positive or negative, depending upon whether the fluid is expanding or contracting.

The derivation of the SPH formulation for the heat diffusion term, allowing for a temperature dependent thermal conductivity, is similar to that of the viscous terms of the momentum equation described in the above section. The final result reads
The mass fraction equation of species is written:

\[
\frac{\partial}{\partial t} \left( \rho Y_s \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \sum_{ss=1}^{Species} \frac{\partial}{\partial x} \left( \rho Y_s \frac{D_{ss,m}}{X_s} \frac{\partial X_{ss}}{\partial x} \right) + \sum_{ss=1}^{Species} \frac{\partial}{\partial y} \left( \rho Y_s \frac{D_{ss,m}}{X_s} \frac{\partial X_{ss}}{\partial y} \right) + \left( \dot{R}_s \right) = 0
\]

which can also be written in a way similar to Eq. (4-27). Note that in order to avoid the nested summation and the associated increase in computational cost, the correction velocity is written in vector form.
4.3 Results and Discussion

The RSPH technique is used for the simulation of a laminar, planar, opposed-jet burner (Figure 51). Diffusion flames are of great practical importance since many combustion application include flames dominated by mixing of a gaseous fuel and oxidant. Internal combustion engines, rocket combustion and building fires all share diffusion flame phenomena. Here, a hydrogen-air opposed jet diffusion flame is simulated using RSPH.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{geometry.png}
\caption{Geometry of planar opposed-flow diffusion flame}
\end{figure}

A schematic representation of the present study is shown in Figure 51. For the numerical simulations only half of the domain is considered. The inflow conditions for both jets are:

\[ v = 0, \quad u = u_{\text{max}} \left(1 - \frac{y^2}{B^2 / 4}\right), \quad T_{\text{inlet}} = 1 \quad (4-31) \]

and the mole fraction of each jet is given by:

\[ \begin{cases} X_{O_2} = 0.21 \\ X_{N_2} = 0.79 \end{cases} \text{Oxidizer} \quad & \quad \begin{cases} X_{H_2} = 0.40 \\ X_{N_2} = 0.60 \end{cases} \text{Fuel} \quad (4-32) \]

The Reynolds number is defined as

\[ \text{Re} = \frac{u_{\text{max}} \rho_{\text{oxidizer}} B}{\mu_{\text{oxidizer}}} \quad (4-33) \]

The plates are defined as isothermal walls (no-slip, no penetration, T=1), the outflow conditions are those of zero gradient \((du/dx = dv/dx = dY_z/dx = dT/dx = 0)\), and ambient pressure and the axis of symmetry as a zero gradient boundary \((v = dv/dx = dT/dx = d\rho/dx = dY_z/dx = 0)\). In the simulation, the following geometric ratios, H/B=1, and L/B=3 are adopted in all computations, unless otherwise noted.

The numerical simulation of compressible flow requires accurate control of wave reflections from the computational domain. For accurate predictions, it is necessary to eliminate the acoustic waves by a mechanism like non-reflecting or absorbing boundary conditions [276, 219]. All thermodynamic and transport properties depend on temperature [172, 132] and for the time integration, the ordinary differential equation integrator VODEPK [49, 47] is used, which can handle stiff and non-stiff systems accurately and with optimum computational cost.
Table 5 Detailed reaction mechanism for the H₂/Air system adopted in the present study [293].

<table>
<thead>
<tr>
<th>No.</th>
<th>Reactions</th>
<th>A</th>
<th>b</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H₂+M=H+H+M</td>
<td>4.57E+19</td>
<td>-1.4</td>
<td>104000</td>
</tr>
<tr>
<td>2</td>
<td>O+H₂O=OH+OH</td>
<td>2.95E+06</td>
<td>2</td>
<td>13400</td>
</tr>
<tr>
<td>3</td>
<td>O+H₂=H+OH</td>
<td>5.08E+04</td>
<td>2.7</td>
<td>6290</td>
</tr>
<tr>
<td>4</td>
<td>O+O+M=O₂+M</td>
<td>6.17E+15</td>
<td>-0.5</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>H+O₂+O=O₂+OH</td>
<td>1.94E+14</td>
<td>0</td>
<td>16440</td>
</tr>
<tr>
<td>6</td>
<td>H+O₂(+M)=HO₂(+M)</td>
<td>4.52E+13</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>H+O+M=OH+M</td>
<td>4.72E+18</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>OH+H₂=H₂O+H</td>
<td>2.16E+08</td>
<td>1.5</td>
<td>3430</td>
</tr>
<tr>
<td>9</td>
<td>OH+H=H₂O+H</td>
<td>2.24E+22</td>
<td>-2</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>HO₂+O=O₂+OH</td>
<td>1.75E+13</td>
<td>0</td>
<td>-397</td>
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<tr>
<td>11</td>
<td>HO₂+H=H₂+O₂</td>
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<td>0</td>
<td>2130</td>
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<tr>
<td>12</td>
<td>HO₂+H=OH+OH</td>
<td>1.69E+14</td>
<td>0</td>
<td>874</td>
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<tr>
<td>13</td>
<td>HO₂+OH=H₂O+O₂</td>
<td>1.90E+16</td>
<td>-1</td>
<td>0</td>
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<tr>
<td>14</td>
<td>HO₂+HO₂=H₂O₂+O₂</td>
<td>4.20E+14</td>
<td>0</td>
<td>11980</td>
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<tr>
<td>15</td>
<td>HO₂+HO₂=H₂O₂+O₂</td>
<td>1.30E+11</td>
<td>0</td>
<td>-1629</td>
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<td>16</td>
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<td>17</td>
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<td>18</td>
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<td>3590</td>
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<td>19</td>
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<td>4.82E+13</td>
<td>0</td>
<td>7950</td>
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<tr>
<td>20</td>
<td>H₂O₂+OH=H₂O₂+HO₂</td>
<td>1.00E+12</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>21</td>
<td>H₂O₂+OH=H₂O₂+HO₂</td>
<td>5.80E+14</td>
<td>0</td>
<td>9557</td>
</tr>
</tbody>
</table>

a Arrhenius coefficients (pre-exponential factor, temperature exponent and activation energy).
b Third body efficiencies: H₂: 2.5E+00, H₂O: 1.2E+01

Simulations are performed for Re=508.76, which corresponds to fully laminar jets. The Prandtl number is 0.714, and the Mach number is 0.05. A Mach number less than 0.3 corresponds to a practically incompressible flow [215]. All the simulations are performed using a 21-step detailed chemical mechanism shown in Table 5 [293]. The present mechanism involves nine species O₂, H₂, H, O, OH, H₂O, HO₂, H₂O₂ and N₂.

Figure 52 shows the steady state solution, obtained from RSPH using 97200 particles (corresponding to 180x540 grid) for the velocity field, the temperature, and some representative species. For all the reacting two-dimensional simulations that we are presenting in this Chapter, first we obtained the steady state “cold” flow solution, which represents the mixing problem between the fuel and oxidizer jet, and then we introduced a hot spot on the stagnation region which ignited numerically the flame. The computations proceeded until all the transients die out and the steady state is reached in the computational domain.

From the results shown in Figure 52 it is clear that the resolution of RSPH is one essential parameter that we need to investigate. The solution of the species equations can produce results where the gradients (of temperature, and/or of species) may be much higher than the velocity field gradients and a higher resolution may be necessary. The convergence and grid independence study of the RSPH solution is shown in Figure 53, Figure 54 and Figure 55. Apart from the simulation presented in Figure 52 (97200 particles), a coarser particle resolution (44000 particles, corresponds to a grid 120x360) and a finer particle resolution (174000 particles, corresponds to a grid 240x720) is used, so
as to ensure the convergence of the RSPH implementation. The temperature profile along the axis (Figure 53) shows very good agreement between the three simulations.

**Figure 52** Isolines of velocities, temperature and mass fractions of some representative species, from RSPH simulation using 97200 particles. The range of the values is shown above each figure, using 16 equidistant levels.

**Figure 53** Temperature profiles along the axis of symmetry using RSPH. (-) 97200 particles, (- -) 44000 particles, (--- -) 174000 particles.

The difference of the maximum temperature is smaller than 1%. The flame location and thickness are in very good agreement. In Figure 54 the axial velocity plot along the axis of symmetry is shown. The results indicate that the decay of the axial velocity in both fuel and oxidizer sides is the
same, and the location of the stagnation point is exactly the same. Figure 55 shows some representative species distribution along the axis. The solution for all resolutions is practically identical. From Figure 53, Figure 54 and Figure 55, it is clear that the relative error in RSPH is decreasing when we increase the resolution. The results indicate that the RSPH solution (temperature, axial velocity and representative species) is resolved with all resolutions.

\[\text{Figure 54} \text{ Axial velocity profiles along the axis of symmetry. Using RSPH.} (-) 97200 \text{ particles}, (- -) 44000 \text{ particles}, (---) 174000 \text{ particles.}\]

\[\text{Figure 55} \text{ Mass fraction profiles of H}_2, \text{ O}_2, \text{ H}_2\text{O} \text{ and OH along the axis of symmetry using RSPH.} (-) 97200 \text{ particles}, (- -) 44000 \text{ particles}, (---) 174000 \text{ particles.}\]

For numerical convenience the Mach number value of Ma=0.05 has been utilized. The real value of Mach number (Ma=0.008) would require the employment of attractable small time steps. To verify that the above mentioned disparity between employed and real Mach number has negligible impact on the results In Figure 56 - Figure 58 are presented.
These figures show results from RSPH simulations using two different Mach numbers (in addition to \(Ma=0.05\)), one with higher Mach number (\(Ma=0.1\)) and one with lower Mach number (\(Ma=0.025\)). The difference in temperature and velocity is less than 1.5%.

**Figure 56** Temperature profiles along the axis of symmetry using RSPH for different Mach numbers. (-) 97200 particles with \(Ma=0.05\), (---) 97200 particles with \(Ma=0.1\), (-----) 97200 particles with \(Ma=0.025\).

**Figure 57** Axial velocity profiles along the axis of symmetry using RSPH for different Mach numbers. (-) 97200 particles with \(Ma=0.05\), (- -) 97200 particles with \(Ma=0.1\), (----) 97200 particles with \(Ma=0.025\).
4.3 Results and Discussion

**Figure 58** Mass fraction profiles of $\text{H}_2$, $\text{O}_2$, $\text{H}_2\text{O}$ and OH along the axis of symmetry using RSPH for different Mach numbers. (--) 97200 particles with $\text{Ma}=0.05$, (-- -) 97200 particles with $\text{Ma}=0.1$, (---) 97200 particles with $\text{Ma}=0.025$.

One last but crucial parameter in our simulations is the length of the domain, which is strongly related with the outflow boundary conditions. The error that can be introduced in our simulations by the outflow boundary conditions is moreover investigated. In all our simulations the length of the domain is considered $L/B=3$, which is relative small and can lead to errors in the results.

**Figure 59** Temperature profiles along the axis of symmetry using RSPH for different length $L$ of the domain. (--) 97200 particles with $L/B=3$, (-- -) 129600 particles with $L/B=4$. 

81
On the other hand the simulation of reacting flow is computationally expensive and it is preferable to use relative small domains but at the same time it is necessary to ensure that their effect on the results is minimal. For this reason we tested our RSPH implementation in a bigger domain (L/B=4) by keeping all the other parameters (e.g. particle resolution, Mach number) constant. In Figure 59 the temperature profiles along the axis for the two different situations. The effect of the length of the domain in the maximum temperature is very small indeed. The axial velocity profile along the axis is shown in Figure 60, where it is clear that there is no effect (of the domain length) on the stagnation region. Representative species distributions are shown in Figure 61, exhibiting no difference between the two simulations.

**Figure 60** Axial velocity profiles along the axis of symmetry using RSPH for different length L of the domain. (-) 97200 particles with L/B=3, (- -) 129600 particles with L/B=4.

**Figure 61** Mass fraction profiles of H₂, O₂, H₂O and OH along the axis of symmetry using RSPH for different length L of the domain. (-) 97200 particles with L/B=3, (- -) 129600 particles with L/B=4.
The RSPH results are compared with numerical results obtained by a two-dimensional code [277, 145] and with the one-dimensional code OPPDIF [172]. The two-dimensional code is based on spectral element spatial discretization, and solves the low Mach form of the time dependent conservation equations of mass, momentum, energy and species. The integration of the set of equations is based on a time-splitting [277, 145, 278] technique that couples the hydrodynamics with the thermo-chemistry. The diffusion velocities of the species are calculated using the mixture fraction formulation with correction velocities to ensure mass conservation. Mixture-averaged values are used for the thermal conductivity and viscosity. Detailed description of the numerical formulation and some applications can be found in [277, 145, 278, 94, 144].

OPPDIF is a one-dimensional model, based on the introduction of stream function and assumes that temperature, species mass fraction and transport properties are function of x alone along the axis of symmetry [172].

A comparison of the RSPH results for the temperature along the axis of symmetry with the 2-D and the 1-D simulation codes is shown in Figure 62. The comparison between the RSPH and the results from the spectral code is very good. The RSPH simulation is using 97200 particles and the spectral element is using 176 elements with 12th order polynomials in each spatial direction. Flame location and flame thickness are identical. The one-dimensional results obtained from OPPDIF give the same flame location, but flame thickness is smaller and maximum temperature is about 40 K lower. The discrepancy between the one- and two-dimensional simulations is expected as in the one-dimensional case there is less information concerning the boundary conditions (for example parabolic inflow profile)[94].

![Figure 62](image)

*Figure 62* Temperature profiles along the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D code simulation, (- -) OPPDIF simulation.

The axial velocity profiles along the axis of symmetry are shown in Figure 63. The agreement between the RSPH and the 2-D code is also very good. The decay of the fuel and oxidizer jet and the
stagnation point are correctly matched. The species profiles along the axis of symmetry are in very good agreement as well (Figure 64).

The error between the RSPH and the 2-D code for temperature, axial velocity and species is less than 1%. The error is considered to be within the domain of the governing assumptions for both RSPH and the 2-D spectral element code.

\[\text{Figure 63} \text{ Axial velocity profiles along the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D code simulation, (- -) OPPDIF simulation.}\]

\[\text{Figure 64} \text{ Mass fraction profiles of H}_2, \text{ O}_2, \text{ H}_2\text{O and OH along the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D code simulation, (- -) OPPDIF simulation.}\]

The validity and accuracy of the RSPH simulation is demonstrated not only in the axis of symmetry, but also further downstream in the computational domain. In Figure 65 shows the temperature, u-, v-velocities and characteristic species concentrations profiles at distance y=0.5B.
away from the axis of symmetry, where RSPH is compared with the 2-D code. The RSPH seems able to capture all the details of the flow and reaction field. The same stands also further downstream at distance \( y=1.0B \) (Figure 66) and \( y=1.5B \) (Figure 67).

**Figure 65** Temperature, \( u \) and \( v \) velocity (non-dimensional) and mass fraction profiles at distance \( y=0.5B \) from the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D spectral element code simulation.

**Figure 66** Temperature, \( u \) and \( v \) velocity (non-dimensional) and mass fraction profiles at distance \( y=1.0B \) from the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D spectral element code simulation.

### 4.4 Summary

The RSPH methodology is extended for the simulation of chemically reacting flows and applied in the numerical modeling of a laminar, planar, opposed-jet burner. A detailed hydrogen-oxygen mechanism is used involving 9 species and 21 elementary reactions.

An extensive parametric study for the RSPH method is presented. In this study, the effect of: particle resolutions, Mach number, and length of the computational domain are investigated. The
overall behavior of the RSPH method is deemed satisfactory. The results indicate that RSPH is capable for solution of systems with complex chemistry.

In addition, we have to point out, that there are no topological or geometrical assumptions in the RSPH scheme that can limit the applicability of the method in three dimensions. The computational cost of RSPH is considered competitive to other techniques. RSPH is parallelizable in an efficient way (due to its nature as a particle method) and this is an inherent advantage of the technique compared to other methods. Note that the present RSPH algorithm is programmed in a parallel manner; so as to afford the large computational cost of detailed reacting simulations. The technique, which is used in our implementations, is the OpenMP [117]. (OpenMP is a portable, scalable model that gives shared-memory parallel programmers a simple and flexible interface for developing parallel applications on platforms ranging from the desktop to the supercomputer). The speed-up and efficiency of the RSPH are shown in Figure 68.

**Figure 67** Temperature, u and v velocity (non-dimensional) and mass fraction profiles at distance y=1.5B from the axis of symmetry. (-) RSPH simulation using 97200 particles, (-o-) 2-D spectral element code simulation.

**Figure 68** Speed-up and efficiency of the shared memory parallel implementation as a function of the processors number for RSPH simulation using 44000 particles.
Chapter 5
Remeshed Smoothed Particle Hydrodynamics for the simulation of Interfacial flows: A preliminary Study

5.1 Background

A variety of physical phenomena involve propagating interfaces. Interface(s) separate regions, which may differ according to their density, viscosity or chemical type. The complexity of the interface motion ranges from advection of two different liquids, flame propagation and dendrite solidification to formation of droplet clouds and sprays. In most of these processes the interfacial phenomena are the dominant leading to instabilities (e.g. Kelvin-Helmholtz, Rayleigh-Taylor etc). Interfacial phenomena occur at scales of space and time where experimental measurements or visualization is difficult or impossible.

The computation of interfacial phenomena requires the modeling of many important aspects such as interface thickness (a thin or thick region of space), surface forces and thermal effects. As a result, the numerical treatment of these phenomena involves not only the solution of the Navier-Stokes equations, but also of the interface kinematics (tracking interface topology) and physical processes specific to and localized at the interface (surface tension and phase change). Sometimes molecular-level phenomena need to be considered (e.g. adsorption).

This chapter aims in the extension of the RSPH methodology for the simulation of interfacial flows. This modeling involves the interface kinematics and the surface stresses. These processes are totally different (from the numerical modeling point of view), but they are strongly coupled. In this chapter we are considering only the interface kinematics. The extension of RSPH for the calculation of surface stress is not complicated if the interface topology is known [43]. The continuum surface force (CSF) of Brackbill et. al. [43] have been already applied in SPH methodology for the simulation of surface tension [198].

The first step for our RSPH methodology is the implementation of an algorithm capable to track the interface. Several methods and algorithms have been introduced for tracking the interface. They can be divided in two categories:
- tracking methods and
- capturing methods.

Tracking methods are Lagrangian in nature, and the interface is followed by integrating an evolution equation. Representative tracking methods are: moving-grid, front tracking, boundary integral and particle schemes. In capturing methods the interface is not explicitly tracked, but captured using a characteristic function, which evolves using the advection equation. Representative capturing methods are: continuum advection, volume tracking, level set and phase field models.

The Lagrangian nature of the SPH methodology implies that tracking methods are more suitable for modeling the motion of the interface. Particle-based methods are characterized by discrete particles that can model accurately the interface topology. Popular representative of the tracking methods is the Particle In Cell (PIC) developed by Harlow in 1957 [109] and its later variants like
Marker And Cell (MAC) developed by Harlow and Welch [110]. Another prominent tracking method is the interface tracking technique [280, 283, 282], with many applications like bubbly flows, solidification, premix flames, and boiling [128, 279]. The advantage of these methods is the elimination (partial or complete) of the problems of fixed or moving grid methods. Monaghan and coworkers used SPH as a tracking method for free surface modeling to simulate realistic wave breaking [190, 193].

Unlike the implementation of Monaghan [190], the proposed RSPH cannot be used as a tracking technique since remeshing destroys all the discrete particle information-identifications. Under this consideration capturing methods are better-suited techniques for modeling interface kinematics. Advanced well-designed continuum advection algorithms are able to track the interface within two or three cells. Preliminary RSPH results using the continuum advection approach have shown that the interface is captured with 5-7 particles, which leads to prohibitively expensive calculations. Volume tracking methods with most prominent member the Volume Of Fluid (VOF) technique and its variants [207, 295, 114, 239, 234, 238, 245, 73] are difficult to apply in methods for the compressible Navier Stokes [208, 227, 179, 244] like SPH. On the other hand, level set methods [212, 202] appear to be a better candidate for application in RSPH. They have been successfully applied in many fields [248, 270, 1, 2, 251, 211, 249] and show a great potential. The phase field method is a relative new technique first introduced for the simulation of crystal growth problems and Hele-Shaw flows [50, 134, 287, 289]; it was recently applied to the Navier-Stokes equations [121, 122]. Phase field models are based on continuum interface forces by smoothing the interface discontinuities on a thin numerically resolved layer. Furthermore phase field models provide a surface tension in a continuum manner, which is consistent from energetic and thermodynamic point of view. The phase field method is a promising technique for direct numerical simulation of interfaces, but it is relative new compared to other interface capturing techniques.

In this chapter we will introduce the level set methodology in our RSPH implementation, and we will investigate the applicability of the Lagrangian level set scheme. The main advantage of the level set method compared to other techniques is its natural treatment of topological changes such as merging and breaking. Note that it is the first time that the level set method is applied in a Lagrangian method. The advantage in using the level set method in a Lagrangian way is that the numerical scheme is unconditionally stable, and that there are no errors associated with the advection of the level sets.

5.2 Governing Equations, Level Set and RSPH methodology

5.2.1 Governing Equations

The fundamental system of differential equations governing the motion of a viscous, heat conducting, compressible medium consists of the continuity, momentum and energy. The conservation equations for a calorically perfect gas are:
5.2 Governing Equations, Level Set and RSPH methodology

\[
\frac{D\rho}{Dt} = -\rho \frac{\partial u_i}{\partial x_i} \quad (5-1)
\]

\[
\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + ST_i \quad (5-2)
\]

\[
\rho c_v \frac{DT}{Dt} = -\rho \frac{\partial u_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} - \nabla \cdot q \quad (5-3)
\]

where

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad (5-4)
\]

\[
ST_i = \sigma \kappa \delta(d) n_i \quad (5-5)
\]

\[
q = -k \frac{\partial T}{\partial x_i} \quad (5-6)
\]

where index notation with Einstein's summation convention is used for vectors and tensors in Cartesian coordinates (i, j, k=1,2) and \(x_i\) are the components of the position vector, \(u_i\) the velocity vector components, \(\rho\) is the density, \(p\) the pressure, \(g\) the gravitational acceleration component, \(ST\) is the surface tension term, \(\sigma\) the surface tension coefficient, \(\kappa\) the curvature of the interface, \(n\) is the normal to the interface, \(d\) is the distance to the interface, \(\delta(d)\) is the Dirac delta function, \(T\) the temperature, \(\mu\) the viscosity, \(k\) the thermal conductivity, and \(c_v\) the specific heat at constant volume.

The system of the differential equations (5-1) - (5-3) is closed with the equation of state for an ideal gas.

\[
p = \rho RT \quad (5-7)
\]

where \(R\) is the gas constant.

In the above system of equations it is necessary to define the interface, and at this point is coming the Level set formulation. Since the introduction of the Hamiltonian-Jacobi level set formulation by Osher and Sethian [212], the level set method has been used to model interfacial phenomena in the fields of material science, fluid mechanics, computer vision, grid generation, and image enhancement [250]. The mathematical formalism and rigor of the level set method has helped to attract many researchers, resulting in the evolution, widespread promotion and use of the method, increasing simultaneously the range of applicability.

The basic idea behind level set method it to embed the propagating interface \(\Gamma(t)\) as a zero level set of a higher dimensional function \(\phi\), defined as

\[
\phi(x,t = 0) = \pm d , \quad (5-8)
\]

where \(d\) is the distance from \(x\) to \(\Gamma(t=0)\), chosen to be positive or negative if \(x\) is inside or outside the initial \(\Gamma(t=0)\). The zero level set of \(\phi\) is the interface:

\[
\Gamma = \{x \mid \phi(x,t) = 0\} \quad (5-9)
\]

Since the interface moves with the fluid, the evolution of \(\phi\) (without phase change) is given by
5. RSPH for the simulation of Interfacial flows: A preliminary Study

\[
\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = 0 \tag{5-10}
\]

Additionally, the normal and the curvature of the interface can be easily expressed in terms of \( \phi(x,t) \):

\[
n = \left[ \nabla \phi \right]_{\phi=0} \quad \text{and} \quad \kappa = \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right)_{\phi=0} \tag{5-11}
\]

The level set method propagates the interface by integrating the same scalar equation as other capturing methods. The difference in level set methods is that the scalar function \( \phi \) is not a discrete representation of a Heaviside function (H) or a color function but rather a smoothly varying distance function. Here is the big advantage of using the level set method in our RSPH implementation, since \( \phi \) is smoothly varying and can be accurately solved.

Using the formulation of the Continuum Surface Force (CSF) [43] in the level set concept [270, 52, 269] the surface tension (5-5) can be written as:

\[
ST_i = \sigma \kappa \delta(d) n_i = \sigma \kappa \delta(\phi) \frac{\nabla \phi}{|\nabla \phi|} \tag{5-12}
\]

Using this formulation it is clear that the surface tension is a function of the level set. It must be noted that using equation (5-10), only the zero level set is moving correct and after some computational time the non-zero level sets do not correspond to the correct distance of the levels. Reinitializing the level set function \( \phi \) without changing the zero level set can correct the \( \phi \) [270, 269]. One potential disadvantage of this iterative re-initialization scheme is that it can result in a considerable movement of the zero level set [269, 250]. The Dirac delta function, \( \delta \), is represented by a smoothed or mollified delta function [52, 269]

\[
\delta_{\varepsilon}(\phi) = \frac{dH_{\varepsilon}}{d\phi} \tag{5-13}
\]

where \( H_{\varepsilon} \) is a regularized Heaviside function

\[
H_{\varepsilon}(\phi) = \begin{cases} 
0 & \text{if } \phi < -\varepsilon \\
\frac{1}{2} \left(1 + \frac{\phi}{\varepsilon} + \frac{1}{\pi} \sin \left( \frac{\pi \phi}{\varepsilon} \right) \right) & \text{if } |\phi| \leq \varepsilon \\
1 & \text{if } \phi > \varepsilon \tag{5-14}
\end{cases}
\]

where \( \varepsilon \) is a constant related with the thickness interface.

The non-dimensional variables are again obtained from the physical variables as follows:

\[
x_i^* = \frac{x_i}{L_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad t^* = \frac{tU_0}{L_0}, \quad u_i^* = \frac{u_i}{U_0}, \quad T^* = \frac{T}{T_0}, \quad \mu^* = \frac{\mu}{\mu_0}, \quad g_i^* = \frac{g_i}{g_0}, \quad k^* = \frac{k}{k_0}, \quad c_i^* = \frac{c_i}{c_{i0}} \tag{5-15}
\]

where the superscript * and the subscript 0 indicate the non-dimensional and the reference quantities. The quantities \( L_0, \rho_0, U_0, T_0, \mu_0, k_0 \) and \( c_{i0} \) denote the characteristic length, density, velocity,
5.2 Governing Equations, Level Set and RSPH methodology

Temperature, dynamic viscosity, thermal conductivity and specific heat at constant volume respectively. The dimensionless numbers that appear after non-dimensionalisation in the equations are:

\[
\begin{align*}
\text{Re} &= \frac{\rho_0 U_0}{\mu}, \quad M^2 = \frac{U_0^2}{\gamma R T_0}, \quad \text{Pr} = \frac{\mu c_p}{k}, \\
\text{Fr} &= \frac{U_0}{\sqrt{g_0 L_0}}, \quad \text{We} = \frac{\rho_0 U_0^2}{\sigma},
\end{align*}
\]  

(5-16)

where \( \gamma \) is the ratio of the specific heat capacities, and Re denotes the Reynolds number, M the Mach number, Pr the Prandtl number, Fr the Froude number and We the Weber number.

Finally the non-dimensional system of the governing equations can be written:

\[
\begin{align*}
\frac{D\rho^*}{Dt^*} &= -\rho^* \frac{\partial u_i^*}{\partial x_i^*} \\
\rho^* \frac{Du_i^*}{Dt^*} &= -\frac{1}{M^2} \frac{\partial p^*}{\partial x_i^*} + \frac{1}{\text{Re}} \frac{\partial \tau_{ij}^*}{\partial x_j^*} + \frac{1}{\text{Fr}^2} \rho^* g_i^* + \frac{1}{\text{We}^2} \kappa^* (\phi)^{\nabla} \phi \\
\rho^* c_v^* \frac{DT^*}{Dt^*} &= -(\gamma - 1) \rho^* \frac{\partial u_i^*}{\partial x_i^*} + \frac{M^2 \gamma (\gamma - 1)}{\text{Re}} \tau_{ij}^* \frac{\partial u_j^*}{\partial x_i^*} \\
&\quad + \frac{\gamma}{\text{Re} \text{Pr}} \frac{\partial}{\partial x_i^*} \left( k^* \frac{\partial T^*}{\partial x_i^*} \right) \\
p^* &= \rho^* T^*
\end{align*}
\]

(5-17) to (5-20)

where

\[
\tau_{ij}^* = \mu \left( \frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} - \frac{2}{3} \frac{\partial u_k^*}{\partial x_k^*} \right)
\]

(5-21)

5.2.2 Numerical Method

The RSPH (Section 2.3) is used for the discretization and numerical solution of the governing equations. The continuity and the momentum and energy equation for a 2-D flow are discretized in exactly the same way as in Chapter 2:

\[
\begin{align*}
\frac{D\rho_a}{Dt} &= -\rho_a \sum_b V_b (\vec{u}_b - \vec{u}_a) \cdot \nabla_a W (r_a - r_b, h) \\
\left\{ \rho \frac{Du_a}{Dt} \right\} &= -\left\{ \frac{\partial p}{\partial x} \right\}_a + \frac{4}{3} \left\{ \frac{\partial \mu}{\partial x} \frac{\partial u}{\partial x} \right\}_a - \frac{2}{3} \left\{ \frac{\partial \mu}{\partial x} \frac{\partial v}{\partial y} \right\}_a \\
&\quad + \left\{ \frac{\partial \mu}{\partial y} \frac{\partial u}{\partial y} \right\}_a + \left\{ \frac{\partial \mu}{\partial x} \frac{\partial v}{\partial x} \right\}_a + \left\{ \sigma \kappa \delta (\phi) \frac{d\phi}{dx} \right\}_a
\end{align*}
\]

(5-22) to (5-23)

91
\[
\left\langle \frac{Dv}{Dt} \right\rangle = -\frac{\partial p}{\partial t} + 4 \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial y} \right) - 2 \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{\partial v}{\partial x} \right) + \frac{\sigma \kappa}{\phi} \left( \frac{\partial \phi}{\partial y} \right)
\]

\[
\left\langle \rho \ c_v \frac{DT}{Dt} \right\rangle = -p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{2}{3} \mu \left( \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} \right)^2 \right) + \mu \left( \left( \frac{\partial v}{\partial x} \right)^2 \right) + \frac{\partial}{\partial x} \left( \frac{k \partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k \partial T}{\partial y} \right)
\]

where

\[
\left\langle \frac{\partial p}{\partial x} \right\rangle = \sum_b V_b \left( p_b - p_a \right) \cdot \frac{\partial}{\partial x} W(r_a - r_b, h)
\]

\[
\left\langle \frac{\partial p}{\partial y} \right\rangle = \sum_b V_b \left( p_b - p_a \right) \cdot \frac{\partial}{\partial y} W(r_a - r_b, h)
\]

\[
\left\langle \frac{\partial u^k}{\partial x_j} \mu \frac{\partial u^k}{\partial x_j} \right\rangle_a = \left\langle \frac{\partial u^k}{\partial x_j} \right\rangle_a \left\langle \frac{\partial u^k}{\partial x_j} \right\rangle_a + \left\langle \mu \frac{\partial^2 u^k}{\partial x_i \partial x_j} \right\rangle_a =
\]

\[
\left\langle \sum_b V_b \left( \mu_b - \mu_a \right) \cdot \frac{\partial}{\partial x_i} W(r_a - r_b, h) \right\rangle_a \left\langle \sum_b V_b \left( u^k_b - u^k_a \right) \cdot \frac{\partial}{\partial x_j} W(r_a - r_b, h) \right\rangle_a + \mu_a \left\langle \sum_b V_b \left( u^k_b - u^k_a \right) \cdot \frac{\partial^2}{\partial x_i \partial x_j} W(r_a - r_b, h) \right\rangle_a
\]

\[
\left\langle \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) \right\rangle_a = \left\langle \frac{\partial k}{\partial x_i} \right\rangle_a \left\langle \frac{\partial T}{\partial x_i} \right\rangle_a + \left\langle k \frac{\partial^2 T}{\partial x_i^2} \right\rangle_a =
\]

\[
\left\langle \sum_b V_b \left( k_b - k_a \right) \cdot \frac{\partial}{\partial x_i} W(r_a - r_b, h) \right\rangle_a \left\langle \sum_b V_b \left( T_b - T_a \right) \cdot \frac{\partial}{\partial x_i} W(r_a - r_b, h) \right\rangle_a + k_a \left\langle \sum_b V_b \left( T_b - T_a \right) \cdot \frac{\partial^2}{\partial x_i^2} W(r_a - r_b, h) \right\rangle_a
\]

The SPH formulation of the momentum equation terms (equations (5-23) and (5-24)) is obtained in a straightforward manner by combining equations ((5-26)-(5-28)) as needed. Note that equation (5-28) delivers all derivatives of the viscous terms (where i, j, k=1,2 and x_1=x, x_2=y, u_1=u, u_2=v). The compressibility and the viscous dissipation term in the energy equation can be easily discretized by using the general formula of equation (2-18). The curvature \( \kappa \) can be calculated from Eq. (5-11), which in 2-D takes the form:
\[ \langle \kappa \rangle_a = \left\langle \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \right\rangle_a = \]
\[ = \frac{\partial^2 \phi}{\partial x^2} \left\langle \left( \frac{\partial \phi}{\partial y} \right)^2 \right\rangle_a - 2 \left\langle \frac{\partial \phi}{\partial x} \right\rangle_a \left\langle \frac{\partial \phi}{\partial y} \right\rangle_a + \left\langle \frac{\partial^2 \phi}{\partial y^2} \right\rangle_a + \left\langle \left( \frac{\partial \phi}{\partial x} \right)^2 \right\rangle_a \]
\[ = \left( \left\langle \left( \frac{\partial \phi}{\partial x} \right)^2 \right\rangle_a + \left\langle \left( \frac{\partial \phi}{\partial y} \right)^2 \right\rangle_a \right)^{\frac{3}{2}} \tag{5-30} \]
where all the terms can evaluated using the formulas derived in Chapter 2.

The level set equation (Eq. (5-10)) is solved in a Lagrangian fashion following the trajectories of the particles:
\[ \left\langle \frac{D \phi}{D t} \right\rangle_a = 0 \tag{5-31} \]

The equation (5-31) is basically the exact solution using the method of characteristics for the advection equation. It is unconditionally stable and there is no time step restriction during time integration. Note that this is a full Lagrangian scheme and not a semi-Lagrangian [87, 266, 264, 265]. The regular Lagrangian mesh is rapidly distorted resulting in loss of discretization accuracy. As we discussed in Chapter 2, RSPH is basically formed, by solving the problem of grid distortion using a periodic remeshing of particles locations with high-order moment-conserving kernels.

5.3 Results and Discussion - Validation of the interface capturing technique

An acceptable tracking method must translate and rotate fluid bodies without significant distortion or degradation of the interfaces. The translation and rotation serve as useful debugging tests. In addition to standard translation and rotation, more complicated flows are used to evaluate the performance of interface-tracking algorithms. In the presence of vortical structures in the flow any interface can stretch and potentially tear within the flow [235]. For example, a single vortex that spins the fluid elements will stretch them into a filament that spirals toward the vortex center. We examined the validity of the Lagrangian level set scheme for interface tracking using the following basic test cases:
- Expanding and shrinking square
- Rigid body rotation of Zalesak’s Disk
- Single Vortex
- Rayleigh-Taylor Instability

5.3.1 Expanding and shrinking square

A common test for interface tracking algorithms is the expanding and shrinking of a square with a linear velocity field. In all cases the interface moves with an appropriate speed relative to the grid.

\[ u(x, y) = \pm 0.2x, \quad v(x, y) = \pm 0.2y \tag{5-32} \]
In *Figure 69* and *Figure 70* the expansion and shrinkage of a square are shown. The increase of particle resolution improves the results significantly. From the results it is clear that the implementation satisfies the Huygens’ principle, which states that corners moving outward round off into circular arcs (expanding case), while corners moving inward remain sharp (shrinking case).

*Figure 69* Square expansion: (a) Velocity vectors, (b) Square expanding using 3721 particles, (c) Square expanding using 14884 particles, (d) Square expanding using 59536 particles, for three different times (from inside to outside): t=0, t=1.25, t=2.5.

*Figure 70* Square shrinkage: (a) Velocity vectors, (b) Square shrinking using 3721 particles, (c) Square shrinking using 14884 particles, (d) Square shrinking using 59536 particles, for three different times (from outside to inside): t=0, t=1.25, t=2.5.
5.3 Results and Discussion - Validation of the interface capturing technique

5.3.2 Rigid body rotation of Zalesak’s Disk

The second test case considers a slotted circle centered at position \((x,y) = (0.5,0.75)\) with radius 0.15, width 0.05, and slot length 0.25, which rotates in a constant vorticity velocity field [295]. This test case is a good indicator of diffusion errors in an interface capturing method. The constant vorticity velocity field is given by:

\[
\begin{align*}
    u(x, y) &= 0.5 - y \\
    v(x, y) &= x - 0.5
\end{align*}
\]  

Figure 71(a) shows the velocity vectors of the field. Figure 71 (b)-(d) shows the evolution of the circle during one full rotation, for three different particle resolutions. It is clear that increasing the particle resolution improves the solution. Basic error analysis (Table 6) considering the area of the disk gives an estimate of the convergence of the algorithm. The algorithm seems to be 3rd order accurate, which is in agreement with the theoretical order of the remeshing algorithm. The RSPH solution is compared with a level set solution (Eulerian) [268] in Figure 72. The RSPH solution resolves better the corners than the traditional level set. It must be noted, that hybrid capturing techniques, like the resent proposed by Enright et al. [86], and front tracking schemes, show a superior behavior compared to RSPH.

![Figure 71 Zalesak’s disk rotation: (a) Velocity vectors, (b) Disk rotation using 3721 particles, (c) Disk rotation using 14884 particles, (d) Disk rotation using 59536 particles.](image)

Table 6: Zalesak’s disk error analysis

<table>
<thead>
<tr>
<th>No. of particles</th>
<th>Area</th>
<th>Relative Error %</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact</td>
<td>0.05939</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3721</td>
<td>0.07056</td>
<td>-18.80</td>
<td>-</td>
</tr>
<tr>
<td>14884</td>
<td>0.05826</td>
<td>1.90</td>
<td>3.3063</td>
</tr>
<tr>
<td>59536</td>
<td>0.05924</td>
<td>0.26</td>
<td>2.8524</td>
</tr>
</tbody>
</table>
5. RSPH for the simulation of Interfacial flows: A preliminary Study

5.3.3 Single Vortex

Zalesak’s test case [295] does not test the ability of the capturing technique to accurately resolve thin filaments. Such filaments can occur in stretching and tearing flows, and their size can be very small. In such a flow introduced by Bell, Colella and Glaz [24] the flow field results from a non-constant vorticity field centered in a box. The stream function of the velocity field is given by:

\[ \Psi(x, y) = \frac{1}{\pi} \sin^2(\pi x) \sin^2(\pi y) \]  

(5.34)

A circle of radius 0.15 centered at position \((x, y) = (0.5, 0.75)\) is used as initial condition. For comparison, a high-resolution front tracked [283] solution is used. The high-resolution solution is achieved by placing many particles at the interface and move them under the influence of the given velocity field. \(\text{Figure 73 - Figure 75}\) show the evolution of the circle for three different particle resolutions.

\(\text{Figure 73}\) Evolution of the circle in the single vortex flow at time: (a) \(t=0\), (b) \(t=1\), (c) \(t=3\), (d) \(t=5\): (-) RSPH using 3721 particles, (- -) high-resolution front tracked solution.

The coarser resolution remains accurate until time \(t=1\) (\(\text{Figure 73 (b)}\)), but cannot resolve higher stretching of the filament. With 14884 particles there is a clear improvement of the solution,
but the accuracy is still poor at \( t=5 \) (Figure 74 (d)). For the higher particle resolution the level set solution improves even when the filament becomes very thin (Figure 75 (d)). We must note that in the present level set implementation we are not using the re-initialization of the level sets [270], which can improve the capturing capabilities of the technique (as shown in [269]). Preliminary results shown that re-initialization may produce a considerable motion of the zero level set. This is also reported in the literature [250], where the use of an extension velocity is proposed. The performance of the Lagrangian level set is deemed to be very good compared with many other capturing techniques [239].

**Figure 74** Evolution of the circle in the single vortex flow at time: (a) \( t=0 \), (b) \( t=1 \), (c) \( t=3 \), (d) \( t=5 \): (-) RSPH using 14884 particles, (- -) high-resolution front tracked solution.

**Figure 75** Evolution of the circle in the single vortex flow at time: (a) \( t=0 \), (b) \( t=1 \), (c) \( t=3 \), (d) \( t=5 \): (-) RSPH using 59536 particles, (- -) high-resolution front tracked solution.
5.3.4 Rayleigh-Taylor Instability

In order to demonstrate the capability of the coupled RSPH Lagrangian level set approach to deal with complex cases we simulate here the classical test case of air above helium. The first case consists of the example treated by Bell and Marcus [25]. In this problem a heavy fluid (air) lies above a light fluid (helium). The domain has 1m width and 4m height. The densities of the two fluids are 1.172 kg/m³ and 0.164 kg/m³, respectively. The density ratio across the interface is 7.15:1 and the Atwood number \( A_r = \frac{\rho_{\text{air}} - \rho_{\text{He}}}{\rho_{\text{air}} + \rho_{\text{He}}} = 0.755 \). The viscosity for each fluid is \( 3.1305 \times 10^{-3} \) kg/ms, and as a consequence, the velocities are expected to be continuously differentiable. A sinusoidal perturbation with amplitude of 0.05m is applied to the position of the interface, and the surface tension is neglected at the fluid interfaces. The speed of sound of air is taken 10m/s. This is a practical assumption as it leads to reasonable time steps in the integration, and it is equivalent to the assumption of the Mach number used in the previous chapters. The speed of sound of helium is \( c_{\text{He}} = c_{\text{air}} \sqrt{\frac{\rho_{\text{air}}}{\rho_{\text{He}}}} \) which is acceptable from thermodynamic point of view. The initial density profile is exponential function of the height (using the assumption of isothermal regions).

\[
\rho(y) = \rho_0 e^{-\frac{g}{\rho} (y-y_0)} \quad (5-35)
\]

where \( y_0 \) is the interface location, \( \rho_0 \) the density above and below the interface

\[
\rho_0 = \begin{cases} 
1.172 \text{ kg/m}^3 & \text{if } y \geq y_0 \\
0.164 \text{ kg/m}^3 & \text{if } y < y_0 
\end{cases} \quad (5-36)
\]

In Figure 76 - Figure 78 the contours of the level set \( \phi \) are shown, for times t=0, 0.25, …,1.0 sec, for three different particle resolutions. Because of symmetry, the computational domain is half the size in the horizontal direction from that shown in Figure 76 - Figure 78. The particle resolutions used are 7200 (30×240), 28800 (60×480) and 115200 (121×960).

The initial sinusoidal interfacial perturbation, in Figure 76 - Figure 78, grows as expected into a mushroom shaped interface, and develop side rolls. The solution is resolved with all resolution until time 0.5. For longer time integration the lower resolution cannot resolve the small-scale features of the interface.
5.3 Results and Discussion - Validation of the interface capturing technique

Figure 76 Evolution of the Rayleigh-Taylor instability. Contours of level sets $\phi$ at values $-\frac{1}{31}, 0, \frac{1}{31}$, at times: t=0, 0.25, 0.5, 0.75, 1.0 sec, using 7200 particles.

Figure 77 Evolution of the Rayleigh-Taylor instability. Contours of level sets $\phi$ at values $-\frac{1}{31}, 0, \frac{1}{31}$, at times: t=0, 0.25, 0.5, 0.75, 1.0 sec, using 28800 particles.
Figure 78 Evolution of the Rayleigh-Taylor instability. Contours of level sets $\phi$ at values $-\frac{1}{31}, 0, \frac{1}{31}$, at times: $t=0, 0.25, 0.5, 0.75, 1.0$ sec, using 115200 particles.

In order to evaluate the RSPH in more realistic situations, we consider the air/helium Rayleigh-Taylor instability in a domain with dimensions $0.01 \text{m} \times 0.04 \text{m}$. The viscosities of air and helium for this case are $1.77625 \times 10^{-5}$ kg/ms, and $1.941 \times 10^{-5}$ kg/ms, respectively. In this case, the velocity at the interface in not continuously differentiable (there is a jump in the velocity gradient). All the other properties are the same as in the case presented above. In Figure 79 - Figure 82 the contours of the level set $\phi$ are shown, for times $t=0, 0.0025, \ldots, 0.10$ sec, for three different particle resolutions.

Figure 79 Evolution of the Rayleigh-Taylor instability. Contours of level sets $\phi$ at values $-\frac{1}{31}, 0, \frac{1}{31}$, at times: $t=0, 0.025, 0.05, 0.075, 0.10$ sec, using 7200 particles.
The results indicate that the interface is resolved with all the particle resolutions. A difference in the small features of the interface is once more observed. The solution for time $t=0.10$ sec in Figure 80 shows some spurious disorder in the level sets. The smooth remeshing function (2-37) and the lack of the redistance algorithm in our implementation are certainly two reasons for the existence of these spurious values.
The RSPH results are compared with the results of a high order projection scheme coupled with second order volume of fluid [226] in Figure 82. The agreement of the two solutions is fairly good, even in the mushroom cap. The bigger discrepancies between the two solutions appear in the regions where the helium is moving upward.

![Evolution of the Rayleigh-Taylor instability. Contours of the interface using the RSPH – level set (colored) using 28800 particles, and a high order projection scheme coupled with second order volume of fluid [226] (lines), at times: t=0, 0.047, 0.066, 0.088, 0.118 sec.](image)

**Figure 82** Evolution of the Rayleigh-Taylor instability. Contours of the interface using the RSPH – level set (colored) using 28800 particles, and a high order projection scheme coupled with second order volume of fluid [226] (lines), at times: t=0, 0.047, 0.066, 0.088, 0.118 sec.

### 5.4 Summary

The RSPH is coupled with the level set method. The implemented level set method is solved for first time in a Lagrangian manner. The Lagrangian level set is enjoying unconditionally stability and zero dissipation due to the non-linear convection term of the level set equation. On the other hand, remeshing of the level sets introduces numerical errors. The added dissipation induced by remeshing is proportional to the gradients of the field, which are induced by particle-distance distortion. The gradients of level set are generally constant and the remeshing is introducing low dissipation. The performance of the Lagrangian level set in displacement, rotation and stretching of the level sets is deemed satisfactory. The computational cost of the Lagrangian level set is less than 2% of the total computational cost.

The results presented in this chapter show that the level set method is an accurate and efficient approach for capturing interfacial motion. The present study is directly related to the material removal aspect of the process of shown in Figure 2. Level set is capable of representing surface and phase change effects and the formulations and preliminary results presented here are meant to be a first step towards future work.
Chapter 6

Summary & Future Work

A Lagrangian particle numerical method based on smooth particle hydrodynamics has been developed for numerical simulation of low Mach number compressible, viscous, heat conducting, reacting and interfacial flows, (all features of the engineering problem of interest defined in Figure 2). The classical SPH [191] has been extended to accurately account for diffusion effects.

Particle methods generally are enjoying adaptivity and exact unconditionally stable treatment of the non-linear convection terms. In this thesis the main interest was the investigation of accuracy and applicability of SPH in engineering problems. Under this consideration the SPH is coupled with high-order moment-conserving remeshing schemes. Remeshing introduces numerical errors, which may be viewed as aliasing errors due to the implementation of remeshing kernels with finite support. The extra diffusion that the remeshing procedure introduces can be quite large, but it should be pointed out that the added dissipation induced by remeshing is proportional to the gradients of the flow field. These gradients remain very small when remeshing is performed at each time step. Finally, as discussed in [68, 135], the overall effect of remeshing is to act as a subgrid-scale model, which has been shown to have a negligible effect on the overall accuracy of the simulations [135].

The robustness and accuracy of the proposed Remeshed SPH (RSPH) methodology is tested for a number of benchmark problems involving flow and energy transport. The accuracy of the developed RSPH method comes with a minimal additional computational cost, while maintaining the adaptive character of the method. Furthermore, the tensorial character of the remeshing schemes make it easily extendable to three dimensions and no extra algorithmic constraints are imposed by the proposed modeling of the viscous terms in conjunction with remeshing.

Concerning the applicability of RSPH, detailed two-dimensional simulations for the flow and heat transfer characteristics of single and pair slot pulsating jets impinging on a hot surface, has been conducted. The performance of these configurations has been investigated. By varying systematically the characteristics (frequency, amplitude and phase angle) as well as the Reynolds number, we have identified optimum operating regimes. For particular Reynolds numbers, we have identified intermittent behavior of the system (periodic/chaotic) and more importantly, windows of pure periodicity at post-chaotic states.

Moreover, RSPH methodology is applied for the simulation of chemically reacting flows. A laminar, planar, opposed-jet burner is modeled numerically using a detailed hydrogen-oxygen mechanism involving 9 species and 21 elementary reactions. The results indicate that RSPH is capable for solution of systems with complex chemistry. In our RSPH solver, a multithread parallel technique is implemented in order to accelerate the computational time of detailed reacting simulations.

Finally, RSPH methodology is applied in preliminary fashion to the simulation of interfacial and multiphase flows. The level set approach is adopted in order to track the interface topology. The implemented Lagrangian level set is tested against basic interface tracking test cases. The results indicate that the Lagrangian level set is a robust and accurate scheme, which is not suffering from time step limitations that usually are following the Eulerian interface capturing techniques.
Summarizing, we have to point out, that there are no topological or geometrical assumptions in the RSPH scheme that can limit the applicability of the method in three dimensions. The computational cost of RSPH is considered competitive to other grid-based techniques. The present numerical scheme has second-order spatial discretization accuracy. Note that higher-order kernels functions can be easily applied in the present RSPH implementation. However, RSPH in the present formulation is probably not applicable for high Mach number flows and generally in flows with discontinuities (e.g. shocks). We expect that that the remeshing schemes that we are using will probable smear the shock regions.

Future development of the two-dimensional RSPH implementation is mostly concerning algorithmic and applicability improvements. The RSPH implementation can be relative easily extended in three-dimensional flows. Massively parallel computing environment (e.g. Message Passing Interface) is required in order to accelerate the computations and gain from the particle meshfree nature of RSPH. Additional speed up of the computations can be achieved by calculating the forces and fluxes in the discretized equations only once (and not twice, since contributions between the particles are generally in symmetric form). The presented RSPH implementation is based on equidistant particle spacing. Variable particle spacing can be also applied in RSPH, like in vortex methods [69], however the applicability of remeshing in non-equidistant grids is not clear.

RSPH can gain further accuracy from improvements of higher order kernel functions, and/or relevant shock-capturing operators. Developments of other related particle methods (e.g. vortex methods) can be used in the context of RSPH. Other methods can as well have benefit from the high-order remeshing schemes that first used in vortex methods [135, 70] and we applied in SPH.

Further applicability of RSPH is possible in many fields. The results demonstrated that the proposed RSPH methodology is capable of DNS quality simulations while maintaining its robustness and adaptivity. Introduction of turbulent techniques or Large Eddy Simulation (LES) models using RSPH is a feasible extension, which can make RSPH applicable in more engineering problems.

Direct numerical simulation of interfacial phenomena, including surface tension effects and phase change is a challenging engineering area and extension of RSPH in this field is deemed reasonable. The implementation of level set method in RSPH is a significant step in this direction.

Moreover, implementation of immersed boundary algorithms (immersed boundary is an innovative approach to deal with the problem of modeling fluid flows interacting with a flexible, elastic boundary) can extend RSPH in more complex problems. A plethora of interesting physical problems may be investigated using such implementations.
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References


References


References


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