An Improved Ghost-cell Immersed Boundary Method for Compressible Inviscid Flow Simulations

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ABSTRACT

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This study presents an improved ghost-cell immersed boundary approach to represent a solid body in compressible flow simulations. In contrast to the commonly used approaches, in the present work ghost cells are mirrored through the boundary described using a level-set method to farther image points, incorporating a higher-order extra/interpolation scheme for the ghost cell values. In addition, a shock sensor is introduced to deal with image points near the discontinuities in the flow field. Adaptive mesh refinement (AMR) is used to improve the representation of the geometry efficiently. The improved ghost-cell method is validated against five test cases: (a) double Mach reflections on a ramp, (b) supersonic flows in a wind tunnel with a forward-facing step, (c) supersonic flows over a circular cylinder, (d) smooth Prandtl-Meyer expansion flows, and (e) steady shock-induced combustion over a wedge. It is demonstrated that the improved ghost-cell method can reach the accuracy of second order in $L^1$ norm and higher than first order in $L^\infty$ norm. Direct comparisons against the cut-cell method demonstrate that the improved ghost-cell method is almost equally accurate with better efficiency for boundary representation in high-fidelity compressible flow simulations. Implementation of the improved ghost-cell method in reacting Euler flows further validates its general applicability for compressible flow simulations.
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Chapter 1

Introduction

While non-Cartesian body-fitted grid system is advantageous for dealing with general geometry of solid boundaries, the Cartesian grid system is still dominant in some area that uses adaptive mesh refinement (AMR) or direct numerical simulations (DNS) due to its simplicity and regularity. To have solid body geometries in a Cartesian grid system avoiding a stair-case like representation, one may adopt one of the two popular approaches: the cut-cell method or the ghost-cell method.

In the cut-cell method [2–5], near-boundary computational cells are cut by the true boundary. Though cut-cell method can guarantee strict conservation of mass and momentum at the boundary, cell reshaping may generate very small cells, which limit the time-step size satisfying stability condition, resulting in steep increase in the computational cost. To address this small-cell problem, solutions such as cell-merging technique [2, 6], rotating box method [4], and flux-redistribution procedure [3, 7–11], have been proposed.

In the ghost-cell method [12], ghost cells are defined as neighbor cells inside the solid boundary which implicitly incorporates conditions to be satisfied at the boundary. The ghost-cell method is often coupled with a level-set method [13] to deal with complex geometries or interfaces. The detailed ghost-cell/level-set implementation can be found in [14–18]. In general, the ghost-cell method is considered not as accurate as the cut-cell method at the same resolution of the Cartesian grid because
it inherently represents the solid boundary implicitly, and for conventional ghost-cell method, it is non-conservative. However, it is advantageous for implementation and computational efficiency as it does not require to modify flux calculations of existing Cartesian-system based codes, and it does not involve cell reshaping procedure. The accuracy of ghost-cell method is determined by how the ghost-cell variables are extra/interpolated through the boundary. A classical scheme computing ghost-cell values is the bilinear interpolation (trilinear for three-dimensional cases) for symmetrically mirrored points. However, when the mirrored point is too close to the boundary, it may occur that four surrounding points required for the bilinear interpolation, for example in two-dimensional cases, are not all in the fluid domain. If this too-close ghost-cell issue [19] happens, constructing missing points using zeroth order extrapolation [20] or using body-intercepting points instead of the missing points for interpolation [21, 22] can be considered.

In this thesis, an improved approach based on ghost-cell method is proposed to deal with the too-close ghost-cell issue for two-dimensional Euler equations by constructing the value at ghost cells too close to the boundary from a farther points inside the fluid domain that allows complete bilinear interpolations at image points. This idea was first proposed for incompressible flow simulations [23], and is implemented to be suitable for compressible flow simulations in the present study. Subsequently, feasibility of this approach for the reacting Euler flows is validated. To estimate the robustness and accuracy of the proposed ghost-cell method, simulation results over a range of selected test problems are presented and discussed in comparison to those from a ghost-cell method using zeroth order extrapolation [20] for too-close ghost cells, and to those from a cut-cell method available from the Chombo package [24, 25]. Both single-species compressible Euler flows and multiple-species reacting flows are considered in the simulations.
Chapter 2

Formulation and Equations

In this chapter, the governing equations are derived and clarified. The ghost-cell immersed boundary method is verified in compressible flow simulations, where the equations to be solved are compressible Euler equations for inviscid flows and additional species equations for reacting flows.

2.1 Single-species Compressible Flows

The basic equations for single-species compressible flows is the Euler equations,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (2.1)
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{uu}) + \nabla p = 0 \quad (2.2)
\]

\[
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\mathbf{u}) = 0 \quad (2.3)
\]

where \(\rho, \mathbf{u}, p, E\) denote the density, velocity, pressure, and total specific energy, respectively.

We assume that the single-species compressible flows (gas) at standard conditions is calorically perfect. Therefore, for a calorically ideal gas, total specific energy \(E\) and
speed of sound $c$ are written as

$$E = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u^2, \quad c = \sqrt{\frac{\gamma p}{\rho}} \quad (2.4)$$

where gas constant $\gamma$ is defined as the ratio of specific heats,

$$\gamma = \frac{c_p}{c_v} \quad (2.5)$$

Here, $c_p$ is the specific heat at constant pressure and $c_v$ is the specific heat at constant volume. Since the gas is assumed to be calorically perfect, the specific heats are constant values. At standard conditions, for a diatomic gas such as hydrogen, the gas constant is $\gamma = 1.4$.

### 2.2 Multiple-species Non-reacting Flows

The above single-species Euler equations system is able to be modified for multiple species. $N$ species equations need to be added to the governing equations system, $N$ is the number of the species being considered. The species equations added are expressed in a general form,

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho u Y_k) = 0. \quad (2.6)$$

Here, $Y_k$ represents the mass fraction of species $k$, $k = 1, ..., N$.

For a mixture of calorically perfect gases, the specific heats $c_{p,k}$ and $c_{v,k}$ of each species $k$ are constant. Hence, the total specific heats $c_p$ and $c_v$ of the mixture are obtained as

$$c_p = \sum_{k=1}^{N} Y_k c_{p,k} \quad \text{and} \quad (2.7)$$
\[ c_v = \sum_{k=1}^{N} Y_k c_{v,k}. \]  

(2.8)

Using formula (2.7) and (2.8), gas constant \( \gamma \) for the multiple species is represented as

\[ \gamma = \frac{c_p}{c_v} = \frac{\sum_{k=1}^{N} Y_k c_{p,k}}{\sum_{k=1}^{N} Y_k c_{v,k}}. \]  

(2.9)

It is obvious that \( \gamma = \gamma(Y_1, ..., Y_k, ..., Y_N) \) is a function of the mass fractions.

For a mixture of thermally perfect gases, the specific heats \( c_{p,k} \) and \( c_{v,k} \) are also functions of temperature. Thus, \( \gamma = \gamma(Y_1, ..., Y_k, ..., Y_N, T) \) is a function of both temperature and mass fractions.

In practical implementation, the specific heats \( c_p \) and \( c_v \) for multiple species can be calculated with the aid of a chemical kinetics package, Cantera [26].

### 2.3 Compressible Reacting Flows

The multiple-species Euler equations can be further modified to resolve reacting Euler flows when chemical reactions are taken into account. With reacting form source terms added, the general species equations become,

\[ \frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho u Y_k) = \dot{\omega}_k(T, p, Y_1, Y_2, ..., Y_N) \]  

(2.10)

where \( \dot{\omega}_k \) is the mass production rate of species \( k, k = 1, ..., N. \)

Regarding chemically reacting gases, the assumption for thermodynamic properties based on ideal gases is not true. For simplicity, here we just assume a chemically reacting mixture of perfect gases.

Two-dimensional cases are mainly discussed in this work. The following is the full 2D compressible reacting equations in conservative form:

\[ U_t + F(U)_x + G(U)_y = S_{react} \]  

(2.11)
with

$$
U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
E \\
\rho Y_1 \\
\vdots \\
\rho Y_N
\end{bmatrix},
F(U) = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho u(E + p) \\
\rho u Y_1 \\
\vdots \\
\rho u Y_N
\end{bmatrix},
G(U) = \begin{bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
v(E + p) \\
\rho v Y_1 \\
\vdots \\
\rho v Y_N
\end{bmatrix}
$$

(2.12)

and

$$
S_{react} = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\dot{\omega}_1(T, \rho, Y_1, Y_2, ..., Y_N) \\
\vdots \\
\dot{\omega}_N(T, \rho, Y_1, Y_2, ..., Y_N)
\end{bmatrix}.
$$

(2.13)
Chapter 3

Numerical Methods

In this chapter numerical methods are discussed which solve the governing equations numerically both in the internal fluid domain and on the solid boundary. The improved ghost-cell method is introduced in comparison with the conventional ghost-cell method implemented in AMROC package [20].

3.1 Strang Splitting

Strang splitting [27] is a time splitting method which is able to discretize the one time step full governing equations (2.11) into simpler equations in several time steps. This technique splits apart the convection and reaction terms of the 2D compressible convection-reaction equations and is overall second order accurate.

To begin with, the above conservative governing equations (2.11) can be rewritten as

$$\frac{\partial U}{\partial t} = -\nabla \cdot F + S_{\text{react}}$$ (3.1)

where $F$ is the flux vector in general direction, $S_{\text{react}}$ is the reaction source terms. With Strang splitting discretization, to update the conservative variables, $U$, over one time step of size $\Delta t$, we first react for half a time step $\frac{\Delta t}{2}$, then advect for a full time step $\Delta t$ without reacting terms, finally react for another half a time step $\frac{\Delta t}{2}$. In
this way, the discretization of the governing equation (3.1) is basically divided into the following three steps:

\[
U^{n+1/3} = U^n + \frac{\Delta t}{2} S_{\text{react}}^n
\]  

(3.2)

\[
U^{n+2/3} = U^{n+1/3} - \Delta t \nabla \cdot F^{n+1/2}
\]  

(3.3)

\[
U^{n+1} = U^{n+2/3} + \frac{\Delta t}{2} S_{\text{react}}^{n+1}.
\]  

(3.4)

As a result, the problem is simplified to solve one partial differential equation (3.3) (advection equation) and two ordinary differential equations (3.2) and (3.4) (reaction equations).

3.2 Hydrodynamic Advection

The advection equations are discretized by finite volume method and solved by an unsplit 2nd order Godunov method. The time-centered edge states are reconstructed by the piecewise parabolic method (PPM) and the fluxes at the cell edges are then predicted by an approximate Riemann solver.

3.2.1 Godunov method

Using a finite volume method, within each cell \( I_{i,j} = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}; y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}] \), the above advection equation (3.3) is discretized in space and time,

\[
U_{i,j}^{n+2/3} = U_{i,j}^{n+1/3} + \frac{\Delta t}{\Delta x}[F_{i-\frac{1}{2}}^{n+1/2} - F_{i+\frac{1}{2}}^{n+1/2}] + \frac{\Delta t}{\Delta y}[G_{j-\frac{1}{2}}^{n+1/2} - G_{j+\frac{1}{2}}^{n+1/2}]
\]  

(3.5)

with numerical fluxes at cell interfaces given by

\[
F_{i+\frac{1}{2}}^{n+1/2} = F(U_{i+\frac{1}{2}}^{n+1/2}), \quad G_{j+\frac{1}{2}}^{n+1/2} = G(U_{j+\frac{1}{2}}^{n+1/2}).
\]  

The piecewise parabolic method (PPM) introduced by Colella and Woodward [28]
is adopted here for the approximation of time-centered edge states $U^{n+1/2}_{j+1/2}$. In the PPM algorithm, the time-centered edge states of primitive variables $Q(\rho, u, v, p, ...)$ at each cell edge are extrapolated from the base-time data in space and time, using a characteristic wave propagation. To explain in detail, a 4th order spatial interpolation of the cell center values to the high and low edge sides is applied with van Leer slope limiter in the beginning; Then a quadratic profile is constructed using the high and low edge states; For the next step concerning time integration, average value swept out by the quadratic profile across the cell face is computed; Finally the left and right edge states can be extrapolated from the base-time data.

After the left state $Q_L(\rho_L, u_L, v_L, p_L, ...)$ and the right state $Q_R(\rho_R, u_R, v_R, p_R, ...)$ of the cell edge are reconstructed, a Riemann problem is established around each cell edge, the cell edge fluxes $F^{n+1/2}$ and $G^{n+1/2}$ can then be constructed using a Riemann solver.

### 3.2.2 Riemann solver

The Riemann solver used for this study is the primitive variable Riemann solvers (PVRS)\[29\], an approximate Riemann solver using the characteristic equations to obtain approximate solutions for the star values. For x-split, two dimensional time dependent Euler equations, the following differential relations hold true along characteristic directions,

\[
\begin{align*}
\left\{\begin{array}{l}
dp - \rho adu = 0 & \text{along } dx/dt = u - a \\
dp - a^2d\rho = 0 & \text{along } dx/dt = u \\
dp + \rho adu = 0 & \text{along } dx/dt = u + a
\end{array}\right. \tag{3.7}
\]

where $a = \sqrt{\gamma \rho / \rho}$ is the sound speed.

Set $C = \rho a$, and integrate $dp - \rho adu = 0$ along the characteristic of speed $u - a$, with $C$ evaluated at the foot of the characteristic. Then we can get the following
relation
\[ p^* - C_R u^* = p_R - C_R u_R. \] (3.8)

Similarly, integrate \( dp + padu = 0 \) along the characteristic of speed \( u + a \), another relation is obtained,
\[ p^* + C_L u^* = p_L + C_L u_L. \] (3.9)

Combining the above relation (3.8), (3.9) and (3.7), the full solution for star variables can be summarized as

\[ p^* = \frac{C_L p_R + C_R p_L + C_L C_R (u_L - u_R)}{C_L + C_R} \] (3.10)

\[ u^* = \frac{C_L u_L + C_R u_R + (p_L - p_R)}{C_L + C_R} \] (3.11)

\[ \rho_{L,R}^* = \rho_{L,R} + \frac{p^* - p_{L,R}}{a_{L,R}^2} \] (3.12)

\[ (a_{L,R}^*)^2 = \gamma p^*/\rho_{L,R}^* \] (3.13)

\[ \mathbf{v}_{L,R}^* = \mathbf{v}_{L,R}. \] (3.14)

Here, \( \mathbf{v} \) refers to all the advected quantities including transverse velocity components, \( L,R \) represents the left and right states for the Riemann problem and \( ^* \) represents values on the left and right side of the contact discontinuity. For multiple-species flows, the mass fractions \( Y_1, ..., Y_k, ..., Y_{NS} \) are treated as advected quantities.

After the star variables are obtained, we sample the solution to find the interface variables \( \mathbf{Q}^{n+1/2}(0) \). The primitive variables \( \mathbf{Q}^{n+1/2}(0) \) are finally converted to the conservative variables \( \mathbf{U}^{n+1/2}(0) \). Thereby, the Godunov fluxes \( \mathbf{F}^{n+1/2} \) and \( \mathbf{G}^{n+1/2} \) can be computed by equation (3.6).
3.3 Chemical Reaction

The chemical reaction part involves a system of ordinary differential equations. Consider ing equations (3.2) and (2.13), the relation \( \rho_t = (\rho u)_t = (\rho v)_t = E_t = 0 \) is enforced by the first four equations. Hence, \( \rho, u, v \) and \( E \) are kept as constants during the reaction process. The mass production rate of species \( k \) is then represented as \( \dot{\omega}_k(e, \rho, Y_1, Y_2, ..., Y_N) \), which is a function of the species mass fractions \( Y_1, Y_2, ..., Y_N \). The value of \( \dot{\omega}_k \) can be evaluated using Cantera \[26\] when the variables \( e, \rho, Y_1, ... \) and \( Y_N \) are given. Finally the reaction equations (3.2) reduce to the following system of ordinary differential equations,

\[
\begin{pmatrix}
\rho Y_1 \\
\rho Y_2 \\
\vdots \\
\rho Y_N
\end{pmatrix}_t =
\begin{pmatrix}
\dot{\omega}_1(e, \rho, Y_1, Y_2, ..., Y_N) \\
\dot{\omega}_2(e, \rho, Y_1, Y_2, ..., Y_N) \\
\vdots \\
\dot{\omega}_N(e, \rho, Y_1, Y_2, ..., Y_N)
\end{pmatrix}
\]

(3.15)

where \( e \) is the internal energy, \( e \) and \( \rho \) are constants during the ODE solving process.

We use the ODE solver VODE (variable-coefficient ordinary differential equation solver) \[30\] to integrate the above equations which are mathematically stiff. The Jacobian is generated internally by numerical differencing. Finally the mass fractions \( Y_1, Y_2, ..., Y_N \) are updated successfully through the ODE solver.

3.4 Ghost-cell immersed boundary method

A ghost-cell method is adopted to implement boundary conditions for the immersed boundaries while keeping the overall finite-volume method intact. In the ghost-cell method, the boundary conditions are incorporated implicitly by defining ghost-cell values appropriately. In the present study, the surface of the immersed geometries are assumed to be slip wall \( (u_n = \frac{\partial u}{\partial n} = 0) \) satisfying non-catalytic \( (\frac{\partial Y_k}{\partial n} = 0) \) and
adiabatic \( \frac{\partial T}{\partial n} = 0 \) conditions, where \( n \) is the local normal to the boundary, \( Y_k \) is the \( k^{th} \) species, \( u_n \) is the velocity component normal to the boundary and \( u_t \) is the velocity component tangential to the boundary.

### 3.4.1 Adaptive mesh refinement

Representation of immersed boundaries in the Cartesian grid system can be improved using adaptive mesh refinement (AMR) which can be applied not only to regions of large gradient in the fluid domain but also to the boundaries of geometry. A block-structured AMR method based on Boxlib \[31\] is implemented to the present study. The Boxlib library supports all the functionality needed to write a parallel AMR application. For the present hyperbolic system, the refinement of the nested grid hierarchy is simultaneous in both time and space.

The AMR technique can ensure refined mesh located in the areas of interest, such as regions where solid boundary lies or high gradients exist. By adaptively distributing different levels of meshes in the flow field, a more efficient use of the CPU and storage is possible. To make tags for the areas of interest which need finer refinements, sensors are created which mark the cells where the gradients of the flow properties exceed the prescribed values. In each level of refinement, the marked cells are divided into several smaller cells depending on the refinement ratio, the smaller cells are then calibrated and marked again for the next level of refinement. Overall, with adaptive refinements, physical shocks and detonations are captured precisely, solid boundary geometry is resolved accurately and the computing resources are utilized efficiently.

### 3.4.2 Level set method

To accurately represent the solid wall boundary which intersects with the Cartesian grid and to store the necessary geometric information for the ghost cell projection process, we implement the level set method, which has been introduced by Osher and
Sethian[32] to represent the interface in the computational domain. Details on the level set method can be found in [13, 33, 34].

Two-dimensional, stationary level set cases are considered in the present study. A level set function \( \phi(x, y) \) is defined using the signed distance from point \((x, y)\) to the immersed boundary. Specifically, \( \phi(x, y) \) is positive inside the fluid domain and negative outside. \( \phi(x, y) = 0 \) represents points exactly on the interface. Hence, the level set function \( \phi(x, y) \) is able to represent different complex geometries, giving the geometry parameters which are necessary to construct \( \phi(x, y) \). In this study, the absolute distance to the interface \( |\phi(x, y)| \) and the normal vector \( \nabla \phi(x, y) \) of the isoline of \( \phi \) are utilized to determine the relative positions of the image points of ghost cells and to compute the extrapolated ghost cell values.

### 3.4.3 Baseline ghost-cell method

The conventional bilinear interpolation scheme which can be found in AMROC package [20] for example is referred to a baseline ghost-cell method in the present study. In the baseline ghost-cell method (Fig. 3.1), an image point of a ghost cell is symmetrically mirrored through the boundary, satisfying

\[
\mathbf{r}_{\text{image}} = -\mathbf{r}_{\text{ghost}}
\]  

(3.16)

where \( \mathbf{r}_{\text{image}} \) is the distance vector from the projection point to the image point and \( \mathbf{r}_{\text{ghost}} \) is the distance vector from the projection point to the ghost point, i.e. the center of the ghost cell. Then the state values at the image point can be defined using a bilinear interpolation from surrounding cell-centered values available. The baseline ghost-cell method finds the values at the image points using a complete bilinear interpolation for the case A but using an incomplete bilinear interpolation for the case B when the ghost cell is too close to the boundary. When there are missing
points to construct bilinear interpolation, they are arbitrarily extrapolated from either the horizontal neighboring point or the vertical neighboring point depending on the sequential order of interpolation.

Once the location and values of the image points of the ghost cells are identified, boundary conditions for the projection points can be applied to construct ghost cell values as

$$q_{\text{ghost}} = q_{\text{image}}, \quad \text{and}$$

$$u_n|_{\text{ghost}} = -u_n|_{\text{image}},$$

where $u_n$ is the velocity component normal to the boundary and $q$ contains all the rest of primitive variables including $u_t$, the velocity component tangent to the boundary.

![Figure 3.1: Relative positions of ghost cells, projection points, image points and the surrounding fluid cells for a bilinear interpolation.](image)

The baseline ghost-cell method is simple to implement and known to be robust enough. However, when incomplete bilinear interpolation is applied to those ghost cells closer to the boundary, there may arise a concern of decreased accuracy, which motivates the improvement suggested in the present study.
3.4.4 Improved ghost-cell method

An improved ghost-cell method is proposed, which can ensure complete bilinear interpolations in the construction of image point values. This concept has been introduced by Pan and Shen [23] for incompressible flows, and we extend its application to compressible flows here. In this method, when the distance between ghost-cell node and the immersed boundary is smaller than a threshold, the image point is projected to a farther distance in fluid domain as shown in Fig. 3.2. The distance $\delta$ should be large enough to ensure the image point to be enclosed by a complete set of four neighboring fluid cells, but an excessive large distance $\delta$ is inappropriate and may result in incorrect modeling of the boundary. Thus it is suggested that a threshold distance is defined as $\delta = \sqrt{2}\Delta x$ in two-dimensional cases, $\Delta x$ is the cell size. Besides, for a quadratic extrapolation for the boundary conditions, an extra image point with a distance vector from the image point to the extra image point is defined as $r_{\text{extra}}$.

For a non-catalytic, adiabatic, slip wall boundary condition, we have the relation

\begin{align}
\left. u_n \right|_{\text{proj}} &= 0 \\
\left. \frac{\partial q}{\partial n} \right|_{\text{proj}} &= 0
\end{align}

(3.19) (3.20)

where $n$ is the coordinate normal to the wall boundary, $u_n$ is the velocity component normal to the boundary, and $q$ contains all the rest of primitive variables including $u_t$ (velocity component tangent to the boundary).

We assume that the normal gradients $\frac{\partial q}{\partial n}$ at the ghost cell, at the projection point, and at the image point are linear each other. For the normal component of the velocity $u_n$, a quadratic extrapolation is applied. We first derive the ghost-cell value for $q$ that incorporates the boundary condition (3.20), then for $u_n$ at the ghost cell that satisfies the boundary condition (3.19).
A relation obtained from the assumption of linear normal gradients is

$$\frac{\partial q}{\partial n}|_{\text{ghost}} = \frac{\partial q}{\partial n}|_{\text{proj}} - |r_{\text{ghost}}| \cdot s_0$$  \hspace{1cm} (3.21)

where $s_0$ is the slope defined by

$$s_0 = \frac{\frac{\partial q}{\partial n}|_{\text{image}} - \frac{\partial q}{\partial n}|_{\text{proj}}}{\delta}$$  \hspace{1cm} (3.22)

Once the boundary condition (3.20) is applied, equation (3.21) can be written as

$$\frac{\partial q}{\partial n}|_{\text{ghost}} = 0 - |r_{\text{ghost}}| \cdot \frac{\frac{\partial q}{\partial n}|_{\text{image}} - 0}{\delta}$$

$$= -|r_{\text{ghost}}| \cdot \frac{\frac{\partial q}{\partial n}|_{\text{image}}}{\delta}$$  \hspace{1cm} (3.23)

It is impossible to directly compute $q|_{\text{ghost}}$ from (3.23). Here the symmetrically mirrored point which satisfies $r_{\text{mirror}} = -r_{\text{ghost}}$ should be considered as shown in Fig.
3.3 The relation between the symmetrically mirrored point and the ghost cell has to meet the boundary condition (3.20), thus we have

\[ \mathbf{q}|_{\text{ghost}} = \mathbf{q}|_{\text{mirror}} \] and

\[ \frac{\partial \mathbf{q}}{\partial n}|_{\text{ghost}} = -\frac{\partial \mathbf{q}}{\partial n}|_{\text{mirror}}. \] (3.25)

Using the approximations

\[ \frac{\partial \mathbf{q}}{\partial n}|_{\text{mirror}} \approx \frac{\mathbf{q}|_{\text{image}} - \mathbf{q}|_{\text{mirror}}}{\delta - |\mathbf{r}_{\text{mirror}}|} \] and

\[ \frac{\partial \mathbf{q}}{\partial n}|_{\text{image}} \approx \frac{\mathbf{q}|_{\text{extra}} - \mathbf{q}|_{\text{image}}}{|\mathbf{r}_{\text{extra}}|} \] (3.26, 3.27)

with (3.24), (3.25) then substitute them into equation (3.23), we get the sought relation

\[ \mathbf{q}|_{\text{ghost}} = \mathbf{q}|_{\text{image}} - \delta - |\mathbf{r}_{\text{ghost}}| \frac{\mathbf{q}|_{\text{extra}} - \mathbf{q}|_{\text{image}}}{\delta}. \] (3.28)

As the approximations (3.26) and (3.27) are one-sided first-order differencing, the sought expression (3.28) does not satisfy the boundary condition (3.20) exactly, especially in the case when \(|\mathbf{r}_{\text{ghost}}|\) is very small. Even though, the first-order approximations would not decrease the accuracy of the boundary too much.

For the normal component of the velocity, a quadratic relation approximated between the ghost cell and the projection point can be expressed as

\[ u_n|_{\text{ghost}} = u_n|_{\text{proj}} - |\mathbf{r}_{\text{ghost}}| \cdot \frac{\partial u_n}{\partial n}|_{\text{proj}} + \frac{|\mathbf{r}_{\text{ghost}}|^2}{2} \cdot \frac{\partial^2 u_n}{\partial n^2}|_{\text{proj}} \] (3.29)

Besides, between the extra image point and the image point following quadratic relation holds true:

\[ u_n|_{\text{extra}} = u_n|_{\text{image}} + |\mathbf{r}_{\text{extra}}| \cdot \frac{\partial u_n}{\partial n}|_{\text{image}} + \frac{|\mathbf{r}_{\text{extra}}|^2}{2} \cdot \frac{\partial^2 u_n}{\partial n^2}|_{\text{image}} \] (3.30)
With a quadratic assumption, second order derivatives at the projection point and at the image point meet
\[
\frac{\partial^2 u_n}{\partial n^2}_{\text{proj}} = \frac{\partial^2 u_n}{\partial n^2}_{\text{image}}
\]  
(3.31)
and the average slope between the projection point and the image point meets
\[
\frac{\frac{\partial u_n}{\partial n}_{\text{proj}} + \frac{\partial u_n}{\partial n}_{\text{image}}}{2} = \frac{u_n}_{\text{image}} - \frac{u_n}_{\text{proj}} \frac{\delta}{\delta}
\]  
(3.32)

For simplicity, we may define the location of the extra image point such that \( r_{\text{extra}} = -r_{\text{ghost}} \). Subtract (3.30) from (3.29) and consider the relations (3.31) and (3.32), the sought expression for the normal component of the velocity at the ghost cell can be obtained as
\[
u_n|_{\text{ghost}} = u_n|_{\text{extra}} - u_n|_{\text{image}} - |r_{\text{ghost}}| \cdot \frac{2u_n|_{\text{image}}}{\delta} = u_n|_{\text{extra}} - (1 + \frac{2|r_{\text{ghost}}|}{\delta})u_n|_{\text{image}}
\]  
(3.33)

Figure 3.3: Relative positions of ghost cells, projection points, mirrored points, farther image points and extra image points.

Using equation (3.28) and (3.33), values at the ghost cells can be extrapolated
from the image points and the extra image points eventually. The values at the image points and the extra image points can be obtained using a complete bilinear interpolation.

For compressible flows that may involve discontinuity such as shock waves, higher order extrapolation may result in nonphysical values for the ghost cells. For instance, when a shock wave happens to be positioned between the image point and the extra image point, the extrapolation from these image points may result in negative density or pressure at the ghost cell. Therefore, a shock sensor $\alpha$ is introduced for the improved ghost-cell method to address this issue. The shock sensor proposed is defined using the ratio of pressures at the extra image point and the image point as

$$\alpha = \frac{p|_{\text{extra}}}{p|_{\text{image}}} \quad (3.34)$$

Once a threshold $\alpha_0$ for the sensor is chosen, the extrapolation for the ghost cells can be reduced to the first order when the shock sensor is larger than the threshold while keeping the quadratic extrapolation elsewhere as

$$q|_{\text{ghost}} = \begin{cases} 
q|_{\text{image}} - \frac{\delta - |r_{\text{ghost}}|}{\delta}(q|_{\text{extra}} - q|_{\text{image}}) & \text{if } \alpha < \alpha_0 \\
q|_{\text{image}} & \text{if } \alpha \geq \alpha_0 
\end{cases} \quad (3.35)$$

The choice of threshold $\alpha_0$ is subject to the conditions of given problems. Based on the experience of the authors, it can be chosen as $1.2 \leq \alpha_0 \leq 2.0$, trading off the robustness at lower values and the higher accuracy at higher values.
Chapter 4

Numerical Results

We present a set of numerical tests verifying the accuracy of the ghost-cell immersed boundary method in dealing with compressible flow problems, illustrating the improved solutions comparing to those from the baseline ghost-cell method and proving the advantage of the improved ghost-cell method. For selected cases, the solutions with the improved ghost-cell method is compared with those with a cut-cell method as an effort to compare both approaches directly. Finally, the improved ghost-cell method is verified for reacting flows as well as non-reacting flows.

4.1 Double Mach reflection on a ramp

Double Mach reflection test, which was suggested as a benchmark for numerical methods for solving Euler equations by Woodward and Colella [35], is a useful tool to check the quality of a numerical scheme because the jet formed along the boundary is known to be highly sensitive to the numerical scheme used. A non-dimensionalized, two-dimensional computational domain of a $2 \times 1$ rectangle is used. A single-species gas with gas constant $\gamma = 1.4$ occupies the whole fluid domain. An initial planar shock wave of Mach 10 is set at point $x = \frac{1}{6}, y = 0$. The pre-shock values of density and pressure are $\rho_0 = 1.4$ and $p_0 = 1$.

Figure 4.1(a) shows the ghost-cell immersed boundary case where the boundary
Figure 4.1: Baseline ghost-cell boundary calculation of DMR: 30 contours of density from 1.4 to 23. Fixed grid 400×200, cfl=0.8, t=0.09.
for a ramp starting from $x = \frac{1}{6}$ with an angle of 30° to the x-axis is not aligned with the Cartesian grid. The shock wave travels to the right in a direction normal to x. Figure 4.1(b) shows the equivalent grid-aligned case conceived by rotational transformation, where the shock wave moves with an angle of 30° to the x-axis and the domain boundary at the bottom is reflective from $x = \frac{1}{6}$. The moving shocks relative to the solid boundaries are identical in both cases. In Fig. 4.1(c) the density contours of the ghost-cell method case (red) are overlapped with the grid aligned case (grey) if it is rotated by 30°, which means the slip-wall boundary condition implicitly represented by the ghost-cell method is valid.

Figure 4.2 shows the results for the same problem with finer resolution, with which detailed structure of the flow involving Mach stems is well resolved. While the structure of the jet along the wall is captured well in the grid-aligned case (Fig. 4.2(b)), the jet along the ramp wall with the baseline ghost-cell method (Fig. 4.2(a)) is more diffusive, hence the detachment of the jet front and the leading Mach stem is not clear. This discrepancy may be attributed to the implicit representation of the boundary in the ghost-cell method. This becomes clear when the ghost-cell immersed boundary method is compared directly with a cut-cell method in the later part of this section.

Figure 4.3 shows the results of the improved ghost-cell method at resolutions of 400×200 and 800×400, respectively. Compared to the baseline ghost-cell method, the jet structure in double Mach region for the improved ghost-cell method is in better agreement with the corresponding grid-aligned case. In particular, in both cases, the leading edge of the jet intersects the boundary at a right angle, which is regarded as correct representation of a realizable jet. In comparison of Fig. 4.2(a) and Fig. 4.3(a) at the same resolution of 400×200, one may find the smeared out structure from the baseline ghost-cell method is improved with the improved ghost-cell immersed boundary method.
Figure 4.2: Baseline ghost-cell boundary calculation of DMR: 30 contours of density from 1.4 to 23. Fixed grid $800 \times 400$, $\text{cfl}=0.8$, $t=0.09$
Figure 4.3: Improved ghost-cell boundary calculation of DMR: 30 contours of density from 1.4 to 23, cfl=0.8, t=0.09.
Figure 4.4: Cut-cell boundary (Chombo) calculation of DMR: 30 contours of density from 1.4 to 23, cfl=0.8, t=0.09.
With the same test case, solutions with a cut-cell method from the simulation using Chombo package \[24, 25\], is presented in Fig. 4.4. In the cut-cell method readily available in EBAMRGodunov solver of Chombo package, an equivalent PPM reconstruction using van Leer limiter for characteristic variables for the fourth order slope calculation and the same choice of primitive variable Riemann solver are used. Hence, we find the comparison between the present ghost-cell immersed boundary method and the cut-cell method is fair by sharing the equivalent second order finite volume method. In the result with cut-cell method, the Mach stem and jet structure developed along the ramp wall is resolved accurately. Comparing Fig. 4.2(a), Fig. 4.3(b) and Fig. 4.4(b) at a same resolution of 800×400, it is verified that the improved ghost-cell immersed boundary method resolves the solution along the immersed boundary as accurately as the cut-cell method.

Finally, A detailed comparison between the improved ghost-cell method and the cut-cell method is presented with the AMR capability activated. Figure 4.5 is the result obtained from the cut-cell method. Figure 4.6 is get from the improved ghost-cell method. In Fig. 4.5(b) mesh in the boundary grids are not refined, finer refinements only take place around the Mach stems and jet structure in fluid domain. That is because the geometry resolution is independent of the mesh resolution in this slope boundary case, the geometry is dealt by the cut-cell method automatically. Through comparison, it is also found that the relative distance from the jet front to the front mach stem is farther in Fig. 4.6 and the relative distance in Fig. 4.5 is more approximate to the results in \[35\]. Thus, it is proved that the cut-cell method would be slightly more accurate representing the physical boundary in the double Mach reflection case.

In fact, even with AMR technique, the initial-value problem for the multidimensional Euler equations cannot converge to a weak solution near the shear layer due to the ill-posed governing equations. One way to make the equations well-posed is to do
a self-similar transformation from hyperbolic equations to mixed hyperbolic-elliptic equations as in [36, 37]. In the initial-value problems in this thesis, AMR is still useful to enhance the computational efficiency and achieve finer local resolution near the discontinuities and boundary.

Figure 4.5: Cut-cell boundary (Chombo) calculation of DMR. The effective grid resolution at the finest level is $1600 \times 800$, cfl=0.8, t=0.09.
Figure 4.6: Improved ghost-cell boundary calculation of DMR. The effective grid resolution at the finest level is $1600 \times 800$, $cfl=0.8$, $t=0.09$. 

(a) 30 density contours from 1.4 to 23.

(b) density plot with AMR grid hierarchy.
4.2 A Mach 3 supersonic flow in a wind tunnel with a forward-facing step

The classical Woodward-Colella test for a forward facing step \[35\] is chosen to verify the robustness and accuracy of the improved ghost-cell immersed boundary method for the grid-aligned geometries. The domain is a $3 \times 1$ rectangle. A forward-facing step starts from $x = 0.6$ and its height is 0.2. The initial flow field is defined with a density $\rho = 1.4$, a pressure $p = 1.0$ and a horizontal velocity of Mach number $M = 3$, with $\gamma = 1.4$ for a single-species ideal gas. The top boundary of the channel is set to be a slip wall.

![Figure 4.7: Cut-cell boundary (Chombo) calculation of forward facing step problem: density field. Above: 30 contours from 0 to 6.5. Below: Pseudocolor plot with contours. The effective grid resolution at finest level is 480×160, cfl=0.8, t=4.00237.](image)

In Fig. 4.7 the boundary is treated by the cut-cell method, it is compared with Fig. 4.8 obtained from the improved ghost-cell method. In the test, overexpansion flow strikes the upper surface of the step, causing weak oblique shock. Both of the two boundary treatments show well-resolved contact discontinuity. However, the result
4.3 Supersonic flows over a circular cylinder

Circular cylinder case is used to demonstrate the capability of the improved ghost-cell method dealing with curving boundary. In this case, the computational domain is $4cm \times 4cm$ rectangle. At the center of the domain, there is a circular cylinder with radius $r = 0.5cm$. Initially, a uniform supersonic flow is in the whole domain with pressure $p_0 = 10^5 Pa$ and Mach number $M_0 = 3$. CFL number of 0.5 is used in the computation.

Figure 4.9 shows the comparison of density and pressure contours when the su-
(a) Density, cut-cell method  
(b) Density, improved ghost-cell method  
(c) Pressure, cut-cell method  
(d) Pressure, improved ghost-cell method  

Figure 4.9: Comparison between the cut-cell method and the improved ghost-cell method for a Mach 3 supersonic flow over a circular cylinder. Fixed grid $350 \times 350$, $cfl=0.5$, $t=1.5$. 
personic flow pasts the circular cylinder. As the flow behind the cylinder does not have any physical significance, the domain of interest can be zoomed in to a partial domain $[1 : 2] \times [1 : 3]$. A bow shock occurs after the flow meets the front part of the cylinder. In both plots, the bow shock is well resolved.

The pressure coefficient along the cylinder surface is calculated as:

$$C_p = \frac{p}{p_0} - 1 = \frac{1}{\frac{1}{2} \gamma M_0^2}$$

(4.1)

Figure 4.10 shows the pressure coefficient along the cylinder surface as function of the x-coordinate, the cut-cell method and the improved ghost-cell method are compared with the body-fitted grid case from [1]. Both methods are using fixed grid with approximately the same number of grid points placed on the solid body. It is obvious that the pressure coefficient curves of the cut-cell method and the improved ghost-cell method are all in good agreement with the body-fitted grid case.

Figure 4.10: Comparison of pressure coefficients for a Mach 3 supersonic flow over a circular cylinder obtained from the improved ghost-cell method, the cut-cell method and the result for body-fitted grid from [1].
4.4 Smooth Prandtl-Meyer expansion flows

Steady state calculation of the Prandtl-Meyer expansion wave is often chosen to evaluate the accuracy of the immersed boundary quantitatively [8, 39]. In this study we calculate a Mach 1.3 flow turning through an angle of 20°. The exact solution is a smooth flow with constant entropy \( S = p/\rho^\gamma \). Figure 4.11 shows the density contour plot for a uniform 200×200 grid when the flow reaches steady state. The error for entropy in the fluid domain is tabulated in Table 4.1. Under the assumption that the errors can be expressed as \( C h^p \) where \( h \) is the cell size and \( C \) is constant, the order of accuracy \( p \) can be obtained numerically. The convergence results in Table 4.1 suggest that \( L^\infty \) norm error converges more quickly in the improved ghost-cell method than in the baseline ghost-cell method. Besides, the improved ghost-cell method produces smaller absolute errors in the same grid resolutions. Therefore, it is demonstrated

Figure 4.11: Density contours for Prandtl-Meyer expansion wave resulting from a Mach 1.3 flow turning through an angle of 20°.
Table 4.1: Convergence rate of entropy

<table>
<thead>
<tr>
<th>Method</th>
<th>grid(h)</th>
<th>$L^1$ order</th>
<th>$L^2$ order</th>
<th>$L^\infty$ order</th>
</tr>
</thead>
<tbody>
<tr>
<td>baseline ghost-cell method</td>
<td>50×50</td>
<td>1.06e-05</td>
<td>4.32e-05</td>
<td>4.74e-04</td>
</tr>
<tr>
<td></td>
<td>100×100</td>
<td>3.11e-06</td>
<td>1.77</td>
<td>1.42e-05</td>
</tr>
<tr>
<td></td>
<td>200×200</td>
<td>9.73e-07</td>
<td>1.68</td>
<td>5.45e-06</td>
</tr>
<tr>
<td></td>
<td>400×400</td>
<td>2.51e-07</td>
<td>1.95</td>
<td>1.60e-06</td>
</tr>
<tr>
<td>improved ghost-cell method</td>
<td>50×50</td>
<td>6.44e-06</td>
<td>2.47e-05</td>
<td>1.58e-04</td>
</tr>
<tr>
<td></td>
<td>100×100</td>
<td>1.82e-06</td>
<td>1.82</td>
<td>9.00e-06</td>
</tr>
<tr>
<td></td>
<td>200×200</td>
<td>4.60e-07</td>
<td>1.98</td>
<td>2.89e-06</td>
</tr>
<tr>
<td></td>
<td>400×400</td>
<td>1.19e-07</td>
<td>1.95</td>
<td>9.41e-06</td>
</tr>
</tbody>
</table>

Quantitatively, that the improved ghost-cell method has better accuracy compared to the baseline ghost-cell method. Overall, the improved ghost-cell method can reach second-order in $L^1$ and higher-order in $L^\infty$. From the convergence study in [10], it is known that the cut-cell method in Chombo is second-order accurate in $L^1$, and first-order accurate in $L^\infty$, which is comparable to the accuracy of the improved ghost-cell method.

### 4.5 CPU time comparison

To compare the efficiency of the cut-cell method and the improved ghost-cell method, CPU time is calculated with one core for these two methods in double Mach reflection case and circular cylinder supersonic flow case. The following Table 4.2 shows the CPU time comparison result.

Table 4.2: CPU time comparison

<table>
<thead>
<tr>
<th>CPU time (s)</th>
<th>improved ghost-cell Method</th>
<th>cut-cell method</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMR case</td>
<td>185</td>
<td>303</td>
</tr>
<tr>
<td>Cylinder case</td>
<td>894</td>
<td>1880</td>
</tr>
</tbody>
</table>

It is evident that the computing speed using the improved ghost-cell method is almost twice than that using the cut-cell method, which means the improved ghost-cell method is more efficient.
4.6 Steady shock-induced combustion over a wedge

Supersonic flow of a reactive mixture around a wedge is simulated to verify the improved ghost-cell method for reacting flows. The wedge half-angle is 35°. Initially, there is a stoichiometric hydrogen-air mixture in the fluid domain with pressure \( p = 0.266\ atm \) and temperature \( T = 300K \). The supersonic flow has horizontal velocity with Mach number \( M = 7 \). The chemical kinetics mechanism used in the computation is the Balakrishnan and Williams model [40], which involves 9 species \((H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, N_2)\) and 21 elementary reactions. The reaction mechanism is described in the following Table 4.3. The detailed setup of the simulation can be seen in [41].

Table 4.3: Reaction mechanism for \( H_2 \)-air combustion: \( A \) in (cm, mol, s), \( E \) in (cal/mol).

<table>
<thead>
<tr>
<th>Reactions</th>
<th>( A )</th>
<th>( \beta )</th>
<th>( E )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H + O_2 \rightleftharpoons OH + O )</td>
<td>3.52e16</td>
<td>-0.7</td>
<td>17070.</td>
</tr>
<tr>
<td>( H_2 + O \rightleftharpoons OH + H )</td>
<td>5.06e4</td>
<td>2.67</td>
<td>6290.</td>
</tr>
<tr>
<td>( H_2 + OH \rightleftharpoons H_2O + H )</td>
<td>1.17e9</td>
<td>1.3</td>
<td>3626.</td>
</tr>
<tr>
<td>( OH + OH \rightleftharpoons H_2O + O )</td>
<td>1.51e9</td>
<td>1.14</td>
<td>99.</td>
</tr>
<tr>
<td>( H + O_2 + M \rightleftharpoons HO_2 + M )</td>
<td>6.76e19</td>
<td>-1.42</td>
<td>0.</td>
</tr>
<tr>
<td>( H + H + M \rightleftharpoons H_2 + M )</td>
<td>1.80e18</td>
<td>-1.0</td>
<td>0.</td>
</tr>
<tr>
<td>( H + OH + M \rightleftharpoons H_2O + M )</td>
<td>2.20e22</td>
<td>-2.0</td>
<td>0.</td>
</tr>
<tr>
<td>( O + OH + M \rightleftharpoons HO_2 + M )</td>
<td>1.00e16</td>
<td>0.0</td>
<td>0.</td>
</tr>
<tr>
<td>( H + O + M \rightleftharpoons OH + M )</td>
<td>6.20e16</td>
<td>-0.6</td>
<td>0.</td>
</tr>
<tr>
<td>( O + O + M \rightleftharpoons O_2 + M )</td>
<td>6.17e15</td>
<td>-0.5</td>
<td>0.</td>
</tr>
<tr>
<td>( H + HO_2 \rightleftharpoons H_2 + O_2 )</td>
<td>4.28e13</td>
<td>0.0</td>
<td>1411.</td>
</tr>
<tr>
<td>( H + HO_2 \rightleftharpoons OH + OH )</td>
<td>1.70e14</td>
<td>0.0</td>
<td>874.</td>
</tr>
<tr>
<td>( H + HO_2 \rightleftharpoons O + H_2O )</td>
<td>3.10e13</td>
<td>0.0</td>
<td>1720.</td>
</tr>
<tr>
<td>( O + HO_2 \rightleftharpoons OH + O_2 )</td>
<td>2.00e13</td>
<td>0.0</td>
<td>0.</td>
</tr>
<tr>
<td>( OH + HO_2 \rightleftharpoons H_2O + O_2 )</td>
<td>2.89e13</td>
<td>0.0</td>
<td>-497.</td>
</tr>
<tr>
<td>( HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2 )</td>
<td>3.02e12</td>
<td>0.0</td>
<td>1390.</td>
</tr>
<tr>
<td>( HO_2 + M \rightleftharpoons OH + OH + M )</td>
<td>1.20e17</td>
<td>0.0</td>
<td>45500.</td>
</tr>
<tr>
<td>( H_2O_2 + OH \rightleftharpoons H_2O + HO_2 )</td>
<td>7.08e12</td>
<td>0.0</td>
<td>1430.</td>
</tr>
<tr>
<td>( H_2O_2 + H \rightleftharpoons H_2O + OH )</td>
<td>1.00e13</td>
<td>0.0</td>
<td>3590.</td>
</tr>
<tr>
<td>( H_2O_2 + H \rightleftharpoons HO_2 + H_2 )</td>
<td>4.79e13</td>
<td>0.0</td>
<td>7950.</td>
</tr>
<tr>
<td>( H_2 + O_2 \rightleftharpoons OH + OH )</td>
<td>1.70e13</td>
<td>0.0</td>
<td>47780.</td>
</tr>
</tbody>
</table>

Third-body efficiencies:
\[ a = f_{H_2O} = 12., f_{H_2} = 2.5, f_{N_2} = f_{O_2} = 1.0 \]
\[ b = f_{H_2O} = 6.5, f_{H_2} = 1.0, f_{N_2} = f_{O_2} = 0.4 \]
\[ c = f_{H_2O} = 15., f_{H_2} = 2.5, f_{N_2} = f_{O_2} = 1.0 \]
Figure 4.12: Steady shock-induced combustion over a wedge using the improved ghost-cell immersed boundary approach. The effective grid resolution at finest level is $640 \times 640$. 

(a) Density contours

(b) $H_2O$ mass fraction contours
According to the Arrhenius law, the chemical production rates are calculated from

\[ k_f = AT^\beta \exp(-E/RT). \]  

The calculation procedure is performed by the Cantera package.

Figure 4.12 shows the density and the \( \text{H}_2\text{O} \) mass fraction contours obtained by the improved ghost-cell method when the flow reaches steady state. A detonation wave (Fig. 4.12(b)) is triggered by the oblique shock wave (Fig. 4.12(a)). Figure 4.13 shows the position of the shock wave and the reaction front which are indicated by two temperature contours. Starting from the wedge boundary, the distance between the shock wave and the reaction front is gradually reduced up to the triple point, and then remain coupled in the downstream.

![Figure 4.13: Position of the shock wave and reaction front obtained by the improved ghost-cell method](image)

An equivalent grid-aligned case is simulated to compare with the improved ghost-cell immersed boundary solutions. With similar initial flow conditions, a Mach 7
Figure 4.14: Steady shock-induced combustion over a wedge with body-fitted Cartesian grids. The effective grid resolution at finest level is $640 \times 640$. 
oblique flow is coming from the left inflow boundary and moving with an angel of $35^\circ$ to the x-axis. The lower domain boundary satisfies the non-catalytic, adiabatic, slip wall boundary condition. In this way, the flow relative to the solid boundary in the grid-aligned case resembles that in the immersed boundary case. Figure 4.14 shows the density and the $H_2O$ mass fraction contours of the grid-aligned case. Figure 4.15 shows the position of the shock wave and the reaction front in the grid-aligned solutions.

![Figure 4.15: Position of the shock wave and reaction front obtained with body-fitted grids](image)

To compare the immersed boundary solutions with the grid-aligned solutions in a more distinct way, Fig. 4.13 is rotated by $35^\circ$ and matched with Fig. 4.15. It can be seen from the overlap Fig. 4.16 that the position of the shock wave, reaction front and the triple point in the immersed boundary solution are similar to those in the grid-aligned solution. However, the shape of the reaction front near the solid boundary seems not well resolved in the immersed boundary case. This discrepancy
is more clear when comparing Fig. 4.12(b) with Fig. 4.14(b). One possible reason is that the high gradients of mass fractions (the reaction front) near the boundary is diffused away from the boundary by the quadratic and linear assumption in the improved ghost-cell method and bilinear interpolation. This kind of numerical errors can be reduced by the AMR technique when the mesh is refined to be finer near the solid boundary.

Figure 4.16: Comparison between the immersed boundary case (the red contours) and the grid-aligned case (the blue contours)
Chapter 5

Concluding Remarks

In this thesis, a modified ghost-cell method combined with a level set method is proposed and implemented for accurate and efficient boundary treatment in compressible flow simulations. The study mainly attempts to resolve a major deficiencies in the conventional ghost-cell method whose accuracy is deteriorated due to the incomplete bilinear interpolation when the ghost cell is too close to the boundary. The proposed approach improves the accuracy by employing a complete bilinear interpolation and higher-order extrapolation scheme. The method reaches the accuracy of second order in $L^1$ norm and higher than first order in $L^\infty$ norm. Compared to the standard ghost-cell method, the improved ghost-cell method is found to be more accurate for boundary treatment, demonstrated by various test simulations.

In comparison with the cut-cell method at comparable resolution, the improved ghost-cell method also yields the solutions at comparable accuracy for solid boundary representation, and at higher computational efficiency. Furthermore, the improved ghost cell method is easier to implement and does not need to treat special cells cut by the interface.

As an extension of the computational implementation, the method has been successfully implemented in chemically reacting flow simulations and some test simulations are demonstrated. The implementation is fully compatible with the adaptive mesh refinement in the Boxlib library. The study successfully demonstrates an alter-
native computational method to represent solid bodies in compressible reacting flow simulations at higher accuracy and efficiency.
REFERENCES


APPENDICES
A Other Boundary Conditions

The improved ghost-cell method can be modified to deal with other boundary conditions as well as slip wall boundary condition. Dirichlet boundary condition, Neumann boundary condition and mixed boundary condition are considered here for general illustration.

For Dirichlet boundary condition, the variables $q$ on the boundary is specified as

$$q|_{proj} = a$$  \hspace{1cm} (A.1)

where $a$ is a given vector of constant values. A quadratic relation is assumed for the values near the boundary. Hence, the relation between the ghost cell and the projection point can be approximated as

$$q|_{ghost} = q|_{proj} - |r_{ghost}| \cdot \frac{\partial q}{\partial n}|_{proj} + \frac{|r_{ghost}|^2}{2} \cdot \frac{\partial^2 q}{\partial n^2}|_{proj}.$$  \hspace{1cm} (A.2)

Similarly, relation between the extra image point and the image point satisfies the following expression

$$q|_{extra} = q|_{image} + |r_{extra}| \cdot \frac{\partial q}{\partial n}|_{image} + \frac{|r_{extra}|^2}{2} \cdot \frac{\partial^2 q}{\partial n^2}|_{image}.$$  \hspace{1cm} (A.3)

From chapter 3 we have known that the following relations hold true with a quadratic assumption:

$$\frac{\partial^2 q}{\partial n^2}|_{proj} = \frac{\partial^2 q}{\partial n^2}|_{image}.$$  \hspace{1cm} (A.4)
\[
\frac{\partial q}{\partial n}|_{proj} + \frac{\partial q}{\partial n}|_{image} = \frac{q|_{image} - q|_{proj}}{\delta} \quad (A.5)
\]

As the extra image point is defined to satisfy \( r_{extra} = -r_{ghost} \), the sought expression for the ghost cell values can be obtained by subtracting \( (A.3) \) from \( (A.2) \),

\[
q|_{ghost} = q|_{proj} + q|_{extra} - q|_{image} - |r_{ghost}| \cdot \frac{2q|_{image}}{\delta}
\]

\[
= a + q|_{extra} - (1 + \frac{2|r_{ghost}|}{\delta})q|_{image}. \quad (A.6)
\]

For Neumann boundary condition, the normal gradients of the variables on the boundary is specified as

\[
\frac{\partial q}{\partial n}|_{proj} = b \quad (A.7)
\]

where \( b \) is a given vector of constant values. Assuming that the normal gradients \( \frac{\partial q}{\partial n} \) at the ghost cell, at the projection point, and at the image point are linear, a relation can be obtained,

\[
\frac{\partial q}{\partial n}|_{ghost} = \frac{\partial q}{\partial n}|_{proj} - |r_{ghost}| \cdot s_0 \quad (A.8)
\]

where \( s_0 \) is the slope defined by

\[
s_0 = \frac{\frac{\partial q}{\partial n}|_{image} - \frac{\partial q}{\partial n}|_{proj}}{\delta}. \quad (A.9)
\]

Combining \( (A.8) \) and \( (A.9) \) with relation \( (A.7) \), the following formula can be obtained

\[
\frac{\partial q}{\partial n}|_{ghost} = b - |r_{ghost}| \cdot \frac{\frac{\partial q}{\partial n}|_{image} - b}{\delta}. \quad (A.10)
\]

Using the approximations

\[
\frac{\partial q}{\partial n}|_{image} \approx \frac{q|_{extra} - q|_{image}}{|r_{extra}|}, \quad (A.11)
\]
\[
\frac{\partial q}{\partial n}\bigg|_{\text{proj}} \approx \frac{q|_{\text{image}} - q|_{\text{proj}}}{\delta} \quad \text{and} \quad (A.12)
\]

\[
\frac{\partial q}{\partial n}\bigg|_{\text{ghost}} \approx \frac{q|_{\text{proj}} - q|_{\text{ghost}}}{|r_{\text{ghost}}|}, \quad (A.13)
\]

then substitute them into equation (A.10), we can get the sought expression for \(q|_{\text{ghost}}\) as

\[
q|_{\text{ghost}} = q|_{\text{image}} - \frac{|r_{\text{ghost}}|}{\delta}(q|_{\text{image}} - q|_{\text{extra}}) - \frac{b|r_{\text{ghost}}|^2 + b\delta|r_{\text{ghost}}| + b\delta^2}{\delta}. \quad (A.14)
\]

For mixed boundary conditions which satisfy Dirichlet condition for some variable components and Neumann condition for other variable components on the boundary, the construction of the ghost cell values should combine the above two expressions (A.6) and (A.14). In this way, the improved ghost-cell method is able to represent general boundary conditions.
B Piecewise Parabolic Method

Piecewise parabolic method (PPM) is a higher-order extension of Godunov’s method. A brief description of this technique is presented here.

The ultimate goal of PPM reconstruction is to get the time-centered cell edge states $q_{i+rac{1}{2},L}^{n+1/2}$ and $q_{i+rac{1}{2},R}^{n+1/2}$. Following this goal, Taylor expansion is applied both in space and in time from the base-time cell center states to the time-centered cell edge states. Here we take the reconstruction of $q_{i+rac{1}{2},L}^{n+1/2}$ for example:

$$q_{i+rac{1}{2},L}^{n+1/2} = q_i^n + \frac{\Delta x}{2} \frac{\partial q}{\partial x} \bigg|_i + \frac{\Delta t}{2} \frac{\partial q}{\partial t} \bigg|_i + ...$$

$$\approx q_i^n + \frac{1}{2} \left[ 1 - \frac{\Delta t}{\Delta x} A_i \right] \Delta q_i. \quad \text{(B.1)}$$

where $\Delta q_i$ is the reconstructed slope of the variables in cell $i$.

Recognizing that $A = RAL$ and considering the limited slope $\overline{\Delta q_i}$, the above equation (B.1) is rewritten as

$$q_{i+rac{1}{2},L}^{n+1/2} = q_i^n + \frac{1}{2} \left[ RL - \frac{\Delta t}{\Delta x} RAL \right] \overline{\Delta q_i}. \quad \text{(B.2)}$$

Furthermore, the equation can be expressed as

$$q_{i+rac{1}{2},L}^{n+1/2} = q_i^n + \frac{1}{2} \sum_{v; \lambda^{(v)} \geq 0} \left[ 1 - \frac{\Delta t}{\Delta x} \lambda_i^{(v)} \right] (l_i^{(v)} \overline{\Delta q_i}) r_i^{(v)} \quad \text{(B.3)}$$

where $\lambda_i^{(v)}$ is the eigenvalue, $l_i^{(v)}$ and $r_i^{(v)}$ are the corresponding left and right eigenvectors respectively, and $v$ represents different waves.
It is a linearization of the quasi-linear system to decompose $\mathbf{A}$ in terms of left and right eigenvectors [42]. To minimize the effect caused by this characteristic projection, the reference state $\bar{q}+$ is introduced into the equation (B.3), the full expression for the time-centered cell edge state becomes

$$q_{n+1/2}^{r} = \bar{q}+ - \sum_{v; \lambda^{(v)} \geq 0} I_{i}^{(v)} \{ \bar{q}+ - q_i^n + \frac{1}{2}(1 - \frac{\Delta t}{\Delta x} \lambda_i^{(v)} \Delta q_i) \} r_i^{(v)} (B.4)$$

and

$$q_i^n + \frac{1}{2}(1 - \frac{\Delta t}{\Delta x} \lambda_i^{(v)} \Delta q_i) \approx \frac{1}{\lambda \Delta t} \int_{x_i+1/2 - \lambda \Delta t}^{x_i+1/2} \mathbf{q}(x)dx. \quad (B.5)$$

The integral on the right side of equation (B.5) represents the average of $\mathbf{q}$ that can reach the right interface of cell $i$ over timestep $\Delta t$, moving at the wavespeed $\lambda$. We define the integral

$$I_{+}^{(v)}(q_i) = \frac{1}{\sigma^{(v)} \Delta x} \int_{x_i+1/2 - \sigma^{(v)} \Delta x}^{x_i+1/2} \mathbf{q}(x)dx \quad (B.6)$$

with $\sigma^{(v)} = |\lambda^{(v)}| \Delta t / \Delta x$. Then, equation (B.4) is simplified to be

$$q_{n+1/2}^{r} = \bar{q}+ - \sum_{v; \lambda^{(v)} \geq 0} I_{i}^{(v)}(\bar{q}+ - I_{+}^{(v)}(q_i)) r_i^{(v)}. \quad (B.7)$$

The reference state $\bar{q}+$ is chosen as

$$\bar{q}+ = \begin{cases} I_{+}^{(v)}(q_i) & \text{if } u + c > 0 \\ q_i & \text{otherwise.} \end{cases} \quad (B.8)$$

To compute the integral $I_{+}^{(v)}(q_i)$, the parabolic form of $\mathbf{q}(x)$ has to be determined. As described in the original PPM paper [28], the reconstruction is

$$\mathbf{q}(x) = \mathbf{q}_- + \xi(x)(\Delta \mathbf{q} + \mathbf{q}_6(1 - \xi(x))) \quad (B.9)$$
with $\Delta q = q_+ - q_-$. $q_-$ and $q_+$ are the values of the polynomial on the left and right edges of the current cell, respectively. The variables $q_6$ and $\xi(x)$ are defined as

$$q_6 \equiv 6[q_i - \frac{1}{2}(q_- + q_+)] \quad (B.10)$$

and

$$\xi(x) = \frac{x - x_{i-1/2}}{\Delta x} \quad (B.11)$$

To obtain the values of $q_-$ and $q_+$, fourth order interpolation scheme is applied with van Leer limiter. In the end, the integral in equation (B.6) is computed as

$$I^{(+)}(v)(q_i) = q_{i+1/2} - \sigma_i \cdot \frac{1}{2} \left[ \Delta q_i - q_6,i(1 - \frac{2}{3}\sigma_i^{(v)}) \right]. \quad (B.12)$$

Similar expression can be derived for the right state $(q_{i+1/2}^{n+1/2})$ at the left interface of the cell $i$

$$q_{i+1/2}^{n+1/2} = \tilde{q}_- - \sum_{\nu, \lambda^{(v)} \leq 0} I^{(v)}_i(\tilde{q}_- - I^{(v)}(q_i)) r_i^{(v)}. \quad (B.13)$$

The reference state is

$$\tilde{q}_- = \begin{cases} \ I^{(-)}(q_i) & \text{if } u - c < 0 \\ q_i & \text{otherwise} \end{cases} \quad (B.14)$$

and the integral is

$$I^{(-)}(q_i) = q_{i-1/2} - \sigma_i^{(v)} \cdot \frac{1}{2} \left[ \Delta q_i - q_6,i(1 - \frac{2}{3}\sigma_i^{(v)}) \right]. \quad (B.15)$$

Using equations (B.7) and (B.13), the time-centered edge states $q_{i+1/2}^{n+1/2}$ and $q_{i+1/2}^{n+1/2}$ can be finally determined.
C Publications

• Cheng Chi, Bok Jik Lee, and Hong G. Im, “An Improved Ghost-cell Immersed Boundary Method for Compressible Flow Simulations”, In Preparation.