Chapter 5

Numerical Method

In this chapter, an accurate and stable method is described for the solution of the time-dependent incompressible Navier-Stokes equations with finite differences on structured body-fitted overlapping grids in one, two or three space dimensions. For the incompressible Navier-Stokes equations, there is no direct link for the pressure between the continuity and momentum equations; the governing equations are said to be decoupled. To establish a connection between the two equations, mathematical manipulations are introduced. The numerical method presented is a split-step scheme, second-order accurate in space and time and solves the momentum equations for the velocity together with a Poisson equation for the pressure (the so called pressure-Poisson equation or PPE), this system of equations is known as the velocity-pressure formulation of the incompressible Navier-Stokes equations.

5.1 Primitive Variable Formulation of the Incompressible Navier-Stokes Equations

In primitive variables (u, v, w, p), the initial-boundary-value problem (IBVP) for the incompressible Navier-Stokes equations is

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \frac{-\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} \qquad \text{for} \quad \mathbf{x} \in \mathcal{D}, \qquad t > 0, \tag{5.1}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{for} \quad \mathbf{x} \in \mathcal{D}, \qquad t > 0, \tag{5.2}$$

with the following boundary conditions and initial conditions

$$\begin{aligned} B(\mathbf{u}, p) &= \mathbf{g} && \text{for} \quad \mathbf{x} \in \partial\mathcal{D}, \quad t > 0, \\ \mathcal{D}\mathring{\mathbf{Q}}(\mathbf{x}, 0) &= \mathbf{q}_0(\mathbf{x}) && \text{for} \quad \mathbf{x} \in \mathcal{D}, \quad t = 0. \end{aligned} \tag{5.3}$$

in this IBVP, $\mathbf{x} = (x, y, z)$ (for $\mathbb{N} = 3$ where $\mathbb{N}$ is the number of space dimensions) is the vector containing the Cartesian coordinates in physical space $\mathcal{P}$, $\mathcal{D}$ is a bounded domain in $\mathcal{P} \in \Re^{\mathbb{N}}$ ($\mathbb{N} = 1, 2, 3$), $\partial\mathcal{D}$ is the boundary of the domain $\mathcal{D}$, t is the physical time, $\mathbf{u} = (u, v, w)$ is the vector containing the velocity field in $\mathcal{P}$, p is the pressure, ν is the kinematic viscosity which is equal to $\nu = \mu/\rho$, B is a boundary operator, $\mathbf{g}$ is the boundary data and $\mathbf{q}_0$ is the initial data. The system of equations eq. 5.1, eq. 5.2 and eq. 5.3 will be called the velocity-divergence formulation of the governing equations in primitive variables [78, 84, 118].

Typical boundary conditions for the system of equations eq. 5.1 and eq. 5.2 might be those for a non-penetrating no-slip wall

$$\begin{aligned} \mathbf{u} \cdot \hat{\mathbf{n}} = 0 \quad & \text{for} \quad \partial \mathcal{D}_{wall} \quad \text{“no-through-flow (Dirichlet boundary condition)”} \\ \mathbf{u} \cdot \hat{\mathbf{t}} = 0 \quad & \text{for} \quad \partial \mathcal{D}_{wall} \quad \text{“no-slip (Dirichlet boundary condition)”} \end{aligned} \tag{5.4}$$

or those for an inflow such as

$$\mathbf{u} = \mathbf{g} \quad \text{for} \quad \partial \mathcal{D}_{in} \quad \text{“inflow (Dirichlet boundary condition)”} \tag{5.5}$$

Specifying the pressure, its normal derivative, or a combination of the two at the outflow is also often used

$$\begin{aligned} \hat{n} \cdot \nabla p = g \quad & \text{for} \quad \partial \mathcal{D}_{out} \quad \text{“outflow (Neumann boundary condition)”} \\ \alpha p + \beta \hat{n} \cdot \nabla p = g \quad & \text{for} \quad \partial \mathcal{D}_{out} \quad \text{“outflow (Mixed boundary condition)”} \end{aligned} \tag{5.6}$$

with α and β suitable coefficients.

Also, the specification of zero velocity gradient at the outflow may be appropriate for most applications

$$\nabla \mathbf{u} = 0 \quad \text{for} \quad \partial \mathcal{D}_{out} \quad \text{“outflow (Neumann boundary condition)”} \tag{5.7}$$

Before continuing with our discussion of the numerical method, it is important to make a few comments with regard to the velocity-divergence formulation of the incompressible Navier-Stokes equations.

- The governing equations are a mixed elliptic-parabolic system of equations which are solved simultaneously. The unknowns in the equations are velocity field $\mathbf{u} = (u, v, w)$ and pressure p.
- There is no direct link for the pressure between the continuity and momentum equations. To establish a connection between the two equations, mathematical manipulations are introduced. Generally speaking there are three procedures for this purpose. The first is that of generating a Poisson equation for the pressure (the so-called PPE equation), which is developed in this chapter; the second is the introduction of artificial compressibility into the continuity equation, and the third is the use of projection methods, which encompasses similarities with the PPE approach. Projection methods also produce a Poisson equation that is solved for the pressure in the incompressible flow, this new equation is obtained by using Hodge decomposition theorem, which basically decompose the velocity field into a sum of a divergence-free part (solenoidal) and curl-free part (irrotational) [45]. Note that this difficulty does not exist for the compressible Navier-Stokes equations. That is because in the compressible case there is a link between the continuity and momentum equations through the density which appears in both equations.
- Straight-forward discretizations of eq. 5.1 and eq. 5.2 can lead to checker-board instabilities [81, 118]. Centred finite-difference approximations on unstaggered grids permit discrete

satisfaction of the divergence-free constraint by non-physical velocity fields. Similarly, centred finite-differences approximations to the pressure gradient terms (on unstaggered grids) in the momentum equations allow non-physical pressure fields to go undetected and thus, uncorrected (spurious oscillations).

- Many approaches require extra boundary conditions, either for the pressure or for an intermediate velocity field, which can be non-trivial to choose and difficult to implement.
- For efficiency, it is useful to decouple the solution of the velocity from the solution of the pressure (split-step scheme).

5.2 Pressure-Poisson Equation (PPE) or Velocity-Pressure Formulation in Primitive Variables

In this formulation, the PPE equation for the pressure is used in place of the continuity equation eq. 5.2. The new IBVP is expressed as follows

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \frac{-\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} \qquad \text{for} \quad \mathbf{x} \in \mathcal{D}, \qquad t > 0 \tag{5.8}$$

$$\frac{\nabla^2 p}{\rho} + \nabla u \cdot \mathbf{u}_x + \nabla v \cdot \mathbf{u}_y + \nabla w \cdot \mathbf{u}_z = 0 \qquad \text{for} \quad \mathbf{x} \in \mathcal{D}, \qquad t > 0 \tag{5.9}$$

with the following boundary and initial conditions

$$\begin{aligned} B(\mathbf{u}, p) &= \mathbf{g} && \text{for} \quad \mathbf{x} \in \partial\mathcal{D}, \quad t > 0 \\ \nabla \cdot \mathbf{u} &= 0 && \text{for} \quad \mathbf{x} \in \partial\mathcal{D}, \quad t > 0 \\ \mathcal{D}\mathring{\mathbf{Q}}(\mathbf{x}, 0) &= \mathbf{q}_0(\mathbf{x}) && \text{for} \quad \mathbf{x} \in \mathcal{D}, \quad t = 0 \end{aligned} \tag{5.10}$$

The system of equations eq. 5.8, eq. 5.9 and eq. 5.10 will be called the velocity-pressure formulation of the governing equations in primitive variables. Equation eq. 5.9 implies that the pressure can be calculated provided the velocity field is known. This is the form of the equations that will be discretized in the method described in this chapter (where the equations are solved on unstaggered grids), and which is based in the method developed by Brown *et al.* [25], Chesshire and Henshaw [37], Henshaw [78], Hewshaw, Kreiss and Reyna [80] and Henshaw and Petterson [81], for solving the velocity-pressure formulation of the incompressible Navier-Stokes equations on overlapping grids. The pressure equation (eq. 5.9) is derived by taking the divergence of the momentum equation eq. 5.1 and using the divergence-free constraint $\nabla \cdot \mathbf{u} = 0$, then, eq. 5.2 is replaced by the elliptic equation for the pressure. For the system of equations eq. 5.8 and eq. 5.9 an extra boundary condition is required in order to make the problem well-posed. The condition $\nabla \cdot \mathbf{u} = 0$ for $\mathbf{x} \in \partial\mathcal{D}$ is added as the extra boundary condition. This latter condition is an essential boundary condition for this formulation and ensures that the system of equations (eqs. 5.8 - 5.10) is equivalent to the original formulation (eqs. 5.1 - 5.3).

5.3 Remarks on the Pressure Boundary Condition

Perhaps, it is appropriate to make some remarks regarding the choice of $\nabla \cdot \mathbf{u} = 0$ as the extra boundary condition for the velocity-pressure formulation. The extra boundary condition required by the velocity-pressure formulation should satisfy three general conditions. First, it should be chosen so that eq. 5.8 and eq. 5.9 are well posed. Second, it should be consistent with the original formulation eq. 5.1 and eq. 5.2. And lastly, it should be chosen so that the velocity-pressure formulation is equivalent to the velocity-divergence formulation. These three conditions are satisfied by the boundary condition $\nabla \cdot \mathbf{u} = 0$, which, despite not looking like a pressure boundary condition, is in some sense the natural extra condition to be added in order to fulfill the three requirement previously mentioned.

There has been a great deal of confusion as to the proper boundary condition for the PPE equation (*i.e.* eq. 5.9). Several articles (*e.g.*, [61, 78, 80, 92, 126, 142, 159]), discuss the issue whether it is appropriate to use the tangential or normal component of the momentum equation on the boundary as a boundary condition for the pressure equation or another type of boundary condition. However, it appears that these methods also impose (implicitly or explicitly) the boundary condition $\nabla \cdot \mathbf{u} = 0$ on $\partial\mathcal{D}$. Often the fact that this condition is applied is not emphasized [81].

In [61], Gresho and Sani proposed an important hypothesis regarding the pressure Poisson equation (PPE) for the incompressible Navier-Stokes equations. They stated there (but did not prove it) a so-called equivalence theorem that claimed that if the Navier-Stokes momentum equation is solved simultaneously with the PPE equation whose boundary condition is the Neumann boundary condition obtained by applying the normal component of the momentum equation on the boundary on which the normal component of velocity is specified as a Dirichlet boundary condition, the solution $(\mathbf{u}, p)$ would be exactly the same as if the primitive equations (in which the PPE equation plus Neumann boundary condition is replaced by the usual divergence-free constraint $(\nabla \cdot \mathbf{u} = 0)$) were solved instead. This issue is explored in sufficient detail by Sani *et al.* in [159], so as to actually prove the theorem for at least some situations. Additionally, like the primitive equations that require no boundary condition for the pressure, the new results establish the same requirement when the PPE equation approach is employed.

5.4 Spatial Discretization of the Velocity-Pressure Formulation of the Incompressible Navier-Stokes Equations

We now describe in more detail how we discretize equations (5.8 - 5.10). But before continuing, let us recall some basic features of overlapping grids (as illustrated in figure 4.7). An overlapping grid $\mathbb{G}$ of the domain $\mathcal{D}$ in $\mathbb{N}$ space dimensions, consists of a set of $\mathcal{N}$ structured component grids $\mathcal{G}_g$,

$$\mathbb{G} = \{\mathcal{G}_g\}, \qquad g = 1, 2, ..., \mathcal{N}$$

that entirely cover the domain $\mathcal{D}$ and overlap where the component grids $\mathcal{G}_g$ meet. Each component grid is a logically rectangular structured grid in $\mathbb{N}$ space dimensions and is defined by a smooth mapping $\mathbf{M}_g$ from the computational space $\mathcal{C} = \mathcal{C}(\xi, \eta, \zeta, \tau)$ to the physical space $\mathcal{P} = \mathcal{P}(x, y, z, t)$, such that

$$\mathcal{P} = \mathbf{M}_g(\mathcal{C}), \qquad \mathcal{C} \in [0, 1]^{\mathbb{N}}, \qquad \mathcal{P} \in \Re^{\mathbb{N}}$$

Here $\mathcal{P}$ is equal to $\mathbf{x} = (x, y, z)$ (for $\mathbb{N} = 3$) and contains all the coordinates in physical space and

$\mathcal{C}$ is equal to $\mathbf{r} = (\xi, \eta, \zeta)$ (for $\mathbb{N} = 3$) and contains the logically uniform array in computational space. Variables defined on a component grid, are stored in rectangular arrays. The grid vertices are represented as the array

$$\mathbf{x}_{\mathbf{i}}^{g} : \text{grid vertices}, \qquad \mathbf{i} = (i_1, \ldots, i_{\mathbb{N}}), \qquad i_\alpha = 0, \ldots, N_\alpha^g, \qquad \alpha = 1, \ldots, \mathbb{N}$$

where N_α^g is the number of grid points or nodes in the i_α-*coordinate* direction. Each component grid is usually created with one or more lines of ghost points, which are useful for applying boundary conditions. Domain connectivity is obtained through proper interpolation of the overlapping areas of the component grids $\mathcal{G}_g$.

For ease of presentation we describe here the solution of the velocity-pressure formulation of the incompressible Navier-Stokes equations in two space dimensions on a square grid $\mathcal{G}_g = \mathbf{G}$ in physical space $\mathcal{P}$ with grid spacing $h_{i_\alpha} > 0 (h_{i_\alpha} = 1/N_{i_\alpha})$ and with $h_{i_1} = h_{i_2}$, such that

$$\mathbf{G} = \{\mathbf{x}_{\mathbf{i}} = (x_{1\mathbf{i}}, x_{2\mathbf{i}}) = (x_{\mathbf{i}}, y_{\mathbf{i}}) = (ih, jh) \quad \text{for} \quad i, j = -1, 0, 1, \ldots, N+1\}$$

here $\mathbf{i} = (i_1, i_2) = (i, j)$ is a multi-index. We include one row of ghost points at the boundaries to aid in the discretization. The discretization on the unit square in the transformed computational space $\mathcal{C}$ is straightforward and is done by replacing the Cartesian derivatives in the velocity-pressure formulation by their equivalent in the transformed computational space $\mathcal{C}$ (*i.e.*, eq. 3.28), as explained in Chapter 3, Section 3.

The equations defining the velocity-pressure formulation are discretized using second-order centred finite-difference approximations on overlapping grids. Let $\mathbf{U}_{\mathbf{i}}(t)$ and $P_{\mathbf{i}}(t)$ denote the numerical approximations to $\mathbf{u}$ and p so that

$$\mathbf{U}_{\mathbf{i}}(t) \approx \mathbf{u}(\mathbf{x}_{\mathbf{i}}, t) \qquad \text{and} \qquad P_{\mathbf{i}}(t) \approx p(\mathbf{x}_{\mathbf{i}}, t)$$

Here $\mathbf{U}_{\mathbf{i}}(t) = (u_{1\mathbf{i}}(t), u_{2\mathbf{i}}(t)) = (u_{\mathbf{i}}(t), v_{\mathbf{i}}(t))$ is the vector containing the Cartesian components of the numerical approximation of the velocity. The spatial approximations of equations (5.8 - 5.10) are

$$\frac{d\mathbf{U}_{\mathbf{i}}}{dt} = -(\mathbf{U}_{\mathbf{i}} \cdot \nabla_h)\mathbf{U}_{\mathbf{i}} - \frac{\nabla_h P_{\mathbf{i}}}{\rho} + \nu \nabla_h^2 \mathbf{U}_{\mathbf{i}}, \qquad i, j = 0, 1, 2, \ldots, N, \tag{5.11}$$

$$\frac{\nabla_h^2 P_{\mathbf{i}}}{\rho} = -\sum_{m=1}^{\mathbb{N}} \nabla_h u_{m,\mathbf{i}} \cdot \frac{\partial \mathbf{U}_{\mathbf{i}}}{\partial x_m}, \qquad i, j = 0, 1, 2. \ldots, N, \tag{5.12}$$

$$B_h(\mathbf{U}_{\mathbf{i}}, \mathbf{P}_{\mathbf{i}}) = \mathbf{g}(\mathbf{x}_{\mathbf{i}}, t) \equiv (g_u(\mathbf{x}_{\mathbf{i}}, t), g_v(\mathbf{x}_{\mathbf{i}}, t)), \qquad i = 0, j = 0, 1, 2, \ldots, N, \tag{5.13}$$

$$\nabla_h \cdot \mathbf{U}_{\mathbf{i}} = 0, \qquad i = 0, j = 0, 1, 2, \ldots, N, \tag{5.14}$$

$$\mathcal{D}\mathring{\mathbf{Q}}(\mathbf{x}_{\mathbf{i}}, 0) = \mathbf{q}_0(\mathbf{x}_{\mathbf{i}}, 0), \qquad i, j = 0, 1, 2. \ldots, N, \tag{5.15}$$

For the purposes of this discussion, the boundary conditions have only been specified at $i = 0, 0 < j < N$; at this boundary, we have considered a Dirichlet boundary condition for the velocity such as

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{g}(\mathbf{x}, t) \qquad \text{for} \quad \mathbf{x} \in \partial\mathcal{D} \tag{5.16}$$

similar or more general expressions for the boundary conditions will hold at other boundaries (if there are other boundaries), although some of the details of implementation may vary [61, 92, 159]. In equations (5.11 - 5.15), subscript h denotes the order of accuracy of the numerical approximation, which for our case is equal to $h = 2$ (second-order centred finite-difference approximations). For the sake of simplicity, the subscript h will be dropped for the remainder of this dissertation.

Higher-order accurate methods based on the velocity-pressure formulation have been successfully used for solving the incompressible Navier-Stokes equations. Henshaw, Kreiss and Reyna [80] developed a fourth-order finite difference scheme based on this approach and also gave a stability analysis. They also presented a general principle for deriving numerical boundary conditions for higher-order accurate difference schemes. In addition, Henshaw [78], adapted the scheme to compute three-dimensional flows on complex domains using overlapping grids, where he introduced extra boundary conditions to make the scheme accurate and stable. Moreover, Browning [27], used sixth-order finite-difference methods on overlapping grids to solve the shallow water equations on a sphere. In [214], Wright and Shyy present a fourth-order accurate pressure-based composite grid method for solving the incompressible Navier-Stokes equations on domains composed by an arbitrary number of overlain grid blocks, where a conservative internal boundary scheme is devised to ensure that global conservation is maintained.

The discrete operators appearing in equations (5.11 - 5.15), are defined as follows,

$$\begin{aligned}
\nabla \cdot \mathbf{U_i} &= D_{0x} u_{\mathbf{i}} + D_{0y} v_{\mathbf{i}}\,, \\
\nabla^2 \mathbf{U_i} &= \left(D_{+x} D_{-x} + D_{+y} D_{-y}\right) \mathbf{U_i} \\
\nabla P_{\mathbf{i}} &= \left(D_{0x} P_{\mathbf{i}}, D_{0y} P_{\mathbf{i}}\right)^T \\
\nabla \mathbf{U_i} &= \left(D_{0x} u_{\mathbf{i}}, D_{0y} v_{\mathbf{i}}\right)^T
\end{aligned}$$

where

$$\begin{aligned}
D_x \mathbf{U_i} = D_{0x} \mathbf{U_i} &= \frac{\mathbf{U}_{i+1,j} - \mathbf{U}_{i-1,j}}{2h} \approx \frac{\partial}{\partial x}\,, \\
D_y \mathbf{U_i} = D_{0y} \mathbf{U_i} &= \frac{\mathbf{U}_{i,j+1} - \mathbf{U}_{i,j-1}}{2h} \approx \frac{\partial}{\partial y}\,, \\
D_{+x} \mathbf{U_i} &= \frac{\mathbf{U}_{i+1,j} - \mathbf{U}_{i,j}}{h} \approx \frac{\partial}{\partial x}\,, \\
D_{-x} \mathbf{U_i} &= \frac{\mathbf{U}_{i,j} - \mathbf{U}_{i-1,j}}{h} \approx \frac{\partial}{\partial x}\,, \\
D_{+y} \mathbf{U_i} &= \frac{\mathbf{U}_{i,j+1} - \mathbf{U}_{i,j}}{h} \approx \frac{\partial}{\partial y}\,, \\
D_{-y} \mathbf{U_i} &= \frac{\mathbf{U}_{i,j} - \mathbf{U}_{i,j-1}}{h} \approx \frac{\partial}{\partial y}\,, \\
D_x^2 \mathbf{U_i} = D_{0x}^2 \mathbf{U_i} = D_{+x} D_{-x} \mathbf{U_i} = D_{+x} \mathbf{U_i} - D_{-x} \mathbf{U_i} &= \frac{\mathbf{U}_{i+1,j} - 2\mathbf{U}_{i,j} + \mathbf{U}_{i-1,j}}{h^2} \approx \frac{\partial^2}{\partial x}\,, \\
D_y^2 \mathbf{U_i} = D_{0y}^2 \mathbf{U_i} = D_{+y} D_{-y} \mathbf{U_i} = D_{+x} \mathbf{U_i} - D_{-x} \mathbf{U_i} &= \frac{\mathbf{U}_{i,j+1} - 2\mathbf{U}_{i,j} + \mathbf{U}_{i,j-1}}{h^2} \approx \frac{\partial^2}{\partial y}\,,
\end{aligned}$$

where D_{+x} is the forward divided difference operator, D_{-x} is the backward divided difference operator and $D_x = D_{0x}$ is the centred divided difference operator, with analogous definitions for the y direction.

Notice that by using compact difference approximations discretization, the checker-board instability is avoided [81]. The lack of a proper explicit boundary condition for the PPE equation has traditionally been a troubling point when designing or implementing numerical schemes based on the velocity-pressure formulation of the incompressible Navier-Stokes equations. Here, as a boundary condition for the PPE equation (eq. 5.9), we use the normal component $\hat{\mathbf{n}}$ of the momentum equation eq. 5.8 at the boundary $i = 0, 0 < j < N$, as discussed by Gresho and Sani [61], Henshaw [78], Johnston and Liu [92], Petersson [142] and Sani *et al.* [159], where

$$\left.\frac{\partial p}{\partial \hat{\mathbf{n}}}\right|_{\partial\mathcal{D}} = \left.\hat{\mathbf{n}}\right|_{\partial\mathcal{D}} \cdot \left(-\mathbf{g}_t - (\mathbf{g}\cdot\nabla)\,\mathbf{u} + \nu\nabla^2\mathbf{u}\right)\rho\,, \tag{5.17}$$

and we extrapolate the tangential component $\hat{\mathbf{t}}$ of the velocity, such as

$$(D_+)^{pe}\, v_{\mathbf{i}} = 0\,, \qquad \text{for} \qquad i = -1, j = 0, 1, 2, \ldots, N \tag{5.18}$$

where pe is the order of the polynomial extrapolation.

We call eq. 5.17 the div-grad pressure boundary condition and is obtained by taking the dot product between the momentum equation (eq. 5.8) and the unit normal $\hat{\mathbf{n}}$ to the boundary $\partial\mathcal{D}$. Note that by itself it adds no new information to the continuous PDE (since the momentum equation already is satisfied on the boundary) and cannot replace $\nabla\cdot\mathbf{u} = 0$ as the extra essential boundary condition required by the velocity-pressure formulation [81, 142]. Let us now obtain the discrete form of eq. 5.17,

$$D_{0x}P_{0j} = \nu D_{+x}D_{-x}u_{0j}\,, \qquad i = 0, j = 0, 1, 2, \ldots, N, \tag{5.19}$$

where for simplicity we assume $\mathbf{g}|_{\partial\mathcal{D}}$ to be equal to $\mathbf{g}|_{\partial\mathcal{D}} = 0$ (no-slip wall), which can be done without loss of generality [159]. Note that eq. 5.19 requires the value of a flow variable outside the physical domain $\mathcal{P}$ (ghost points), namely $u_{-1,j}$. If we discretize the divergence-free boundary condition $\nabla\cdot\mathbf{u} = 0$ (eq. 5.14) of the velocity-pressure formulation, we obtain

$$0 = \nabla\cdot\mathbf{U_i} = D_{0x}u_{\mathbf{i}} + D_{0y}v_{\mathbf{i}} = D_{0x}u_{\mathbf{i}} + 0 = D_{0x}u_{\mathbf{i}}\,, \qquad i = 0, j = 0, 1, 2, \ldots, N, \tag{5.20}$$

from eq. 5.20 it is obvious that $u_{1,j} = u_{-1,j}$. This implies that in eq. 5.19 one should take $u_{1,j} = u_{-1,j}$, resulting in the following approximation for the Neumann boundary condition eq. 5.19 for the PPE equation

$$D_{0x}P_{0j} = \nu\frac{2}{h}D_{+x}u_{0j}\,, \qquad i = 0, j = 0, 1, 2, \ldots, N, \tag{5.21}$$

We can now see how $\nabla\cdot\mathbf{u} = 0$ provides a boundary condition for the pressure; the discrete divergence-free boundary condition eq. 5.14 determines the ghost line value of the normal component of the velocity $u_{-1,j}$, which is used in the right hand side of eq. 5.19. It is important to emphasizes that in order to achieve a stable scheme using eq. 5.17, it is extremely important to also enforce the essential boundary condition $\nabla\cdot\mathbf{u} = 0$ [81, 142].

5.5 Time-Stepping Algorithm for the Velocity-Pressure Formulation of the Incompressible Navier-Stokes Equations

The method of lines approach is used to solve the discretized equations in time. The method of lines (MOL) [65, 160, 210], is a technique for solving partial differential equations (PDEs) where all but one dimension is discretized. The resulting semi-discrete problem is a set of ordinary differential equations (ODEs) or differential algebraic equations (DAEs) that is then integrated in the undiscretized dimension. The basic idea of the MOL is to replace the spatial (boundary value) derivatives in the PDE with algebraic approximations. Once this is done, the spatial derivatives are no longer stated explicitly in terms of the spatial independent variables. Thus, in effect only the initial value variable (typically time t) remains. In other words, with only one remaining independent variable, we have a system of ODEs that approximate the original PDE. Once this is done, we can apply any integration algorithm for initial value ODEs to compute the approximate numerical solution of the PDE. One significant advantage of the MOL is that it allows the use of existing and generally well established numerical methods for ODEs. For PDEs where it is suitable, MOL is an efficient solution method [65].

After discretizing the equations in space on an overlapping grid system $\mathbb{G}$, one can regard the resulting system as a system of ordinary differential equations ODEs of the form

$$\frac{d\mathbf{U}}{dt} = \mathcal{F}\left(t, \mathbf{U}, P\right)$$

where the pressure P is considered to be a function of the velocity, $P = p(\mathbf{U})$. Now we can use any time integrator on a MOL fashion to solve equations eq. 5.11, eq. 5.12, eq. 5.13, eq. 5.14, eq. 5.18 and eq. 5.19.

In order to keep the solution of the pressure equation decoupled from the solution of the velocity components, we choose a time stepping scheme for the velocity components that only involves the pressure from the previous time steps (split-step scheme). Let us introduce the operators $\mathbb{L} = \mathbb{L}_{\mathbf{E}} + \mathbb{L}_{\mathbf{I}}$ representing the various terms in the momentum equations, as follows

$$\begin{aligned}
\mathbb{L} = \mathbb{L}\mathbf{U_i} &\equiv -\left(\mathbf{U_i} \cdot \nabla\right)\mathbf{U_i} - \frac{\nabla P_{\mathbf{i}}}{\rho} + \nu\nabla^2\mathbf{U_i}\,, \\
\mathbb{L}_{\mathbf{E}} = \mathbb{L}_{\mathbf{E}}\mathbf{U_i} &\equiv -\left(\mathbf{U_i} \cdot \nabla\right)\mathbf{U_i} - \frac{\nabla P_{\mathbf{i}}}{\rho}\,, \\
\mathbb{L}_{\mathbf{I}} = \mathbb{L}_{\mathbf{I}}\mathbf{U_i} &\equiv \nu\nabla^2\mathbf{U_i}\,,
\end{aligned}$$

where $\mathbb{L}_{\mathbf{E}}$ and $\mathbb{L}_{\mathbf{I}}$ are the operators that we treat explicitly and implicitly respectively. Then, the equations (5.11 - 5.14) and (5.18 - 5.19) are integrated using a semi-implicit multistep method, that uses a Crank-Nicolson scheme for the viscous terms and a second-order Adams-Bashforth predictor-corrector approach for the advection terms and pressure. We choose to implicitly treat the viscous terms because if they were treated explicitly we could have a severe time step restriction, proportional to the spatial discretization squared.

By using this time-stepping scheme, the velocity is advanced in time using a second-order Adams-Bashforth predictor step as follows

$$\frac{\mathbf{U}_{\mathbf{i}}^{p}-\mathbf{U}_{\mathbf{i}}^{n}}{\Delta t} = \frac{3}{2}\mathbb{L}_{\mathbf{E}}^{n}-\frac{1}{2}\mathbb{L}_{\mathbf{E}}^{n-1}+\alpha\mathbb{L}_{\mathbf{I}}^{p}+(1-\alpha)\,\mathbb{L}_{\mathbf{I}}^{n}, \qquad \text{for} \qquad i,j=1,2,\ldots,N-1, \tag{5.22}$$

followed by a second-order Adams-Moulton corrector step or the form

$$\frac{\mathbf{U}_{\mathbf{i}}^{c}-\mathbf{U}_{\mathbf{i}}^{n}}{\Delta t} = \frac{1}{2}\mathbb{L}_{\mathbf{E}}^{p}+\frac{1}{2}\mathbb{L}_{\mathbf{E}}^{n}+\alpha\mathbb{L}_{\mathbf{I}}^{c}+(1-\alpha)\,\mathbb{L}_{\mathbf{I}}^{n}, \qquad \text{for} \qquad i,j=1,2,\ldots,N-1, \tag{5.23}$$

where only one corrector step has been used (one may optionally correct more than one time as that should be inexpensive and allows a bigger time step for moving grids [71]). In equations eq. 5.22 and eq. 5.23 the super-script p stands for predicted value, the super-script c stands for corrected value, α is the implicit parameter and $\mathbf{U}_{\mathbf{i}}^{n} \approx \mathbf{u}(\mathbf{x}_{\mathbf{i}}, n\Delta t)$. For $\alpha = 1/2$ we obtain a second-order Crank-Nicolson method, whereas for $\alpha = 1$ we obtain a first-order backward Euler method.

Equations eq. 5.22 and eq. 5.23 are advanced to time $n+1$ together with the following equations

$$\begin{aligned}
\mathbf{U}_{\mathbf{i}}^{n+1} &= \mathbf{g}\left(\mathbf{x}_{\mathbf{i}}, t^{n+1}\right), && \text{for} \quad i=0, j=0,1,2,\ldots,N, && (5.24)\\
D_{0x}u_{\mathbf{i}}^{n+1} &= -D_{0y}g_v\left(\mathbf{x}_{\mathbf{i}}, t^{n+1}\right), && \text{for} \quad i=0, j=0,1,2,\ldots,N, && (5.25)\\
\left(D_{+}\right)^{pe} v_{-1j}^{n+1} &= 0, && \text{for} \quad i=-1, j=0,1,2,\ldots,N, && (5.26)
\end{aligned}$$

Equations (5.22 - 5.26), determine $\mathbf{U}_{\mathbf{i}}^{n+1}$ at all points including the ghost points. We then solve for the pressure at time $n+1$ using

$$\begin{aligned}
\frac{\nabla^2 P_{\mathbf{i}}^{\,n+1}}{\rho} &= -\sum_{m=1}^{\mathbb{N}} \nabla u_{m,\mathbf{i}}^{n+1}\cdot\frac{\partial \mathbf{U}_{\mathbf{i}}^{n+1}}{\partial x_m}, && i,j=0,1,2.\ldots,N, && (5.27)\\
D_{0x}P_{\mathbf{i}}^{n+1} &= \nu D_{+x}D_{-x}u_{\mathbf{i}}^{n+1}+B_p\left(\mathbf{U}_{\mathbf{i}}^{n+1},\mathbf{g}_{\mathbf{i}}^{n+1}\right), && i=0, j=0,1,2,\ldots,N, && (5.28)
\end{aligned}$$

where the boundary forcing $B_p(\mathbf{U},\, \mathbf{g})$ satisfies

$$B_p(\mathbf{U},\,\mathbf{g}) = -\frac{\partial g_u}{\partial t} - g_u D_{0x}u - g_v D_{0y}g_v + \nu D_{+y}D_{-y}g_u \tag{5.29}$$

5.6 Velocity-Pressure Formulation for Moving Overlapping Grids

On a non-moving overlapping grid system $\mathbb{G}$, each component grid $\mathcal{G}_g$ is defined by a smooth mapping $\mathbf{M}_g$ from the computational space $\mathcal{C} = \mathcal{C}(\xi,\eta,\zeta,\tau)$ to the physical space $\mathcal{P} = \mathcal{P}(x,y,z,t)$, such that

$$\mathcal{P} = \mathbf{M}_g\left(\mathcal{C}\right) \qquad \text{or equivalently} \qquad \mathbf{x} = \mathbf{M}_g\left(\mathbf{r}\right)$$

where $\mathbf{x}$ denotes the coordinates in physical space $\mathcal{P}$ and $\mathbf{r}$ denotes the coordinates in computational space $\mathcal{C}$. On a moving grid, the moving mapping depends on time, such as

$$\mathbf{x} = \mathbf{M}_g\left(\mathbf{r}, t\right)$$

On moving grids we solve the governing PDE in a frame that moves with the grid. Thus, if we are solving the velocity-pressure formulation of the incompressible Navier-Stokes equations in physical space $\mathcal{P} = \mathbf{x}$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \frac{-\nabla p}{\rho} + \nu \nabla^2 \mathbf{u}$$
$$\frac{\nabla^2 p}{\rho} + \nabla u \cdot \mathbf{u}_x + \nabla v \cdot \mathbf{u}_y + \nabla w \cdot \mathbf{u}_z = 0$$

then on each moving component grid $\mathcal{G}_g$ of the overlapping grid system $\mathbb{G}$, we make the change of variables from $\mathcal{P} = \mathbf{x}(x, y, z, t)$ to $\mathcal{C} = \mathbf{r}(\xi, \eta, \zeta, \tau)$ defined by

$$\begin{aligned} \mathbf{x} &= \mathbf{M}_g(\mathbf{r}, \tau) \\ t &= \tau \\ \mathbf{u}(\mathbf{x}, t) &= \mathbf{u}(\mathbf{M}_g(\mathbf{r}, \tau)) \equiv \mathbf{U}(\mathbf{r}, \tau) \end{aligned}$$

and as already outlined in Chapter 4, Section 3.1, the time derivative of $\mathbf{u}(\mathbf{x}, t)$ at a fixed point of the physical space $\mathbf{x}$ is related to its time-derivative of a fixed point of the computational space $\mathbf{r}$ by the following equation

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{\partial \mathbf{U}}{\partial \tau} - \dot{\mathbf{G}} \cdot \nabla \mathbf{u} = \frac{\partial \mathbf{U}}{\partial t} - \dot{\mathbf{G}} \left(\nabla_{\mathbf{x}} \mathbf{r} \cdot \nabla_{\mathbf{r}} \right) \mathbf{U} \tag{5.30}$$

where

$$\dot{\mathbf{G}} = \frac{\partial \mathbf{M}_g(\mathbf{r}, t)}{\partial t} \tag{5.31}$$

is the grid velocity.

By replacing equations eq. 5.30 and eq. 5.31 into the incompressible Navier-Stokes equations eq. 5.8 and eq. 5.9 we obtain,

$$\frac{\partial \mathbf{U}}{\partial t} + \left[\left(\mathbf{U} - \dot{\mathbf{G}} \right) \cdot \nabla_{\mathbf{r}} \right] \mathbf{U} = \frac{-\nabla_{\mathbf{r}} p}{\rho} + \nu \nabla_{\mathbf{r}}^2 \mathbf{U} \tag{5.32}$$
$$\frac{\nabla_{\mathbf{r}}^2 p}{\rho} + \sum_{m=1}^{\mathbb{N}} \nabla_{\mathbf{r}} \mathbf{U}_m \cdot \partial_{\mathbf{x}_m} \mathbf{U} = 0 \tag{5.33}$$

which is the velocity-pressure formulation of the incompressible Navier-Stokes equations expressed in a moving frame in computational space $\mathbf{r}$.

5.6.1 Boundary Conditions for Moving Walls

The new governing equations expressed in the moving reference frame, must be accompanied by the proper boundary conditions. For a moving body with a corresponding moving wall, only one constraint may be applied and this corresponds to the velocity on the wall

$$\mathbf{U}(\mathbf{r},t) = \dot{\mathbf{G}}(\mathbf{r},t) \qquad \text{for a no-slip wall} \tag{5.34}$$

$$\hat{\mathbf{n}} \cdot \mathbf{U}(\mathbf{r},t) = \hat{\mathbf{n}} \cdot \dot{\mathbf{G}}(\mathbf{r},t) \qquad \text{for a slip wall} \tag{5.35}$$

On a moving no-slip wall the boundary condition for the pressure equation is obtained by dotting the normal $\hat{\mathbf{n}}$ into the momentum equation

$$\frac{1}{\rho}\frac{\partial p}{\partial \hat{\mathbf{n}}}\bigg|_{\partial\mathcal{D}_{wall}} = \hat{\mathbf{n}}\bigg|_{\partial\mathcal{D}_{wall}} \cdot \left(-\ddot{\mathbf{G}} + \nu\nabla^2_{\mathbf{r}}\mathbf{U}\right) \tag{5.36}$$

Note that the acceleration of the wall appears on the right hand side of eq. 5.36.

5.7 Boundary Conditions

Imposing appropriate boundary conditions to the incompressible Navier-Stokes equations is of paramount importance for the success of every numerical algorithm. The type of boundary conditions to be imposed are dependent on the physics of the flow once the geometry and topology of the selected problem have been determined. In this dissertation, the applications and the flow geometry solved in general belong to external flow problems, where the normal unit vector out of the solid surface points away from the surface towards the computational domain (see figure 5.1).

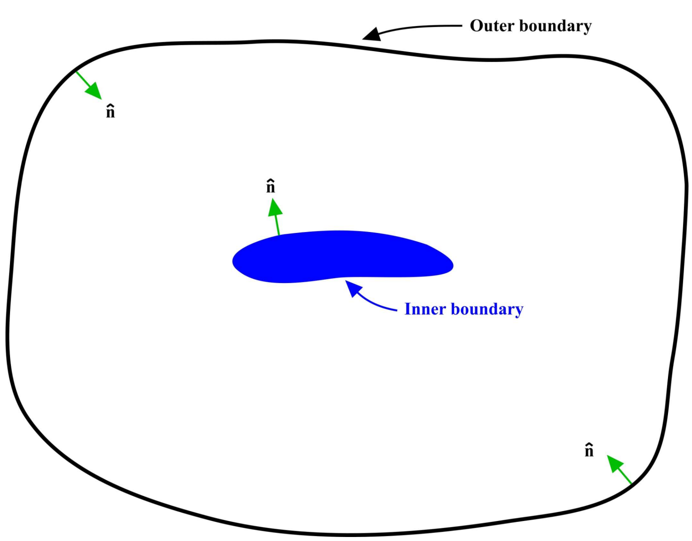

Figure 5.1: *General boundary configuration for external flows.*

The incompressible Navier-Stokes equations in their velocity-pressure formulation are numerically solved using the Overture[1] framework together with the PETSc[2] library. Using Overture, elementary boundary conditions such as Dirichlet boundary conditions, Neumann boundary conditions and mixed boundary conditions, extrapolation boundary conditions, symmetry boundary

[1] https://computation.llnl.gov/casc/Overture/
[2] http://www-unix.mcs.anl.gov/petsc/petsc-as/

conditions and so on, can be easily implemented. Besides the boundary conditions enforced in the velocity-pressure formulation, the following boundary conditions may be used,

$$\text{No-slip wall} = \begin{cases} \mathbf{u} = \mathbf{g} & \text{velocity specified} \\ \nabla \cdot \mathbf{u} = 0 & \text{zero divergence} \end{cases}$$

$$\text{Slip wall} = \begin{cases} \hat{\mathbf{n}} \cdot \mathbf{u} = g & \text{normal velocity specified} \\ \partial_{\hat{\mathbf{n}}} \left(\hat{\mathbf{t}} \cdot \mathbf{u} \right) = 0 & \text{normal derivative of} \\ & \text{tangential velocity is zero} \\ \nabla \cdot \mathbf{u} = 0 & \text{zero divergence} \end{cases}$$

$$\text{Inflow with velocity given} = \begin{cases} \mathbf{u} = \mathbf{g} & \text{velocity specified} \\ \partial_{\hat{\mathbf{n}}} p = 0 & \text{normal derivative of the pressure zero} \end{cases}$$

$$\text{Outflow} = \begin{cases} \text{extrapolate } \mathbf{u} & \text{velocity specified} \\ \alpha p + \beta \partial_{\hat{\mathbf{n}}} p = g & \text{mixed derivative of } p \text{ given} \end{cases}$$

$$\text{Dirichlet boundary condition} = \begin{cases} \mathbf{u} = \mathbf{g} & \text{velocity specified} \\ p = P & \text{pressure given} \end{cases}$$

$$\text{Symmetry} = \begin{cases} \hat{\mathbf{n}} \cdot \mathbf{u} : \text{odd}, \ \hat{\mathbf{t}} \cdot \mathbf{u} : \text{even} & \text{vector symmetry} \\ \partial_{\hat{\mathbf{n}}} p = 0 & \text{normal derivative of the pressure zero} \end{cases}$$

On moving walls, the boundary conditions are those specified in the previous section (equations eq. 5.34, eq. 5.35 and eq. 5.36).

5.8 Discrete Divergence Damping

Due to truncation errors and because of the interpolation between the component grids $\mathcal{G}_g$ of the overlapping grid system $\mathbb{G}$, the divergence ($\delta = \partial u/\partial x + \partial v/\partial y$) will not be identically zero in the numerical computation. Hence, an extra-term, namely discrete divergence damping $\alpha_{\mathbf{i}} \nabla \cdot \mathbf{U}_{\mathbf{i}}$, is often added in the pressure equation eq. 5.12 in order to suppress the spurious divergence. Equation 5.12 becomes,

$$\frac{\nabla_h^2 P_{\mathbf{i}}}{\rho} = \alpha_{\mathbf{i}} \nabla \cdot \mathbf{U}_{\mathbf{i}} - \sum_{m=1}^{\mathbb{N}} \nabla_h u_{m,\mathbf{i}} \cdot \frac{\partial \mathbf{U}_{\mathbf{i}}}{\partial x_m}, \qquad i, j = 0, 1, 2 \ldots, N, \tag{5.37}$$

This technique of adding a damping term is well known and has been used previously by a number of researchers in the field of incompressible flows (*e.g.*, the MAC method of Harlow and Welch [66] or the fourth-order velocity-pressure method of Henshaw, Kreiss and Reyna [80]). This term can be seen as a divergence sink, since it appears as a sink in the PPE equation, helping to keep the discrete divergence small. A detailed description of the coefficient $\alpha_{\mathbf{i}}$ is given by Henshaw in [72, 78] and Henshaw and Kreiss in [79].

One might wonder whether this divergence damping term, which is a potentially order one addition to the pressure equation, will destroy the accuracy of the method. In [79], Henshaw and Kreiss presented an analysis of this damping term using normal-mode stability analysis and showed why this term does not degrade the accuracy of the numerical method. They also found that increasing $\alpha_{\mathbf{i}}$ will result in a decrease of the maximum divergence (up to a point), but it can also increase the error in the pressure.