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Abstract Domain decomposition (DD) is a powerful approach to numerically solve partial differential equations, and it has become popular and indispensable in simulations of fluid flows, especially those that arise from models of the real world that require large-scale, parallel computation. Domain decomposition methods (DDMs) were originally introduced for problems on "complex" geometries, and they are now popular as parallel algebraic solvers and preconditioners for solutions of various problems. Research in theory and practical application of DDMs for fluid flows has seen considerable progress with a substantial amount of work published in the past forty years. This paper makes a comprehensive review of the development and current status of the DDMs, and, for both beginners and experts in this area, it surveys the concepts, algorithms, and the utilization of DD to compressible flows, incompressible flows, and flows in various applications. Along with numerical examples, difficulties are highlighted with potential methods to overcome them, and topics for future study are identified.

Keywords: fluid flow, compressible, incompressible, multiscale, multiphysics, domain decomposition, Schwarz iteration, precondition, multiblock, parallel computation, interface, model coupling

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Fig. 1: Number of journal papers published in each year. The numbers result from a search within Web of Science with four pairs of phrases: "domain decomposition, flow", "multiblock (or multi-block), flow", "domain decomposition, fluid", and "multiblock (or multi-block), fluid".

1 Introduction

The idea of domain decomposition (DD) was proposed to solve partial differential equations (PDEs) by Schwarz more than one hundred years ago [309], and now DD has evolved into an important computational approach to simulate fluid flows. Essentially, the idea is to split a large, complicated problem into smaller, simpler sub-problems, solve them individually, and then recombine their solutions to provide a global solution. Originally, domain decomposition methods (DDMs) for fluid flows, also frequently referred to as zonal methods, or multiblock methods, or composite mesh methods [147,145], were primarily used to overcome difficulties in dealing with complex geometries in mesh generation. Since early the 1980s, research on DDMs has flourished in the simulation of fluid flows with complicated boundaries. Extensions have also been developed in many situations, such as simulations on meshes in relative motion, or whenever a global remeshing is impossible or is too expensive – with sliding meshes or Chimera grids [314, 154]. Currently, DD is an indispensable approach for parallel computation of fluid flows, and it has become a main avenue to feasible, accurate simulation of multiscale and multiphysics flow problems in the real world [183].

In the past forty years, research dedicated to the theory and application of DDMs for fluid flows has seen a rapid and steady increase among the communities of computational mathematics, sciences, and engineering. Fig. 1 presents a survey on the numbers of journal papers published during this period. These numbers of the papers are obtained by searching the Web of Science database with phrases related to DD and fluid flows as "topics", which appear in the articles’ titles, abstracts, and keywords. Additionally, there are various seminars, workshops, and conferences dedicated to the study of DD. The main conference on DDMs is the International Conference on Domain Decomposition Methods. Its first meeting was held in Paris in 1987, and since then it is held every one or two years with publication of a well-respected refereed proceedings [2]. There are also conferences which provide a platform for research on DDMs for fluid flows, such as the International Conference on Computational Fluid Dynamics [1].
Since the 1990s, there have been a number of reviews and surveys related to DD and fluid flows. These reviews cover theory [355, 269, 118], algorithms [108, 135, 61, 154], and computation of fluid flows [379, 244, 183]. They focused mainly on DD for model or simplified problems [355, 118], specific techniques [379], and particular types of flows [244, 287]. These reviews do not reflect recent progress, for example in the simulation of multiphysics flow problems. This paper intends to fill the gaps and present a comprehensive review on the development over the past forty years for flows of fluids. Our goal is to serve both laymen as well as experts on this topic by introducing the concepts and fundamentals of DDMs and discuss their application in various flow problems. It should be noted that, since there is a tremendous amount of literature, as seen in Fig. 1, it is impossible to include and review all related publications, and only representative and sample articles will be discussed in this paper.

2 Concepts and Fundamentals

2.1 Schwarz methods

The idea of DD originated from German mathematician H. A. Schwarz in the 19th century. In a study of the Laplace equation subject to Dirichlet boundary conditions

\[
\begin{align*}
\Delta u(x) &= 0, \quad x \in \Omega, \\
 u(x) &= g(x), \quad x \in \partial \Omega,
\end{align*}
\]

he divided the domain \( \Omega \) into two overlapping subdomains \( \Omega_1 \) and \( \Omega_2 \), as shown in Fig. 2a, and proposed the following iterative algorithm: for \( n = 0, 1, 2, \ldots \) solve

\[
\begin{align*}
\Delta u_1^{n+1} &= 0, \quad x \in \Omega_1, \\
u_1^{n+1} &= u_2^n, \quad x \in \Gamma_1, \\
u_1^{n+1} &= g(x), \quad x \in \partial \Omega_1 \setminus \Gamma_1, \\
\end{align*}
\]

\[
\begin{align*}
\Delta u_2^{n+1} &= 0, \quad x \in \Omega_2, \\
u_2^{n+1} &= u_1^{n+1}, \quad x \in \Gamma_2, \\
u_2^{n+1} &= g(x), \quad x \in \partial \Omega_2 \setminus \Gamma_2,
\end{align*}
\]

starting from an initial guess \( u_0^2 \) prescribed along \( \Gamma_1 \) [355]. Algorithm (2) is called the (overlapping) alternating Schwarz method. In algorithm (2), \( \Gamma_1 \) and \( \Gamma_2 \) are artificial interfaces or internal boundaries introduced in the interior of \( \Omega \). The boundary conditions on the interfaces, referred
to as transmission conditions [118], exchange solutions between the two subdomains. Schwarz showed, [309], that both \( u^n_1 \) and \( u^n_2 \) converge to the solution of problem (1). More than one hundred years later, Lions made a correction in the proof of Schwarz and proposed a modification of the alternating Schwarz method (2) by setting \( u^{n+1}_2 = u^n_1 \) for \( x \in I_2 \) [216,217]. With this modification, the subproblems on \( \Omega_1 \) and \( \Omega_2 \) are completely independent at each iteration, opening the door to parallel computation. This modified method is called the parallel Schwarz method.

A domain may also be partitioned into non-overlapping (disjoint) subdomains, which overlap with each other only at their interfaces (Fig. 2b). Without overlap, the alternating or parallel Schwarz methods introduced above do not converge, as the interface solution stagnates at its initial value. To recover convergence, the above algorithm must be appropriately modified. One remedy is the non-overlapping alternating Schwarz method given by: for \( n = 0, 1, \ldots \), solve

\[
\begin{align*}
\Delta u^{n+1}_1(x) &= 0, & x &\in \Omega_1, \\
(\partial/\partial n_1 + \alpha_1)u^{n+1}_1(x) &= (\partial/\partial n_2 + \alpha_2)u^{n+1}_2(x), & x &\in \Gamma, \\
u^{n+1}_1 &= g(x), & x &\in \partial \Omega_1 / \Gamma,
\end{align*}
\]

\[\begin{align*}
\Delta u^{n+1}_2(x) &= 0, & x &\in \Omega_2, \\
(\partial/\partial n_2 + \alpha_2)u^{n+1}_2(x) &= (\partial/\partial n_1 + \alpha_1)u^{n+1}_1(x), & x &\in \Gamma, \\
u^{n+1}_2 &= g(x), & x &\in \partial \Omega_2 / \Gamma,
\end{align*}\]

in which \( \alpha_1, \alpha_2 = \text{const} \). Noting that \( n_1 = -n_2 \), whenever \( \alpha_1 + \alpha_2 \neq 0 \), should this algorithm converge, the limiting solutions, \( u_1 \) and \( u_2 \), satisfy \( u_1 = u_2 \) and \( \partial u_1 / \partial n_1 = \partial u_2 / \partial n_1 \), respectively, on the interface [218]. This coupling method can be applied to overlapping subdomains as well, as in the Dirichlet-Robin method [157]. Additional algorithms which solve problem (1) on non-overlapping subdomains, include the Dirichlet-Neumann algorithm and the Neumann-Neumann algorithm [355]. More variants of DDMs for problem (1) can be found in literature [355,98].

Algorithms (2) and (3) are Schwarz methods at the continuous level, where no discretization is involved. These algorithms may be naturally extended to more than two subdomains and applied to many classes of PDEs. As we will see later, Schwarz methods are widely used as solvers, or solution procedures, in practical problems. However, the convergence of the methods depend on the equation parameters, the interface conditions, the overlap size, and the shapes and sizes of the subdomains, and it is difficult to predict and control in practice. As a consequence, Schwarz methods used as a solver typically suffer from slow or a lack of convergence [118], and thus much focus has shifted to using the DD philosophy as a preconditioner at the algebraic level as discussed in the following section. A review on history and development of Schwarz methods can be found, for instance, in [355,118].

2.2 Domain decomposition at the algebraic level

Discretization of problem (1) by finite differences or a finite element method leads to a linear algebraic system

\[ AU = f, \quad (4) \]

where \( U \) is a solution vector, \( A \) is the coefficient matrix, and \( f \) is the right-hand-side vector. The linear system can be solved using the so-called multiplicative Schwarz method (e.g., [61]). The method solves the system by iteration using a DD scheme at the algebraic level. In particular, suppose the coefficient matrix \( A \) is split into two smaller local matrices \( A_j \) (\( j = 1, 2 \)) that are formed by so-called restriction matrices \( R_1 \) and \( R_2 \) by

\[ A_j = R_j A R_j^T, \quad (5) \]
where

\[
R_1 = \begin{bmatrix} 1 & 0 \cdots & 0 \\ 0 & 1 \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0
\end{bmatrix} \quad \text{and} \quad R_2 = \begin{bmatrix} 0 \cdots & 0 & 1 & 0 & 0 \\ 0 \cdots & 0 & 0 & 1 & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1
\end{bmatrix}.
\]

The multiplicative Schwarz method to solve (4) reads as

\[
\begin{aligned}
U^{n+1/2} &= U^n + R_1^T A_1^{-1} R_1 (f - AU^n), \\
U^{n+1} &= U^{n+1/2} + R_2^T A_2^{-1} R_2 (f - AU^{n+1/2}),
\end{aligned}
\]

where \(n\) is the iteration index.

It can be shown that, for a one-dimensional (1D) problem, the multiplicative Schwarz method is just a block Gauss-Seidel method if the splitting is non-overlapping, that is, if \(R_1^T R_1 + R_2^T R_2 = I\) (e.g., [118]). It is further shown that, in the case of a 1D problem, the multiplicative Schwarz method is actually a discretized version of alternating Schwarz method (2) with a minimal overlap (i.e., two nodes of the grid on \(R_1\) overlap with two nodes of the grid for \(R_2\)). To understand this easily, let us decompose the original problem in block notation as

\[
A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix}, \quad f = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},
\]

which corresponds to the situation when \(R_j\) is non-overlapping, and \(A_{jj} = A_j\) in Eq. (5). Therefore, the multiplicative Schwarz method (7) reads as

\[
\begin{aligned}
\begin{bmatrix} U_1^{n+1/2} \\ U_2^{n+1/2} \end{bmatrix} &= \begin{bmatrix} U_1^n \\ U_2^n \end{bmatrix} + \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \begin{bmatrix} f_1 - A_{11} U_1^n - A_{12} U_2^n \\ f_2 - A_{21} U_1^n - A_{22} U_2^n \end{bmatrix}, \\
\begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \end{bmatrix} &= \begin{bmatrix} U_1^{n+1/2} \\ U_2^{n+1/2} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \begin{bmatrix} f_1 - A_{11} U_1^{n+1/2} - A_{12} U_2^{n+1/2} \\ f_2 - A_{21} U_1^{n+1/2} - A_{22} U_2^{n+1/2} \end{bmatrix}.
\end{aligned}
\]

Simplifying these two equations, one eventually obtains

\[
\begin{aligned}
\begin{bmatrix} U_1^{n+1/2} \\ U_2^{n+1/2} \end{bmatrix} &= A_{11}^{-1} (f_1 - A_{12} U_2^n), \\
\begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \end{bmatrix} &= \begin{bmatrix} U_1^{n+1/2} \\ U_2^{n+1/2} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} (f_2 - A_{21} U_1^{n+1/2}) - A_{22} U_2^{n+1/2},
\end{aligned}
\]

which is actually the two-step block Gauss-Seidel method: the first step solves the original problem in subdomain 1 using the first node of subdomain 2 as a Dirichlet boundary condition (achieved by casting the term \(A_{12} U_2^n\) to the right-hand side); the second step solves in subdomain 2 using the value at the last node of subdomain 1 as a Dirichlet boundary condition (hence the term \(A_{21} U_1^{n+1/2}\) in the right-hand side), as shown in a simple 1D example in Fig. 3. Thus the Gauss-Seidel method is equivalent to selecting non-overlapping \(R_j\) in multiplicative Schwarz method (7) with minimal overlap, i.e., with two nodes.

To allow parallel computation, the additive Schwarz method [102] is proposed to solve (4). For a 1D problem and two subdomains, it reads as

\[
U^{n+1} = U^n + (R_1^T A_1^{-1} R_1 + R_2^T A_2^{-1} R_2) (f - AU^n).
\]

The term \(R_1^T A_1^{-1} R_1 + R_2^T A_2^{-1} R_2\) is called a preconditioner for this simple Richardson iteration, and this preconditioner plays a crucial role in convergence of the iteration [355]. If \(R_j\) is not
overlapping, the additive Schwarz method is equivalent to the discretization of the aforementioned parallel Schwarz method at the continuous level (3) proposed by Lions. If $R_j$ is overlapping, the additive Schwarz method does not converge (e.g., [355,118]). Accidentally, it was found that after a slight modification to $R_1$ and $R_2$ in (11), the additive Schwarz method becomes convergent in the overlapping situation [55]. The resulting method is called the restricted additive Schwarz (RAS) method, and it is equivalent to the discretization of the parallel Schwarz method at the continuous level.

2.3 Schur complement system

Partitioning the domain into non-overlapping subdomains, discretizing Laplace’s equation, and re-ordering the unknowns leads to a linear system $AU = f$ where

$$
U = \begin{bmatrix}
U_1 \\
U_2 \\
U_{\Gamma}
\end{bmatrix}, \quad A = \begin{bmatrix}
A_{11} & 0 & A_{1\Gamma} \\
0 & A_{22} & A_{2\Gamma} \\
A_{\Gamma1} & A_{\Gamma2} & A_{\Gamma\Gamma}
\end{bmatrix}, \quad \text{and} \quad f = \begin{bmatrix}
f_1 \\
f_2 \\
f_{\Gamma}
\end{bmatrix}.
$$

The subscript 1 and 2 indicate unknowns at grid nodes in the interior of $\Omega_1$ and $\Omega_2$, respectively, and the subscript $\Gamma$ indicates unknowns at grid nodes on the interface of the two subdomains [61,269], see Fig. 2b. After elimination of $U_i$ ($i = 1, 2$), a so-called Schur complement system, $SU_{\Gamma} = g_{\Gamma}$, for the solution on the interface, $U_{\Gamma}$, is found where

$$
S = A_{\Gamma\Gamma} - A_{\Gamma1}A_{11}^{-1}A_{1\Gamma} - A_{\Gamma2}A_{22}^{-1}A_{2\Gamma}.
$$

$S$ is referred to as the Schur complement of $A$, and $g_{\Gamma}$ is a vector. The Schur complement system (13) is smaller in size than the original system (12), and once the former is solved, the solution for the latter is readily obtained [269] as

$$
\begin{cases}
U_1 = A_{11}^{-1}(f_1 - A_{1\Gamma}U_{\Gamma}), \\
U_2 = A_{22}^{-1}(f_2 - A_{2\Gamma}U_{\Gamma}).
\end{cases}
$$

These equations independently solve for $U_1$ and $U_2$ in the interior of subdomains using the interface value $U_{\Gamma}$ as Dirichlet conditions. The Schur complement system serves as a basis for study.
of a number of DD algorithms including the Dirichlet-Neumann algorithm and the Neumann-Neumann algorithm. More information may be found in [355, 269].

2.4 Time dependent problem

DDMs have also been proposed and studied for time dependent problems. A standard approach is to apply DD solvers and preconditioners to semi-discretized problems in time and solve the sequence of resulting elliptic spatial problems as discussed above, see for example [240]. A more recent approach is Schwarz waveform relaxation, which supplies an iterative solution by working directly on the time dependent problem [119]. The approach partitions the spatial domain but then solves the resulting time dependent problems on each subdomain over a time window. Traces of the solution in time on each subdomain are then communicated to neighbouring subdomains to allow the solution to be updated.

Suppose we wish to solve the parabolic problem

\[ u_t = \Delta u, \quad (x,t) \in \Omega \times (0, T), \]
\[ u(x,0) = u_0(x), \quad x \in \Omega, \]
\[ u(0, t) = g_0(t), \quad 0 \leq t \leq T, \]
\[ u(L,t) = g_L(t), \quad 0 \leq t \leq T, \]

where \( \Omega = (0, L) \). As shown in Fig. 4, the space-time domain \( \Omega \times [0, T] \) is partitioned into two overlapping space-time subdomains \( \Omega_1 \times [0, T] \) and \( \Omega_2 \times [0, T] \), where \( \Omega_1 = (0, \beta_1 L) \) and \( \Omega_2 = (\beta_2 L, L) \) with \( 0 < \beta_2 < \beta_1 < L \). Define \( u_1^n(x,t) \) and \( u_2^n(x,t) \) to be approximations to \( u(x,t) \) on \( \Omega_1 \times [0, T] \) and \( \Omega_2 \times [0, T] \), respectively, and \( u_1^n(\beta_1 L, t) \) and \( u_2^n(\beta_2 L) \) be given. The (classical) Schwarz waveform relaxation algorithm would attempt to solve this problem using the following iteration: for \( n = 1, 2, \ldots \), solve

![Fig. 4: Space-time domain partition.](image-url)
\[
\begin{align*}
\left\{ \begin{array}{l}
\frac{u^n_{1,t}}{=} \Delta u^n_{1}, \\
\frac{u^n_{1}(x, 0)}{=} u_0(x), \\
\frac{u^n_{1}(0, t)}{=} g_0(t), \\
\frac{u^n_{1}(\beta_1 L, t)}{=} u_2^{n-1}(\beta_1 L, t), \\
\frac{u^n_{2,t}}{=} \Delta u^n_{2}, \\
\frac{u^n_{2}(x, 0)}{=} u_0(x), \\
\frac{u^n_{2}(\beta_2 L, t)}{=} u_1^{n-1}(\beta_2 L, t), \\
\frac{u^n_{2}(L, t)}{=} g_L(t),
\end{array} \right. \\
(x, t) \in \Omega_1 \times (0, T], \\
x \in \Omega_1, \\
0 < t \leq T, \\
0 < t \leq T,
\end{align*}
\]

(16)

Convergence of the above Schwarz waveform relaxation algorithm is shown in [119,125]. Such convergence generally depends on the specifics of the transmission conditions in space-time, the size of the overlap (if overlapping partitions are used), the nature of the PDEs themselves, and the length of the time window. In an effort to speed up convergence, optimal and optimized Schwarz waveform relaxation methods are proposed by adapting better transmission conditions (e.g., [232, 233]). Commonly the convergence rate improves as the time window is made smaller. One does, however, have to balance the size of the time window with the frequency of communication and size of the messages between subdomains. Schwarz waveform relaxation methods have also been studied for hyperbolic problems [37]. Another variant, space-time DD [212], is available. A review of these approaches is available in [118].

2.5 Domain partitioning

DD methods require a partitioning of a domain into overlapping or non-overlapping subdomains. In the case that DD is used for geometrical purposes: in order to perform local refinement, to simplify the meshing (e.g., multiblock, patching grids), or to follow moving components (e.g., sliding mesh), the partitioning is a priori imposed by the geometrical configuration of the problem. Examples include sliding mesh methods for simulation of rotating devices – when simulating a wind turbine, one mesh is attached to the turbine and another attached to the tower [375,192]. In the case DD is used as an algebraic solver, the partitioning should be carried out on a conforming mesh to obtain a load balancing among the different grids which will be assigned to different processes. At the same time, it is desired to minimize the size of the interfaces to reduce the communication cost (which often limits the strong scalability of a DDM [101]).

Partitioning can be done as a preprocessing step or at runtime. In both cases, there exist two main families of partitioners: topological and geometric. Topological partitioners based on graph partitioning divide the vertices of the mesh graph into sets of equal size to provide good load balance, while limiting the number of edges connecting these sets to limit the communications between the processes. Achieving such a partitioning is a well studied NP-complete problem [120] and is generally addressed by means of multilevel heuristics [21,178]. Usually, the implementation is sequential so that their costs become prohibitive for large graphs. Among such partitioners, we cite the open source libraries METIS [177] and Scotch [273]. To lessen this cost, parallel counterparts have been developed, such as ParMETIS and PT-Scotch. However, the efficiency of such parallel partitioners in terms of load balancing degrades with the number of CPUs [12], thus compromising the overall performance of the simulation cycle. In [81], the authors study the effect of different partitionings obtained with METIS on the convergence of a DDM solver (parAINV), for two families of SPD systems [29]. We also mention a surprising alternative based on “Heuristics from Nature”, where an ant-colony algorithm is developed for \(k\)-way partitioning [193].
Geometric partitioners are based on vertex coordinates (and possibly some weights). Examples include the octree partitioning [243], the multi-jagged method [89], the recursive coordinate bisection method [30], and the space-filling curve (SFC) partitioning [276,44]. Significant advantages of geometrical methods include the fast computational time, the easy parallelization, and the well balanced subdomains that provide a certain space locality. However, no control on the interface size is possible, and thus the overall efficiency of the solver depends on the communication efficiency in the DD solver (e.g. by hiding communications using non-blocking messages). To illustrate the difference between topological and geometrical partitioners, Fig. 5 compares the 16 partitions of a cube obtained with METIS and SFC.

![Fig. 5: Partitioning of a cube into 16 subdomains.](image)

An important issue, often neglected, is the influence of the subdomain geometries and connectivities on the convergence of DDM solvers. A class of problems for which these two factors have a great impact on convergence is transport in highly heterogeneous media. An example of such a study can be found in [110] in the context of the FETI method. In [20], the authors study the influence of mesh partitioning in the case of dominating convection and anisotropic diffusion for generic advection-diffusion equations. They also address the convergence of a Schwarz method applied to the solution of a porous media flow with high heterogeneity [140]. In this work, the graph of the matrix is partitioned based on the entries of the input matrix, by simply modifying the weight of the graph edges used by the graph partitioner. A pioneering theoretical work on the influence of the subdomain shapes and aspect ratios on the convergence of a Schwarz method is presented in [60].

2.6 Mathematical issues of study

DDMs involve a number of important mathematical issues. It is known that the convergence of the original Schwarz method (2) improves as the size of the overlap increases between two subdomains (e.g., [118]), while its natural extension to the Helmholtz equation fails to converge (e.g., [98]). The transmission conditions that communicate solution information between subdomains play a crucial role in the convergence rate of DDMs [218,249], and this has led to development of a class of optimized Schwarz methods, which design transmission conditions to produce fast convergence (e.g., [334,168,105]). Dirichlet conditions, Neumann conditions, and Robin conditions are commonly employed at interfaces between subdomains [228]. Note that these transmission conditions may not be enforced strictly but instead approximately, e.g., via minimization of the residual between the different subdomains [92].
As the number of subdomains increases, the convergence rate (per iteration) typically decreases due to the lack of rapid exchange of solution information across all the subdomains (e.g., [98]). This indicates that the method is not immediately scalable with respect to the number of subdomains (weak scalability). This scalability issue presents a barrier for large scale parallel computation. Such an issue may be overcome by introducing corrections via a coarse mesh solution. This gives rise to two-level and multilevel Schwarz methods, see for example, [52,355,11]. Balanced DDMs have been proposed by adding a coarse-level scheme to the Neumann-Neumann algorithm for non-overlapping subdomains [229,103]. In [4], the coarse grid correction is obtained algebraically via generalized eigenvalue problems, leading to a condition number independent of the number of domains. Additionally, some issues arising in practical computation, such as artificial oscillation in numerical solutions, also deserve study to achieve a better simulation [337].

3 Compressible Flow

3.1 Equations and grids

In its early development, a main application area of DDMs was aerospace engineering. DDMs were used as a means to handle flow fields with complex geometries by dividing the physical domains into a set of zones with relatively simple shapes, e.g., [147,26]. The governing equations for compressible flows are the Laplace equation (modelling simplified potential flows), the inviscid Euler equations, and the (viscous) Navier-Stokes equations. The equations can be elliptic, hyperbolic, and parabolic, or even a mixture of these types. A major challenge in simulation of compressible flows has been to reliably capture flow structures including shocks, contact discontinuities, and vortices with available computational capabilities.

Corresponding to the non-overlapping and overlapping subdomains mentioned above, the grids used for DDMs for fluid flow problems can broadly be grouped into two categories: 1) non-overlapping grids and 2) overlapping grids, depending on the layout of meshes, see Fig. 6. With non-overlapping grids, the two meshes are connected to each other along a common line or surface known as a grid or artificial interface. Non-overlapping grids are frequently referred to as patched grids [286,379]. In an overlapping grid situation, one grids wholly or partially covers another grid. Examples of overlapping grids include overset grids and the Chimera-grid method (if the two grids overlap arbitrarily) [26,69]. When two patched grids exhibit relative motion along their interface, the grids are called sliding meshes [154].

Both overlapping-grid and non-overlapping-grid methods present artificial interfaces within flow fields, for example, see the curve $\Gamma$ in Fig. 6. An important issue is how to approximate solutions at grid nodes on these interfaces. In an overset-grid method, it is a challenge to correctly and efficiently locate the host cells of interface nodes (i.e., the grid nodes on the interfaces), see the interface node ‘p’ and its host cell ‘1-2-3-4’ in Fig. 6b. This location problem is even harder if parallel computation is used. A systematic description of related techniques is presented in [26].

3.2 Grid interface algorithms

A crucial issue in the design and implementation of DDMs for the simulation of a compressible flow is to develop appropriate interface algorithms – transmission conditions and their discretizations. The Euler equations describe the motion of inviscid compressible flows, they comprise a hyperbolic system of conservation laws. As revealed in the pioneering work of P. D. Lax [205, 206], a hyperbolic system of conservation laws permits discontinuities (shocks and contact discontinuities) in its solution. Instead of strong solutions, weak solutions, or piece-wise smooth
solutions, are sought for the system. Such weak solutions yield conservation of physical quantities. For example, the solution \( u(t, x) \) \((t \text{ – time, } x \text{ – space coordinate})\) of an initial value problem for a scalar conservation law satisfies
\[
\int_{-\infty}^{+\infty} u(t, x) dx = \text{const} \tag{17}
\]
for all \( t \geq 0 \).

A natural and straightforward approach to compute solutions at grid interfaces is the adoption of Dirichlet interface conditions with the boundary values obtained by the interpolation of solutions between the grids, see (e.g., [26,69]). Unfortunately, such an approach is generally nonconservative, i.e., it does not ensure conservation property (17). When a discontinuity, such as a shock, passes an interface, a nonconservative interface algorithm tends to cause substantial errors in its speed and/or strength, and can even lead to a non-physical solution (e.g., [265,340]). Two numerical examples are presented in Fig. 7. In Fig. 7a, by comparing to the exact solution, it is seen that the solution obtained with a nonconservative treatment gives the wrong strength for the shock on the left and a wrong speed for the shock on the right. In Fig. 7b, the interface treatment results in a contact discontinuity with the wrong strength and a non-physical shock moving towards right.

In an effort to construct better algorithms at grid interfaces, conservative algorithms have been developed to ensure that conservation property (17) is satisfied by the discrete solution \( v_i^n \) (where \( i \) and \( n \) are indices of grid node and time step, respectively):
\[
\sum_{i=-\infty}^{+\infty} v_i^{n+1} \Delta x = \sum_{i=-\infty}^{+\infty} v_i^n \Delta x, \tag{18}
\]
where \( \Delta x \) is the grid spacing. Such a conservative algorithm is effective in preventing the computation of spurious solutions that a nonconservative interface algorithm tends to produce. This is illustrated in the two examples in Fig. 7. It is known theoretically, if it converges, a numerical solution associated with a conservative interface scheme converges to a weak solution [32]. Various conservative algorithms have been developed, and indeed they are effective in overcoming the
Fig. 7: Solutions of Riemann problems for the 1D Euler equations modelling gas flows. A variable-interpolation method and the numerical-flux-interpolation method are used as a nonconservative and a conservative treatment (respectively) at the grid interfaces [340,346], with \(CFL = 0.95\). a) The initial condition is: \(\rho = 1, u = 2,\) and \(p = 1\) for \(x < 5; \rho = 1, u = -2, p = 1\) for \(x > 5\). Here \(\rho\) is the density, \(u\) the velocity, and \(p\) the pressure. In the resolution of the Riemann problem, one shock travels to the left, and another shock propagates to the right. The Lax-Wendroff scheme is used. Two grids are patched at \(x = 6\) (the grid interface). The grid spacing for the grid on the left and the right is \(\Delta x_1 = \Delta x_2 = 0.2\). b) The initial condition is: \(\rho = 0.25, u = 1,\) and \(p = 0.2857142\) for \(x < 5; \rho = 1, u = 1,\) and \(p = 3.2857142\) for \(x > 5\). In this solution, the initial discontinuity remains stationary as a contact discontinuity. The MacCormack scheme is used. The grid interface is located at \(x = 5\), where the two grids are patched with \(\Delta x_1 = 0.1\) and \(\Delta x_2 = 0.2\).

Non-conservative interface treatments are easier to implement, and furthermore have advantages and frequently provide reasonable solutions, even in the presence of shocks at grid interfaces. Typically nonconservative schemes are based on linear, quadratic, high-order Lagrangian, and B-spline interpolation (see for example [26,295,315]). Nonconservative schemes based on the method of characteristics and Riemann resolution are also available [72]. As shown in [347, 348], a linear interpolation at interfaces results in solutions with less oscillation in terms of total variation as compared to a conservative scheme, and the error (in conservation) of a nonconservative interface scheme has an upper bound when the solution itself is bounded. The study also indicates that, under certain conditions, which can be verified a posteriori, the numerical
solution converges to a weak solution if it converges. Interestingly, it is argued that, when the Euler equations are discretized by nonconservative schemes, nonconservative treatments at grid interfaces have no major difficulties, even when shocks appear at internal boundaries [69]. When spurious oscillations associated with nonconservative treatments occur at such boundaries, techniques are available to suppress them, such as the filtering algorithms used for high-frequency noise at locations where meshes are suddenly stretched as in [365]. As a result, nonconservative methods are commonly used in computation of engineering problems including many of those in the literature reviewed in the following section. Treatments at the grid interface remain as an important research topic, and more detailed discussions are available in literature, see [379].

3.3 Computation of compressible flow

Since the early 1980s, DD has attracted substantial attention among the computational fluid dynamics (CFD) community given its demonstrated potential for the simulation of compressible flows [58,126,147], and quickly it has become mainstream to apply a Schwarz iteration as a solver – dividing a flow domain into subdomains and then adopting Schwarz iteration. Straightforward adoption of Schwarz iteration as a solver in form of Schwarz waveform relaxation such as those discussed in Sec. 2.1, without the sophisticated techniques on the algebraic level in Sec. 2.2, has provided successful simulations of many problems. Such problems include flows within convergent and divergent nozzles [191,359], inviscid and turbulent flows around airfoils [352,185], and flows of compressible, multiple phase fluids such as gases and liquids [213,91]. The advent of the software package OVERFLOW and its development for flows around space shuttle launch vehicles serve as a good example to illustrate the evolution and current status of DDMs for
actual compressible flows; the software has been a forerunner in the research and application of Chimera-grid techniques since the 1980s [47,62,48,255]. In the past few decades, the package has evolved with better available computing technology, providing more detailed simulations — from using just three grids and 0.3 million volume points in the 1980s to over 600 grids and 100 million volume points in 2010 [48]. In addition, in recent years, the DD computation of compressible flows has begun to take advantage of GPUs [359,115,213].

In the simulation of compressible flows, Schwarz methods have been used widely as solvers, or, solution procedures, in conjunction with various discretization methods, including finite difference methods [286,47,63,213], finite volume methods [310,185,122,395], and finite element methods [352,204]. Also sophisticated numerical schemes have been utilized, such as discontinuous Galerkin methods [180,117,91], spectral methods [191,149], and compact schemes [315,?]. For better computational efficiency, grid partitioning methods and parallel computing architecture are investigated [369,384,395]. Interestingly, it is proposed to split three dimensional (3D) problems into a series of two dimensional (2D) problems on stream surfaces and a 1D problem [211]. Using Schwarz methods, various strategies have been designed for parallel computation [204,310,180,213,395,91]. In the computation, grid interfaces are frequently treated with Dirichlet and Neumann conditions. In general such treatments are nonconservative [47,295,117], but can be conservative in certain situations [191,63].

In the past few decades, DD techniques at the algebraic level have been applied to the algebraic systems resulting from discretization of the governing equations of compressible flows. Krylov methods with DD preconditioners are powerful in solving the algebraic systems, and they have been implemented into software packages. Two such Krylov methods are the conjugate gradient (CG) method for symmetric positive definite systems and the Generalized Minimal RESidual algorithm (GMRES) for non-symmetric systems (e.g., [148,301,353,190,274]). As mentioned previously, when partitioning a flow domain, a frequently used software package is METIS, which uses principles from computational geometry to divide a whole unstructured grid into smaller grids of nearly equal sizes to provide a good load balance of the computation, while minimizing the interface between them [177,395].

As shown in Sec. 2, the development of DDMs at the algebraic level began with elliptic and other simplified model problems, thus extension and further development are necessary to apply the methods to compressible flows. Among such efforts is a method called the algebraic multiblock method that combines DD and multigrid. This method is proposed to solve the Euler equations, and the resulting block diagonal linear system matrix is solved by a CG squared method [174]. A non-overlapping additive Schwarz scheme is proposed to solve a sparse linear system resulting from an implicit discretization of 2D inviscous flows, and Dirichlet conditions for the characteristic variables are used as transmission conditions when marching from a current time level to the next level [99]. Following its successful application to a flow around the NACA0012 airfoil, the convergence rate of the scheme associated with a modified transmission condition is analyzed [100]. In the simulation of compressible flows using an immersed boundary method, a flow domain is divided into subdomains along the flow direction, and a tri-diagonal matrix is rearranged and split into separate smaller matrices corresponding to the individual subdomains [123]. In order to improve the efficiency of solving a hypersonic flow over a flat plate, an interface strip preconditioner is developed and successfully applied to the Schur complement system in a situation where a conventional preconditioner produces no convergent solution [271, 270]. Many other techniques including two-level Schwarz algorithms [9], RAS [368], space-time DD [132], etc. have been explored and their effectiveness has been examined for the computation of compressible flows.
4 Incompressible Flow

4.1 DD technique and application

Since the late 1980s, research on DDMs for incompressible flows has quickly become a main topic among the CFD community [200, 331]. Frequently the projection method or its variants are employed in the discretization, and efficient computation of the resulting elliptic-type Poisson equations is an important task. As a result, DD techniques for the Laplace equation and its extensions, which are discussed in Sec. 2, can be used in simulation of incompressible flows. In addition, many approaches for compressible flows described above, such as patched grids and overset grids, are applicable also. However, there is a substantial difference in the governing equations and thus the numerical strategies. A major difference is that incompressible flows are restricted by the divergence-free condition, which has to be well enforced and becomes a main challenge in the simulations. Moreover, unlike the compressible case, implicit schemes are typically used for incompressible flows. Consequently, DD methods specifically for incompressible problems have been developed.

The study of DD methods for incompressible flows started with solving the Stokes equations [331, 268], soon followed by methods to solve the Navier-Stokes equations [200, 146, 329]. As in the compressible case, Schwarz methods have been applied with various discretization methods, including finite differences [146, 114], finite elements [70, 155, 227, 313], finite volumes [392, 51, 84], compact schemes [187], and spectral methods [225]. It is noted that DD is naturally combined with spectral methods to overcome their limitation to simple geometries, and such studies began as early as the early 1980s [258, 266]. In addition, DD has become a standard approach for parallel computation in large-scale simulation of incompressible flows [227, 134, 187]. In the past few decades, DDMs and their applications to incompressible flows have seen substantial advances in geometry simplification, local refinement, moving objects, interface treatment, and parallel computation, which will be discussed below in this and following sections.

In geometry simplification, a generic term used in the literature to define these methods is the so-called multiblock approach, which adopts Schwarz methods as a solver. In the literature, two approaches have been used. One of them deals directly with the mesh by reconstructing a conforming mesh across the interface (e.g. the HERMESH method to connect non-conforming and possibly overlapping meshes [159]). For non-overlapping meshes, one other possibility consists of applying algorithms like Eq. 3 for finite differences or finite elements, or performing flux interpolation from one side of the interface to the other. For overlapping meshes, typically the Schwarz method with Dirichlet-Dirichlet conditions, a method like (2) is considered. Examples of using DD for the simplification of geometries and meshes include the division of a flow domain into several rectangles and then applying a spectral method in one direction in space and a high-order finite difference method in the other direction [83], simulation of an indoor air flow and heat transfer within an atrium [227], and air flows past rotors and towers of wind turbines [391]. As mentioned spectral methods are not readily applied to problems with complicated geometries, and DD has been used to overcome this in simulations, such as those of forward- and backward-step flows [83, 181], a rotating flow in a T-shape channel [289], and a L-shape cavity flow [210]. More recently, DD computation is presented for a 3D Stokes flow problem that is split into a series of 2D problems in a proper generalized decomposition formulation [124].

Another important application of Schwarz methods is to accurately resolve local flow structures by employing fine local mesh resolution. For instance, large-eddy-simulation (LES) to capture turbulence structures in a channel and at the backward-facing step is carried out using a multiblock method in [230, 28]. A DD approach is employed to resolve near-wall turbulence by splitting a flow domain into a boundary-layer subdomain and an outer-layer subdomain [362].
A DDM is applied to capture effluent thermal plumes discharged from ports with diameters at \( \mathcal{O}(10) \) cm into an ambient flow in a natural river with length at \( \mathcal{O}(10) \) km [341]. This simulation captures small-scale plumes, large-scale river currents, and their interaction simultaneously. More examples can be found in literature, including local refinement within multiblock grids to resolve turbulence [68], and the simulation of flow around individual droplets in turbulent clouds [13].

DD approaches have also evolved into a powerful tool to simulate flows embedded with moving objects. In order to simulate a flow around moving objects, a straightforward approach consists of remeshing the complete computational domain, or performing a local remeshing, as proposed by the Shear-Slip Mesh Update Method [23]. However, remeshing can be a prohibitive option when dealing with very large meshes on massively parallel supercomputers. An alternative is a method of sliding meshes or overset grids. This approach has a stationary mesh along with a mesh that wraps and moves with an object. The meshes are connected at interfaces [314, 154]. If the mesh interface topology does not change, then only the interpolations must be updated. If the topology changes, specific techniques like the one proposed by the Chimera method must first be applied to update the interface before the interpolation. Such an approach has been applied to various flows, including an air flow past a centrifugal fan [158], a flow around flying insects [220], a current over a fish with a pair of moving pectoral fins [383], wind past rotors and towers of wind turbines [391], and water flows around ships and their propellers [314]. The Chimera method can be applied as well with heterogeneous transmission conditions (e.g. one transmission condition of Dirichlet type and the other of Neumann/Robin type [156]).

Solution-based grid adaptive methods are proposed for patched and segmented grids, and it is shown that the methods can substantially reduce the overall computation time while maintaining solution accuracy obtained with fine resolution in the entire domain [68, 298]. LU decomposition is employed to treat the discretization of the Navier-Stokes equations solved by a fractional step method, and a discussion is presented to deal with Chimera grids’ blanked nodes, which are excluded from computation [49]. The idea of DD has been utilized in a finite element method with different types of meshes in two adjacent subdomains [84]. A reduced-order method is applied with its basis functions being restricted within individual subdomains, and overlapping subdomains and penalty terms are introduced for the stabilization of numerical solutions [19]. Flows within overlapping subdomains are solved analytically by particular solutions [50].

4.2 Grid interface algorithms

Interface treatment is also crucial to the simulation of incompressible flows using DD approaches. Frequently used transmission conditions at the grid interfaces are Dirichlet and Neumann conditions [165, 388]. In order to facilitate solution exchange when two subdomains are patched with each other, a Dirichlet condition is used at the interface (a line or a surface) as a boundary condition on one subdomain, and a Neumann condition is imposed at the interface as a boundary condition for the other subdomain, similar to the interface treatment in (3). In addition, interpolation is commonly used to implement the transmission conditions, and the adoption of an interpolation method with an accuracy higher than that of the discretization within subdomains is proposed [145, 392]. It is argued that such higher accuracy is necessary if the overlap size reduces with grid spacing [145, 114], while using the same accuracy for the interpolation is fine if the overlap does not shrink with grid spacing [331].

The use of Dirichlet conditions and Neumann conditions is straightforward, and their implementation via interpolation is easy. However, this process may lead to difficulties. Such difficulties include slow convergence or even divergence in the computation, or, non-physical oscillations in the solutions near the grid interfaces [162, 338]. Figs. 9a, 9b, and 9c present a simulation obtained
with Dirichlet conditions imposed on velocity and pressure and implemented by a tri-linear interpolation. They show spurious oscillations in both pressure and velocity. Such oscillations become severe as the difference in two adjacent meshes’ spacing increases [338,336]. The oscillation not only pollutes the accuracy of the solutions but also may lead to blowup of the computation.

Fig. 9: Simulation of a 3D oscillating cavity flow at \( t = 10 \) with \( Re = 100 \) [338]. \( p \) is pressure, and \( u \) and \( v \) are velocity in the horizontal and vertical direction, respectively. Two overlapping grids are used and arranged vertically. (a), (b), (c) Solutions obtained with interpolation at the grid interfaces. (d), (e), (f) Solutions obtained with MFBI at the grid interfaces.

In pursuing better treatments at the grid interfaces, the development of conservative algorithms has been a main effort. In addition to prevention of non-physical phenomena such as the oscillations as seen in Figs. 9d, 9e, and 9f, the advantages of conservative interface algorithms include faster convergence, lower residual, and better balance of physical properties [162,392,51,338,336]. Using similar techniques as used with compressible flows [286], conservation of mass and momentum has been achieved on 2D patched, aligned composite grids by matching their fluxes segment by segment along a common line of two adjacent grids [376,390].

Unlike the case of patched grids, when Chimera grids are used in a finite difference method, it is very difficult, if not impossible, to strictly realize conservation properties. In this situation, conservation can only be enforced approximately and, so far, this has been achieved for mass conservation only. Frequently such conservation is implemented using schemes for Poisson equations for pressure [162,296]. Such schemes may lead to discontinuity in solutions for pressure or/and velocity at grid interfaces, and later remedies have been proposed to ensure continuity of solutions [7]. Instead of using a Poisson equation, an interface algorithm called the mass flux balance interpolation (MFBI) is proposed for Chimera grids in [338,336]. Consider the two overest
grids shown in Fig. 6b. Along an imaginary line a - b, the algorithm enforces mass conservation between the two grids, and it computes solutions on the grid nodes, at ‘p’, for example, in such a way that

\[
\begin{align*}
U_{1,j,k} &= J_{1,j,k} \left( (U^I / J)_{1,j,k} + (U^I / J)_{2,j,k} - (U / J)_{2,j,k} \right), \\
V_{1,j,k} &= V^I_{1,j,k}, \\
W_{1,j,k} &= W^I_{1,j,k}, \\
p_{1,j,k} &= p^I_{1,j,k}.
\end{align*}
\]

(19)

Here $J$ is the Jacobian of the geometric transformation, and the superscript $I$ indicates interpolation. $U$ is the velocity in $i$ direction normal to a-b, $V$ and $W$ are the velocity in the $j$ and $k$ (coming out of the paper, not shown) directions of grid lines, and $p$ is the pressure. MFBI determines velocity $U$ by mass conservation and interpolates the other two velocities and pressure; MFBI is only a slight modification of the standard interpolation, which interpolates all the four variables (three velocities and pressure), and it can be implemented easily in practical computation. In comparison to the standard interpolation, in addition to effectively removing spurious oscillations, as shown in Fig. 9, MFBI leads to fast convergence, lower residual, and better balance of mass fluxes between subdomains [338,336,381,322,78]. It should be noted that, in general, solutions for incompressible flows are continuous and smooth. A standard interpolation at grid interfaces is justified from the point of view of numerical accuracy. However, from the point of view of the divergence-free condition, frequently such interpolation does not perform well. In addition, it is expected that a standard interpolation leads to over-imposing of the boundary conditions since it specifies all of the four variables (three velocities and pressure).

In a finite element method, apart from classical interpolation, projection may provide global conservation properties across interfaces. A typical projection of a variable $u$ on an interface $\Gamma$ from non-overlapping meshes $B$ to $A$ (see Fig. 6a), consists of solving for $u$ in mesh $A$ by

\[
\int_{\Gamma} u_A \phi_A d\Gamma = \int_{\Gamma} u_B \phi_A d\Gamma,
\]

(20)

where $\phi_A$ is a weight function on mesh $A$ (which frequently corresponds to a coarser mesh). By computing accurately the right-hand side of this equation (e.g. by introducing a sufficient number of integration points on $\Gamma$), we can show that this projection conserves the average value of the unknown on the interface. Should this unknown $u$ be a flux, we thus have a simple way of conserving the total flux on the interface. Note that (20) can be solved very efficiently by using a lumped mass matrix on the left-hand side. In [154], several conservative algorithms are presented. Another option is to constrain the continuity of the interpolated unknown, and a mass conservation algorithm is developed by minimizing the difference of interpolated variables at two adjacent grids, and constraining it by a mass conservation equation [155].

Investigations have also been conducted for other interface treatments. A fourth-order finite difference method together with interpolation at grid interfaces is presented to solve the full Navier-Stokes equations on overset grids [146]. When a spectral discretization is used, continuity of flow variables and their derivatives, and even the divergence-free constraint, are enforced with Dirichlet-Dirichlet, and Neumann-Neumann conditions at interfaces of subdomains [224,181,289]. A least-square method is proposed to deal with an overdetermined system and derive interface conditions [142]. Numerical viscosity, or a filtering technique, in spectral methods is examined and quantified near internal boundaries and in regions away from the boundaries in flows at high Reynolds numbers [90]. A prediction-correction procedure used with compact schemes is implemented to suppress spurious errors at grid interfaces of overset grids [187]. An optimized Schwarz DDM for the Navier-Stokes equations, together with transparent boundary conditions, is presented, and it is shown that such conditions may improve convergence of the method [40].
A main drawback of explicit interface algorithms is that they slow down the overall convergence of DDMs to the global solution (Sec. 2.6). To remedy this, one possibility is to apply the coupling method in an implicit way. By taking a look at Eq. 3, if one gets rid of the iteration index, implicit coupling can be achieved by assembling the interpolated unknowns and flux directly into the matrix of the uncoupled system. The mortar element method is another example of such implicit method for coupling non-overlapping [34] or overlapping [53] non-conforming meshes. Another possibility is explored in [154,153], where the implicit coupling between the non-conforming meshes is achieved by extending the Sparse-Matrix Vector product (SpMV) used in iterative solvers.

4.3 DD at the algebraic level and parallel computation

As the application of Schwarz methods as solvers gradually becomes popular, extensive research has been completed on DD at the algebraic level. Such research stems from DD techniques developed for computation of solutions for Laplace equations, Eq. (1). An example of a DDM designed at the algebraic level for incompressible flows is the element-by-element preconditioned CG algorithm developed to solve a Poisson equation for the pressure [70]. A preconditioner associated with a balanced Neumann-Neumann DDM is proposed for the Schur system resulting from Stokes flows, and its computational performance is shown to be independent of the number of subdomains [127]. The iterative Neumann-Neumann algorithm with a relaxation parameter is applied to a Poisson equation, and the convergence of the solution can be obtained after a limited number of internal iterations [225]. Attempts have been made to extend a balanced DD method to the Stokes equations, and improvement in performance with regard to convergence is confirmed [268]. A Schur complement preconditioner is proposed to solve a Poisson equation, it achieves faster convergence and requires less computation time and memory [71].

In recent years, DD techniques at the algebraic level have also seen a growing number of applications to practical problems. Subdomain partitioning tools associated with a finite element method are used to simulate 2D, low Reynolds number flows in a step channel and past a cylinder [70]. An LES has been accomplished for an unsteady, 3D backward-facing step flow using a non-overlapping strategy associated with a Poisson solver and the Schur complement system [230,28]. As mentioned in Sec. 2, the convergence of DD solvers worsens with the number of subdomains and coarse solvers are therefore usually used to remove this dependence, leading to two-level DD methods. A two-level preconditioner is applied to simulate a 2D cavity flow, and its computational efficiency and the effect of the overlap are discussed [164]. An algorithmic framework that removes the scalability limitations and leads to an optimal allocation of available computational resources is applied to unsteady flows within arterial networks [134]. A balancing DD method is applied to simulation of unsteady dispersion of hydrogen [387]. Newton-Krylov-Schwarz algorithms are used to model flows in a microchannel and around a high-speed train [163,67].

DD at the algebraic level has become an avenue for improvement in computational efficiency and parallel computation. Let $N$ be the number of unknowns in the algebraic system and $P$ be the number of subdomains. The rate of convergence of classical Krylov solvers (CG, GMRES, etc.) with simple preconditioners (Jacobi, Gauss-Seidel, etc.) decreases with the mesh size and thus increases with the number of degrees of freedom $N$ [300,214]. This is mainly due to the fact that the main error propagation mechanism is provided by matrix-vector products, which propagate error from node to node. DD preconditioners remove this dependence as they provide a subdomain-to-subdomain propagation. DD solvers are thus attractive for their robustness, and,
Two level domain decomposition methods, namely, Balancing Neumann-Neumann (BNN) [229], Balancing Domain Decomposition by Constraints (BDDC) [96] and the dual-primal finite element tearing and interconnecting (FETI-DP) [109] for example, permit algorithmic weak scalability (see also [4] in the generic context of abstract Schwarz preconditioners). In actual implementations in a distributed memory environment [139,297], however, the solution of the coarse problem ends up dominating the total computing time at large scales [16,14]. In the case of BDDC, the coarse problem can be solved in parallel with the fine problem and this extends scalability further [17]. A multilevel extension is one good option to reach the extreme scales of future architectures [15].

Parallel computation via DD at the algebraic level has been applied in complicated, realistic problems. In general, the subdomains used in a DD solver coincide with the partitioning used for the assembly of the equations (although they could be different). A two-level additive Schwarz preconditioner is presented for solving steady, incompressible flows [164]. In order to speed up convergence in solving systems of nonlinear algebraic equations resulting from discretization, a Newton-Krylov-Schwarz algorithm in conjunction with GMRES is applied to simulate complicated and large-scale computational problems [163,67]. Efforts towards efficient parallel computation have proceeded via other approaches. A two-stage DDM is proposed to remove the scalability limitation in parallel computation of linear systems, and it is applied to problems with 96,000 computer cores [134]. A 2D "pencil" DDM for parallel computation on distributed-memory systems is used in DNS modeling of a stratified channel flow [141]. DD has emerged as a main approach for large-scale, parallel computation of various complex real-world incompressible flow problems using over 10,000 computer cores, see, e.g., [134,314,320].

5 Flow Problems in Various Applications

5.1 Flow in porous media

Flows in porous media follow Darcy’s law or its variants such as Brinkman’s equation, their governing equations are essentially Poisson equations that are generally elliptic in nature, but also may involve other processes described by parabolic or hyperbolic equations [324,175]. When described by Poisson equations, DD computation of these flows benefit from the existing extensive investigations of standard DD techniques as discussed in Sec. 2.1 and 2.2. However, the simulation of actual problems of flows in porous media remains challenging. The challenge comes from locality of permeability, e.g., high contrast and high frequency in the permeability, the presence of multiphase flows, and the large sizes of the matrices resulting from discretization. These lead to strong multiscale and multiphysics features and frequently even ill-conditioned problems [108, 272,143,175]. DD is a natural approach to overcome these difficulties, and the simulation of actual flows in porous media has been an active area in the study of DDMs.

Theoretical investigations of DDMs for flows in porous media are commonly made at the algebraic level since their governing equations are Poisson-type equations, and DD techniques for such equations, frequently in conjunction with multigrid methods, are available for the flows. It is known that the approximation of the Darcy’s law will be more efficient if a sudden change in permeability is aligned with the coarse grids [278,175]. In order to efficiently solve the large-scale algebraic systems resulting from discretization of Darcy flows with stochastic permeability, a two-level scalable preconditioner is proposed on the basis of the Schur complement system [332]. A two-scale nonlinear preconditioning technique is proposed, and numerical examples demonstrate that its coarse solver improves the scalability properties [325]. Preconditioners based on
a discontinuous Galerkin method and a multigrid technique are presented for solving the Darcy and Brinkman models, and they perform well for flows in porous media with high contrast and high frequency in permeability [175].

In actual porous flows, multiple components, or multiple phases, such as gases and liquids, and transitions among them are commonly present, and this presents challenges to their simulations. In these situations, non-Poisson equations may have to be solved [108,143]. A method is proposed to transform a multiphase problem into an interface problem and then solve the latter using an inexact Newton-GMRES method or a full approximation scheme multigrid V-cycle with Newton-GMRES smoothing [389]. In order to deal with multiple scales in flows, a DD framework is proposed on the basis of an observation that a multiscale finite-volume method is actually a special case of a non-overlapping DD preconditioner [256]. A multiscale finite element method together with several adaptive strategies for both fluid flow and concentration transport is presented to capture the instability of density driven flows [197]. A toolbox utilizing OpenFoam is used for the simulation of flows within porous media, and its capability and parallel computational efficiency are verified in [152].

Other non-standard decomposition methods have also been used for porous media flows. In order to achieve high-fidelity simulations, direct modeling is used for flows within a porous media represented as an array of cylinders or spheres of different sizes, and the flows are treated as Stokes flows and the configuration of flow boundaries are resolved [219,239]. In such efforts, the flow domains are partitioned into many subdomains, and solutions within individual subdomains are obtained, for instance, by a boundary integral method and then with a multiplicative Schwarz approach. Traditionally, the nonlinear algebraic systems resulting from discretization are first linearized, and DD preconditioners are then applied to the linear systems derived from this linearization and thus they do not take nonlinearity of the original problems into account. Unlike the traditional approach, a DD algorithm based on an additive Schwarz preconditioned inexact Newton’s method is directly applied to nonlinear algebraic systems. It is shown that the proposed algorithm can be significantly faster than the standard DD approaches [54,324]. A finite difference method to solve the Biot’s equations is presented, and its DD-based, parallel computation is used to simulate wave propagation within a poro-elastic media [374]. While exploring space-time DD for the advection and diffusion of concentration in porous media, optimized Schwarz waveform relaxation based on Robin transmission conditions is studied and illustrated with numerical examples [151]. A space-time DDM is extended from a so-called enhanced velocity mixed finite element for DD in space to compute incompressible and compressible subsurface flows [318].

5.2 Surface geophysical flow

Surface geophysical flows are present in rivers, lakes, oceans, and the atmosphere. A simplification for such a flow is a potential flow described by the Laplace equation [76]. Frequently, more complicated equations, typically the shallow water equations (SWEs) or the geophysical fluid dynamics equations, are used for practical problems [280,335]. In the SWEs, a flow is fully mixed and has zero velocity in the vertical direction. Since the SWEs comprise a hyperbolic system of conservation laws, to which the governing equations of compressible flows also belong, techniques for the discretization and the DDMs used in compressible flows may also be applicable. In the geophysical fluid dynamics equations, a weak flow motion is permitted in the vertical direction, but in general the hydrostatic assumption is used. With such an assumption, the momentum equation in the vertical direction is simplified as the balance of gravity and pressure, and typically, the discretization of the equations includes an internal and an external mode [65]. It should be noted that full Navier-Stokes equations are also applied occasionally for geophysical
flows, however, due to the computational expense, such applications are frequently restricted to problems at relatively small scales [341, 257].

In computation of SWEs, a finite element method in space and an implicit scheme in time are proposed, and the Schur complement matrix is derived and a modified interface matrix approach is presented to deal with the coupling between subdomains in [250]. An additive Schwarz preconditioning technique for a Poisson equation in the discretization of the SWEs is used in simulation of a coastal flow [261]. A discussion is provided on the partitioning of a flow domain and its relation to the arrangement of the resulting algebraic system [59]. Since they are a hyperbolic system of conservation laws, often the SWEs are solved by explicit schemes, and, when marching from a current time step to the next one, the computation in each subdomain is completely independent of the computation in the other subdomains and hence can be carried out in parallel.

As a result, no iteration is needed in applying a Schwarz method. With such an approach, the SWEs are solved using the MacCormack scheme and the communication of solutions at the internal boundaries of patched subdomains is realized by MPI [288]. By assigning computation in individual subdomains to different processors and using an explicit Runge-Kutta method for the temporal discretization, it is shown that the computation scales well for discontinuous Galerkin and spectral element methods [209]. SWEs are solved by an explicit finite volume method based on an approximate Riemann solver and a TVD technique, which are popular in the computation of compressible flows, and a Schwarz method is used as a solver for parallelization [86]. In order to solve the viscous SWEs with a small Coriolis force, Schwarz waveform relaxation algorithms using Dirichlet-type transmission conditions on the boundaries of overlapping subdomains and also an absorbing boundary condition as the transmission conditions for non-overlapping subdomains are proposed and analyzed [234]. Moreover, a popular coastal ocean model ADCIRC is developed to simulate storm surges on the basis of a finite element method, and both strong and weak stability are achieved for a certain range of problem sizes [335]. In an effort to simulate atmospheric and oceanic flows, a DD spectral method has been developed to solve the SWEs [357]. A lattice Boltzmann scheme in association with a multiblock method is presented to solve solute transport in shallow water flows [222]. SWEs are discretized using explicit schemes and then solved on subdomains with adaptive mesh refinement and an efficient GPU implementation [302]. In conjunction with a Godunov-type scheme, DD techniques are used to split flow domains in computation of flooding [305].

A number of efforts have been made on DD computation of the geophysical fluid dynamics equations and the Navier-Stokes equations, which permit weak vertical motions of flows that the SWEs do not. In order to enhance resolution and better capture local flows in the numerical prediction of global weather, a method known as the “conformal octagon” is presented, which arranges grids in a way so that resolution gradually improves around the zone of interest and parallel computation becomes natural [279]. Partitioning of grids for parallel computation with space-filling curves (Hilbert, Peano, and nested Hilbert m-Peano space-filling curves) is investigated, and numerical tests on atmosphere flows shows that, in comparison with the commonly used partitioning tool METIS, such partitioning achieves a substantial increase in the sustained floating point execution rate [87]. A mesh generator called amatos is developed to facilitate mesh-adaptive simulation of atmospheric and oceanic flows. It partitions grids adaptively with OpenMP parallelization and guarantees optimal load balancing and good data locality by construction and results in rather short interface length [24]. An investigation is made for the solutions of the SWEs on so-called “Yin-Yang” grids on a sphere, i.e., two geometrically identical grids overlapping each other, and it is shown that optimized Schwarz methods associated with specific Robin or higher order transmission conditions lead to faster convergence for certain elliptic problems in [280]. A parallel DD algorithm based on integral linear programming is proposed for a coastal ocean model called sECOM, and its division of a global domain into
subdomains leads to balanced loads in individual processors so that the overall computational time will be reduced [173]. DD techniques for parallel computation are used to generate meshes and solve the full Navier-Stokes equations for the simulation of wind fields, and good scaling is achieved for $10^4$ processors [257].

5.3 Heat transfer and mass transport

Heat transfer and mass transport, frequently combined with other processes such as chemical reaction and phase transition, happen in various flows, both compressible and incompressible. DD simulation of these flows began with relatively simple situations, such as a steady flow in a step channel Since the early 1990s [308], and it has now matured and the simulations are able to deal with complicated, real world problems such as physical and chemical phenomena in nuclear reactors [380]. For flows with heat transfer and mass transport, in addition to the governing equations for pure fluid flows (the continuity and momentum equations), additional governing equations such as those for temperature and concentration, mostly parabolic PDEs, have to be included. These additional equations are coupled with the governing equations, and this complicates the DD analysis and computation. Therefore, many techniques for pure fluid flows, such as those discussed in above sections, may not be generally applicable to flows with heat transfer and mass transport, further extension and development is necessary.

Over the past twenty years, a number of investigations have been made on development of DD methods for flows associated with heat transfer and mass transport. For instance, an iterative solution strategy based on an inexact Newton method with a preconditioned Krylov solver is proposed for computation of a finite element method applied to flows with nonequilibrium chemical reactions, and the numerical results are encouraging with regard to computational efficiency and robustness [311]. A DD meshless method is presented for incompressible flows and conjugate heat transfer, and a flow domain is divided into subdomains in such a way that the condition numbers of the algebraic systems resulting from discretization are effectively reduced [94]. Operator decomposition is investigated for conjugate heat transfer problems [107]. In a multiblock computation of a turbulent flow with heat transfer for a power station boiler, interestingly it is shown that the parallel efficiency increases if the mean temperature and density are calculated a priori and stored, with a speedup of six on eight processors [74]. Governing equations for flows with soot formations are discretized using an implicit finite volume method, and the resulting nonlinear algebraic system is solved with the aid of GMRES [64]. A continuum-fluid model is applied across the domain of a entire-rarefied gas flow with heat transfer, and it is coupled with and corrected by a direct simulation Monte Carlo model in micro regions [95]. More recently, a two-level, space-time DD method is presented for a control problem involving flows with heat transfer, and its parallel scalability and efficiency are demonstrated by numerical examples [386].

DDMs have been applied to simulate various problems involving thermal transfer and mass transport. Multiblock grids are used to simulate conjugate heat transfer problems such as flows by an array of heated cylinders [371,167]. Incompressible turbulence flow and heat transfer within a rotating pipe bend are simulated using a finite-analytic numerical method on Chimera grids enhanced by a mass conservation algorithm at grid interfaces [66]. Continuum-atomistic schemes are used for heat transfer in various micro- and nano-flows [223,244]. In the simulation of heat transfer in a flow near a rough wall, the flow domain is split into two zones, one for the large-scale outer flow, and the other for the small-scale flow next to the wall [166,?]. A free-surface flow domain is split into several subdomains in the vertical direction, and simulation of sediment transport at bottom of a channel induced by a solitary wave is presented [189]. Parallel computation based on DD is made for mass transfer of soluble surfactants in 3D multiphase
flows [247]. A software package named CTF built on DD techniques is used to simulate flow and heat transfer within light water reactors [304]. GMRES is used to solve the algebraic system resulting from a finite element discretization in the simulation of high Reynolds number flows in pressurized water reactors [312]. DD techniques using MPI for parallel computation is used in the software GASFLOW, which is designed for simulation of fluid dynamics with heat transfer, chemical kinetics, aerosol transportation, and other related phenomena in postulated accidents in nuclear reactor containment [380].

5.4 Multiphase flow

Multiphase flows are complicated in that they contain two or more phases interacting with each other. A commonly encountered category of multiple phase flows involve gas/vapour, water, and solid particles [330]. A category of these flows are flows containing different fluids. These are described by mixture models based on governing equations for viscous or inviscous, compressible and/or incompressible flows, plus some auxiliary relations to reflect the effects from individual phases [6]. In such a model, the density consists of percentages from the individual phases and becomes an unknown. DD approaches for compressible and incompressible flows of pure fluids in Sec. 3 and 4 may be applicable or extendable to this situation. Another category of multiphase flows are particle laden flows, and a model is needed to directly resolve and track the particles [303]. With this model, computational loads increase with the number of particles, and it becomes necessary to resort to DD techniques when the number of particles is substantially large [171].

DD is now becoming a common approach in the simulation of multiphase flows using mixture models. In the computation of a steady flow of a gaseous mixture in a boiler using the standard $k-\varepsilon$ model, the flow domain is divided into subdomains that are assigned to different processors [74]. A flow domain is split in the simulation of boiling water in nuclear power generation [25]. Multiblock, structured meshes, are used in simulation of cavitating flows that are represented as a mixture of gas, vapor, and liquid [196]. In another computation of cavitating flows on unstructured grids, implicit schemes are used when marching in time, and a DD procedure is utilized in solving the discretized equations [6]. Again for cavitating flows, a DD procedure is designed to dynamically balance the computational loads among processors in the iteration to solve for the pressure and temperature when different sizes of cavitation regions are present [377]. Moving overset unstructured grids are used to capture cavitation generated by marine propulsors [5]. A wavelet adaptive multiresolution representation algorithm is developed for compressible flows with reaction among gases, and DD techniques are used for its parallelization [262]. An etching multiblock method is used to solve incompressible immiscible liquid-liquid flows [221]. An algorithm with a flow-domain split is presented for the GPU computation of chemical reaction flows [360]. Chimera grids are utilized in simulation of flows of air, vapor, and water around moving solid objects during water entry [254]. A method for partitioning unstructured grids is introduced for the simulation of liquid-vapor flows using a discontinuous Galerkin method and adaptive mesh refinement [91].

In recent years, an increasing number of efforts have been made to directly resolve particles and interaction among themselves and with fluids. For instance, each particle may be assigned a subdomain, and its interactions is restricted to those within a close distance and in the same subdomain and an error estimate (due to this restriction) is obtained [303]. A procedure to split unstructured grids into sub-grids is presented to directly resolve particles in flows [171]. Bubbles entrapped within water are also captured using DD techniques [75]. In order to handle a large number of particles, an existing unstructured-mesh serial software, which is able to deal with the interaction of individual particles, is extended to a parallel version with the aid of DD
techniques, plus the open source PETSc library for matrix operation and the ParMETIS for mesh partitioning [367]. In the simulation of dust particles within turbulence, a Particle Block Domain Decomposition (PBDD) is proposed, by which the numbers of dust particles are evenly distributed amongst computer processors [172]. A parallel solver based on DD techniques to track particles has been implemented into an open source code MFIX, which is widely used for simulation of bubbling and circulating fluidized beds, and good scalability is achieved with \( \sim 10^6 \) particles [129]. For the simulation of flows containing a large number of particles, as large as \( O(10^6) \), parallel computation based on DD techniques achieves good scalability with a moderate to large number of computer processors [354,264]. A procedure to implement a method called the Physalis method for simulation of particle-laden flows using parallel GPU computation is presented, and it is concluded that a speedup of up to 60 times as compared to an existing CPU version is possible [317]. Parallelization strategies for DD computation of time-dependent particulate flows are proposed and compared, and it is found that a so-called communication optimal strategy is more efficient in the case of homogeneously distributed particles [144].

5.5 Non-Newtonian flow

Flows of non-Newtonian fluids such as polymer, biofluid, mud, and sediment are widely encountered in engineering and nature. Typically the governing equations for the flows are similar to those for Stokes flows, and DDMs for such flows may be traced back to the study for elliptic problems [355]. The advection terms in the governing equations may be small and negligible as the fluids move slowly, however their constitutive equations and thus their diffusion terms are highly nonlinear, leading to a significant complication in simulation of their motion. In general non-Newtonian fluids’ viscosity is flow dependent (e.g., shear rate dependent), and moreover their behaviors may exhibit memory [36]. All of these place hurdles in the simulation of their motion, and many DD methods and preconditioning techniques that perform well for Newtonian flows do not work as intended for a non-Newtonian flow.

The partitioning of flow domains together with the adoption of Schwarz iterations are commonly applied to overcome difficulties of complex geometry and to better capture physics in non-Newtonian flows. As a natural approach to overcome difficulties in dealing with irregular boundaries, DD has been applied with spectral methods, and early examples of such applications include simulations for a stick-slip problem of an Oldroyd-B fluid [259] and for the motion of an upper convected Maxwell fluid in porous media [327]. An adaptive DD spectral method in conjunction with a Schwarz iteration method is presented to better simulate microchannel flows in which the computational domain is partitioned into three zones: a high-shear zone next to wall, a low-shear or plug-like zone in the center, and a very thin layer in between. Adaptive mesh refinement is used to guarantee there are enough grid lines within the interfacial layer as the flow evolves in time [80,79]. A finite element method with distinct grid spacing in different subdomains is applied to simulate flows of alloy during its extrusion [385]. The flow field of a viscoelastic upper convected Maxwell fluid is split into subdomains, and then these subdomains are transformed into rectangular shapes on which a finite difference method simulation is carried out [285]. A moving-overset-grids method is employed to simulate motion of an air-bubble within a non-Newtonian fluid [111]. Chimera grids are applied to simulate flows of shear thinning blood within arteries [186]. A multiblock approach together with Casson, power-law, and Quemada models is used to simulate blood flows past a vascular convergent-divergent channel [252]. Parallel computation with MPI is made for viscoelastic channel flows represented by the Oldroyd-B model using staggered grids and a finite difference method [133].
As an effort to develop DD algorithms for computation of non-Newtonian flows, a boundary element method called the dual reciprocity method is presented, which adopts additional equations to ensure continuity of solutions at subdomain interfaces [112]. An investigation has been made on a finite element method to solve the linearized governing equations for an Oseen-viscoelastic flow problem, and it is shown both theoretically and numerically that the solution of DD computation converges to the single-domain solution [169]. A Lagrange multiplier is developed to couple solutions of finite element methods in subdomains at their interfaces [293]. A “pencil” decomposition method is designed for parallelization in the direct numerical simulation of a turbulent viscoelastic channel flow, and it shows that the resulting algorithm scales well up to 16000 cores [351]. A stabilized finite element method associated with a Newton-Krylov-Schwarz algorithm has been proposed, and robustness and fast convergence of the computation are achieved in the simulation of a rotational eccentric annular flow of a power-law fluid [316].

6 Multiscale and Multiphysics Flow

6.1 Multiscale flow

DDMs are now emerging as an approach to simulate multiscale flow phenomena, and, in general, such methods are divided into two categories. In the first category of the methods, the same flow solver is used in the entire flow field, and high resolution is employed for local, small-scale flow phenomena with high variation and complex structures. A method in this category (such as the adaptive mesh refinement (AMR) method [31]), is a multi-resolution approach. The second category of the methods apply distinct flow solvers, which have dissimilar governing equations and numerical methods in different regions of a flow field, providing a heterogeneous DD approach. A common example in this category is the use of a molecular dynamics method in one part of a flow domain, while a Navier-Stokes solver is used in the rest of the domain, see, for instance, [260].

In the past 10 years, numerous researchers have attempted to achieve multiscale simulations of various flows by re-using the same solver but with different resolution in parts of the computational domain (or in subdomains). For instance, in order to fully resolve a thermal effluent discharged from individual ports (at scales of $\mathcal{O}(10)$ cm in diameter) of a realistic diffuser in a natural river (at scales of $\mathcal{O}(1)$ km in width), four levels of overset grids are used in [341]. A smoothed particle hydrodynamics (SPH) method is presented for overlapping subdomains with different resolution [35], and a detailed discussion on multi-resolution simulation by SPH and other particle methods is available in [195]. Multi-resolution may also be built into a solver. An example is a multiscale finite element method together with a robust preconditioner constructed for high contrast permeabilities proposed to simulate flows in porous media [130]. For the same type of flow, a multiscale mortar DDM associated with a two-level preconditioner is presented [11]. An adaptive multiscale finite volume scheme is used to track fronts of pollutants in flows in porous media and resolve their instability [197]. For such a flow, a study concludes that a multiscale control volume method is actually a preconditioner for non-overlapping DD computation [256]. In order to simulate compressible gaseous flows, wavelet adaptive multi-resolution representation algorithms are developed, and then DD based techniques are used for their parallelization [262,251].

To achieve multiscale simulation with a hybrid of different solvers, the integration of conventional hydrodynamics and molecular dynamics began about two decades ago, e.g., [260], and it has now become popular in modeling flow problems. In this approach, flows in (usually) relatively small regions are simulated at the molecular level using methods such as a Monte Carlo method,
and those in the other regions are modeled at the continuum level and then approximated by methods such as finite differences. Examples in the literature include water flow, rarefied gas flow, and micro/nano flow [194, 182, 43]. A time-dependent DD algorithm, together with an indicator for domain partitioning, is developed for the multiscale simulation of flows by splitting a flow domain into a kinetic regime modelled by the full Boltzmann equation, an equilibrium regime simulated by the Euler equations, and a transition zone modelled with the BGK-ES equation [8]. Other examples of hybrid methods include the accurate simulation of multiscale flows containing turbulence and shocks. In [321, 203], the authors propose to switch between low-order schemes (e.g., 3rd-order and lower) and high-order schemes (e.g., 6th-order). A computational domain is partitioned into three patching subdomains, each of which is assigned with a solver for a flow at a particular scale, to simulate multiscale chemical vapor deposition [42]. A hybrid modeling system is proposed to simulate porous media flows from the scale of a pore to that of the continuum [238]. A multiscale universal interface method is proposed for coupling different solvers including a SPH solver and a dissipative particle dynamics solver [349].

NEWLY ADDED PARAGRAPH The coupling 1D, 2D, and 3D flows is also an active area of research, resulting in dimensionally heterogenous/multiscale simulations. A typical application of 1D-3D coupling is to deal with geometries consisting of a network of tubes, where a full 3D simulation would be too expensive. As an example, the broncho-pulmonary tree is made of 23 generations, resulting in more than 8 millions segments (ref??). In addition, such coupling naturally provides outflow conditions (the pressure) to 3D problems (ref??). In [245], a coupling method is applied to the respiratory system, where the upper part of the tree is fully resolved and the small airways are simulated with a 1D simulation. In [326], a 1D-3D approach is applied to cardiovascular hemodynamics. A 1D-3D coupling is applied to the solution of the arterial system, accounting for vessel deformations, where the two unknowns of the 1D model are the area of the vessels and the flow rate [113, 361]. In [370], it is proposed to solve a complex hydraulic system by applying the 3D Navier-Stokes equations to limited zones. Theoretical studies of algorithms coupling flows in different spatial dimensions can be found in [38, 208]. Aiming at reducing computational costs, dimensionally heterogeneous solvers have also been applied to simulation of ocean flows, and examples are high-fidelity simulation of small-scale flows next to structures [116, 188].

6.2 Multiphysics flow

Multiphysics flow problems occur in various fields, and DD style methods are a main avenue to achieve their reliable and efficient simulation. Frequently such multiphysics flows happen at distinct temporal and spatial scales, and conventionally they are separated and then simulated individually because they follow or are better represented by different PDEs. For instance, in the 2010 Gulf of Mexico oil spill, the spill gushed as a jet with initial mixing at $\mathcal{O}(10) \text{ m}$ length scales from a broken pipeline, and then it developed into a drift of floating oil on the water surface spreading horizontally at $\mathcal{O}(10^2) \text{ mile length scales}$ [231]. The oil jet and the oil drift have distinct physical behaviors and take place at vastly different scales, and hence in the past they are simulated separately by existing solvers. However, with a view that such different physical phenomena are coupled with each other in many situations (by ocean currents and waves during hurricanes, for example), their interaction has to be considered, since, if not impossible, separating and then simulating them individually induces considerable errors. As a result, there is an urgent need to simulate them together and simultaneously, and it has become a trend to couple different solvers to simulate multiphysics flows [183].
Some theoretical study has been completed on relevant fundamental issues, primarily on the basis of model/simplified problems. Since solvers for individual phenomena are based on different governing equations and numerical methods, in general, integration of these solvers leads to heterogeneous DD methods that are complicated and difficult to realize. An example is the development of a Newton-GMRES method to solve an interface problem resulting from discretization of a multiphase flow problem (gas, water, and oil) in porous media [389]. In the coupling of diffusion and transport zones, it is proposed to use a higher order of approximation at the interface of the two regions, and no iteration is needed between the two zones [128]. It is shown that when Stokes and Darcy equations are coupled with each other, unconditional stability is possible for a long-time computation [207]. It is argued that interface conditions may strongly affect the convergence of computation in the coupling of hydrostatic and non-hydrostatic equations for geophysical flows [39]. Since individual solvers contain uncertainties, it is important to analyze the propagation and interaction of such uncertainties, and, towards this goal, relevant methods are proposed and tested by numerical examples in [77, 10].

In view of the high nonlinearity and complexity involved in flow solvers, it is difficult to study their integration at the algebraic level, and the focus for multiphysics simulations has been on practical coupling of algorithms to ensure the integrated systems work as intended. Conservative schemes are formulated for coupling Stokes and Darcy equations on patched sub-regions [294, 176]. A parallel algorithm is presented for the computation of two equations representing surface and groundwater flows, which are connected with a Robin-Robin boundary condition and solved by finite element methods [170]. A DDM with Dirichlet-Robin iteration between subdomains is proposed to study gas-water flows in multiple layers of porous media [333]. It is proposed to couple the Stokes and Darcy equations by transforming a flow problem into an optimization problem associated with a Schur-complement system, in which the difference between velocity of the two equations at their interface is minimized [93]. In order to reduce computational expense, a high-fidelity solver based on the Navier-Stokes equations is used in a local flow region of interest, a low-fidelity solver based on a proper orthogonal decomposition is employed in the remainder of the computational domain, together with an error indicator to facilitate the division of the flow domains [33]. As another style of DD approach, high-resolution simulation of wave and crack phenomena in multi-media is achieved using solvers with different equations of state but with the same schemes in individual media, in conjunction with the Riemann resolution at the interfaces of the media [344, 281, 382].

The integration of different solvers has evolved into a popular means for the simulation of various actual multiphysics problems. Such efforts may be traced back to the integrated simulation of inviscous and viscous flows, such as a viscous boundary-layer and a potential flow over a 2D airfoil [299, 396]. Although research on such integration is still active, it has evolved into more complicated problems such as fully 3D flows [165, 76, 267, 393]. The integration of solvers now has a broader spectrum of application. Examples include coupling of the Navier-Stokes equations in the form of primitive variables and those in the vorticity form for the prediction of flows within unbounded domains [136]. The unsteady, compressible Navier-Stokes equations are applied around an airfoil, and linearized steady Euler equations are used away from the airfoil [73]. In order to better simulate flows in different regions, a lattice Boltzmann method and a vorticity-stream function method are coupled with each other [363]. A solver for the Euler equations and the incompressible Navier-Stokes equations are connected to study wind energy, with the former assigned as the meso-scale solver for atmosphere prediction and the latter employed as the micro-scale solver for flows around turbines [328].

An emerging area in the application of solver integration is to couple solvers for the Reynolds Averaged Navier-Stokes (RANS) equations and the LES. The coupling of RANS and LES solvers is presented as an option for saving grid points in the near wall region; the RANS equations are...
solved in the near wall region, and they are coupled to LES in the outer region [201]. A multi-code approach is considered to couple the RANS and LES domains, in which the boundary conditions are exchanged between codes using the MPI library [27]. In this work, pseudo velocity fluctuations are generated at the interface between the LES and the RANS domains. In [236], a one way coupling is presented to couple a RANS solver applied in the compressor and a LES solver in the combustor of a jet engine. An overlapping zonal method is presented to couple a local LES domain to RANS that are solved in the complete computational domain [235], and a review on such embedded LES methods is presented in [323]. In [366], in order to provide outflow boundary conditions to an LES simulation, a RANS solver is placed downstream of an LES domain and coupled to it. Coupling techniques can be applied as well to provide a wall-law type boundary condition to a LES solver by solving the RANS equations in a boundary layer, as presented in [277,57].

Another emerging area in the application of solver integration is simulation of geophysical flows – in rivers, lakes, oceans, and in the ground. Such flows present distinct physical phenomena in different regions, which are conventionally simulated by different solvers because of considerations of computational accuracy and efficiency. Now hybrid solvers have evolved into a common approach to simulate geophysical flows. An example is the integration of a 1D flow equation and the 2D Saint-Venant equations, both of which are discretized by a space-time finite element method [241]. To study wave propagation from offshore to shoreline, a two-way coupling is presented to integrate a 1D horizontal Boussinesq solver and a 2D vertical domain solver for the RANS equations [319]. In [339], a two-way 3D-2D coupling is achieved to couple the SWEs to a finite volume coastal ocean model. A solver for potential flows and a full Navier-Stokes solver, in conjunction with a level-set or a VOF method, are coupled to capture waves impinging structures [76, 267, 393]. Along a similar line, a circulation model and a full Navier-Stokes solver, which are the best available types of solvers in the ocean science community and the coastal engineering community, respectively, are integrated to simulate wave impact on a coastal bridge and a beachfront house [282]. A review of methods to couple hydrologic and hydrodynamic solvers for surface and subsurface flows can be found in [3].

The integration of solvers for fluid flows with those for phenomena in non-fluid media have also been conducted, and fluid-solid interaction (FSI) is a classic example [41]. The simulation of flow-induced vibrations and aeroelasticity is achieved by a parallel preconditioned CG method and the GMRES method [292]. Optimization design, using an electrostatic-fluid-structure system tested in an electrostatically actuated channel and an electrostatically actuated aeroelastic wing, is presented in [290]. With the aid of the Richardson iteration, the Navier-Stokes and Biot equations are solved jointly to study the interaction between fluids and poroelastic structures [18]. A monolithic balancing (non-overlapping) DD method for an acoustic fluid-structure interaction problem, which compares two types of Neumann-Neumann preconditioners and two different coarse problems, can be found in [242]. A fluid-solid system is used as a pulmonary model, and the resulting algebraic equations are solved via a standard block Gauss-Seidel iteration [364]. DDMs are used for parallel computation in the coupling of a Newtonian fluid and an elastic and compressible solid [358]. Conditions for the conservation of rigid body translation, total force across the interface, and virtual work acting on the fluid are studied [22,41].

Another commonly encountered example of fluid and non-fluid integration involves the coupling of hydrodynamics and electromagnetism. The performance of a fully coupled algebraic multilevel preconditioner is examined when applied to the Newton-Krylov solution of a flow-magnetism problems [215]. The numerical solution of the motion of a charged fluid in the presence of an electromagnetic field is studied in [82]. The nonlinear equations resulting from an implicit time stepping strategy are solved by approximate block factorization, and the interaction among
electromagnetism, hydrodynamics, and heat transfer in microchannels of integrated circuits is simulated in [226].

6.3 Model integration

In the past few decades, a number of computational models have been developed and thoroughly tested for specific flow phenomena at specific scales, and now it has become a trend to couple these models into single modeling frameworks to simulate complicated, comprehensive multiscale and multiphysics problems. Here, a model refers to as assembly of governing equations, computational methods, and their computer implementation. Such a model includes a complete I/O system and is a stand-alone software package. Currently, due to limitations in mathematical, numerical, and computational abilities, it is unrealistic to develop a single model that is able to resolve most multiscale, multiphysics phenomena in a complicated event, especially a real-world flow problem. Given the fact that numerical simulation has reached the point where mature models are available for individual phenomena over relatively narrow ranges of scales, integration of these models via DD style methods, which facilitate coupling different models to solve flows in different subdomains, is considered as the most promising approach to overcome difficulties and bridge the distinct scales inherent in multiscale and multiphysics modeling [97, 183].

There have been substantial efforts and successes in the integration of stand-alone models for the simulation of multiphysics flows. An interface code is made to couple ANSYS-FLUENT with a software package called Thermo-Calc to simulate reactions among gas, steel, slag in metallurgical processes [106]. A computer program is developed to couple COMSOL, a commercial multiphysics software, with PHREEQC, a package for a wide variety of aqueous geochemical calculations, to compute thermo-hydro-chemical problems in porous media [248]. TOUGH+ is a family of codes for multi-component, multiphase fluid flows in subsurfaces, and in recent years another two modules – RealGasH2O and RealGas with updated capabilities for gas flows and gas-water mixture flows – have been added to the family [246]. A review of the challenges included in the coupling of molecular dynamics (MD) and lattice Boltzmann (LB), and software design is discussed for integration of MarDyn (a model for massively parallel MD simulation) and Peano (a flow model equipped with a LB method at continuum level) [253]. A 2D lattice physics code HELIOS, a neutron kinetic code REMARK, and a thermal hydraulic system code THEATRe are coupled with each other to analyze safety of nuclear reactors in [184]. DYN3D (a neutron kinetic code) is linked with ANSYS-CFX (a commercial CFD code) to better simulate coolants in reactors [131]. Simulation of wind load on a floating offshore wind turbine is made using the STARCCM+ software for aerodynamics and hydrodynamics and the FAST code for structure behaviors of horizontal-axis wind turbines [356]. The software ROMS is widely used among the coastal ocean community to simulate currents, sediments, etc., and it has been coupled with a wave model called SWAN, which is another popular model among the community for the simulation of surface waves, via the Model-Coupling Toolkit [373]. ESMF (Earth System Modeling Framework) is a software framework for simulation of flows in the atmosphere and oceans [150]. It has been under development for years and various modules such as HEMCO (a stand-alone software component for computing emissions in global atmospheric models) have been connected to the framework [179].

As a particular example, in order to capture realistic local, particularly small-scale, coastal ocean flows, it is proposed to integrate SIFOM, a fully 3D fluid dynamics model, and FVCOM, a geophysical fluid dynamics model, with the former resolving small-scale phenomena and the latter simulating large-scale background ocean flows, permitting solution transition between the two models [345, 378, 342, 283]. Fig. 10 shows a sample simulation in which the background ocean
currents and thermal plumes are simultaneously simulated. The SIFOM-FVCOM integration is the first of its kind, it captures multiscale and multiphysics phenomena that are cannot be handled by conventional models.

Fig. 10: Simulation of thermal discharge from the bottom of the ocean, obtained with the SIFOM-FVCOM [342]. (a) Computational domain and bathymetry. (b) Grids. (c) Simulated instantaneous flow field and thermal plume. The red lines indicate the interface between SIFOM and FVCOM.

The idea of the integration of existing mature models into a single modeling system for multiphysics flows is conceptually straightforward, nevertheless, its realization is not trivial, requiring a great amount of effort. In general, DDMs for such integration are heterogeneous, involving the coupling of different solvers with distinct governing equations, dissimilar numerical algorithms, and unlike meshes. For instance, it has been shown that without discretion and careful design, problems such as non-physical artifacts may occur in the integrated SIFOM-FVCOM system used for the simulation shown in Fig. 10 [343]. As noted in [76], the greater the difference in the solvers, the more challenging such an integration becomes, both theoretically and practically. In addition, existing models for individual phenomena have thousands of lines of code with complicated data structures and I/O systems, and hence a non-invasive coupling is preferred. Such coupling efforts are long term; they require input from researchers in multiple institutions and nations and rely on long-term support from various research agencies (e.g., [138]).
6.4 Parallel computation in the integration of solvers and models

In the integration of different solvers and models to simulate multiphysics problems, an important issue is parallel computation of the overall integrated system, even though parallel computing may already be presented in the individual solvers. An example of such an effort is the simulation of transport of particles in a fluid solved by an asynchronous multi-code approach together with a dynamic load balance strategy at the shared memory level to enhance the computational efficiency: different partitions are used for the particle and fluid solvers, and the coupling between the solvers is carried out by MPI [161]. As mentioned previously, in general different solvers/models use distinct numerical methods, computational patterns, memory and CPU time requirements, etc. In order to fully exploit the computational resources of parallel supercomputers, it is therefore necessary to account for this heterogeneity.

When coupling different solvers/models designed for different physical phenomena, two main coupling approaches are possible (see an exhaustive review in [183]). The first approach is the monolithic approach that generates a single matrix for the complete coupled problem, including the transmission conditions at the interfaces. Frequently this is an intrusive coupling [121,202,198,306]. The other is a non-intrusive, partitioned or staggered approach, in which the physics is solved separately, and transmission conditions are exchanged between the different computational domains using a parallel or sequential Schwarz iteration [284,350,199,137]. This approach allows the use of pre-existing solvers for each physics and is the one generally preferred in parallel computing.

Once transmission conditions (e.g., Dirichlet-Neumann, Dirichlet-Robin, and Robin-Robin) and interface acceleration algorithms have been selected, there remain basically two alternatives to achieve the coupling: the Block Jacobi method and the Block Gauss-Seidel method, which correspond to parallel and sequential Schwarz methods, respectively [284,85,307]. Here, each block represents a specific type of physics. In the first case, the two types of physics are solved concurrently and the transmission conditions are exchanged once each type of physics has been solved. In [237], a Jacobi method is presented together with a Quasi-Newton method to accelerate the convergence of fluid-structure interaction simulation. However, Gauss-Seidel coupling is generally preferred for its better convergence. In this case, the physics are solved one after the other, the exchange of transmission conditions taking place at the end of each simulation [183].

We comment that the choice between coupling methods cannot be solely based on a convergence criterion in a high performance computing context [394]. Although having better convergence, the block Gauss-Seidel method has poor computational efficiency, as the reserved resources for one type of the physics are not being used (CPUs are idle) while the other is being solved. There are runtime techniques to reduce the idle time, and therefore to increase the computational efficiency. One example is given in [160] in which a dynamic load balance is introduced to couple a fluid and Lagrangian particle transport codes in [56] to solve fluid-structure interaction problems.

There exist several generic and open source codes that are examples of model integration with parallel computation, mainly based on MPI. In general, the libraries do not only provide the variable exchange subroutines but accelerate algorithms and provide robustness in the coupling (Quasi-Newton [237], Aitken’s relaxation [88], etc.). Particular examples include PRECICE (Precise Code Interaction Coupling Environment) [46], OpenPalm (Projet dAssimilation par Logiciel Multi-méthodes) [45,275], CWIPI (Coupling With Interpolation Parallel Interface) that is a part of OpenPalm [291,104], and MUI (Multiscale Universal Interface) [349].
7 Achievements, Challenges, and Outlook

In the past few decades, DD style methods have been very successful in the computation of various fluid flow problems. Such successes result from theoretical progress, advances in computer capacity, and the needs in science and engineering applications. However, challenges remain and there are increasing demands for better model fidelity and new capabilities for simulation of many emerging realistic multiscale and multiphysics problems. The following are potentially some of the future topics of increased focus to address these challenges and needs.

**Nonlinear DD methods** Research on DDMs at the algebraic level has focused primarily on linear problems, and these techniques may not perform well in computation of many problems that are strongly nonlinear. As discussed in Sec. 6.1, an additive Schwarz preconditioned inexact Newton’s method, a nonlinear DDM, can be much more efficient than standard DDMs. It is anticipated that nonlinear DDMs will be a focus for future research.

**Space-time DDM** Methods which allow parallelism in both space and time require further development to allow application to flow problems of practical interest. Current studies in this regard have mainly been restricted to model problems. In the computation of unsteady flows using implicit schemes, given that a substantial amount of computational time is needed to solve nonlinear algebraic systems when marching from a current to a next time step, a successful DDM in time, together with parallel computers, will substantially reduce the total amount of time of the computation.

**Interface algorithms** As indicated by the analysis and the computation of realistic problems, the algorithms employed at the interfaces between subdomains and solvers are crucial – not only to obtain the correct solutions but also for efficient DD computation by improving the convergence rate. Interface conditions and their discretizations have been studied intensively for model problems, compressible flows, and incompressible flows, all of which have the same PDEs in all the subdomains. There has been relatively less study in situations with different PDEs in the subdomains. In this situation, Dirichlet transmission conditions are commonly employed when coupling the different software packages. It is unclear how good these transmission conditions are. This requires a systematic investigation, and will likely result in the development of better approaches.

**Methods for multiscale and multiphysics flows** Many new multiscale and multiphysics flow problems are emerging, and there is an urgent need to simulate them with high-fidelity and to a desired accuracy. To address this need, multi-resolution methods are being developed by coupling different flow solvers and integrate different stand-alone software packages. This leads to complicated heterogeneous DD methods, and it is important to assess (and improve) the convergence rate and achievable accuracy of such approaches, especially when applied to realistic flow problems.

In view of their tremendous past success and the need to simulate unresolved existing and emerging flow problems, it is anticipated that DDMs will exert a great influence in these areas in the years to come.

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8 Compliance with Ethical Standards

This article does not contain any studies with human participants or animals performed by any of the authors. For this type of study formal consent is not required. The authors declare that they have no conflict of interest.

References


