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Solving Partial Differential Equations on Overlapping Grids

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Abstract. We discuss the solution of partial differential equations on overlapping grids. This is a powerful technique for efficiently solving problems in complex, possibly moving, geometry. An overlapping grid consists of a set of structured grids that overlap and cover the computational domain. By allowing the grids to overlap, grids for complex geometries can be more easily constructed. The overlapping grid approach can also be used to remove coordinate singularities by, for example, covering a sphere with two or more patches. We describe the application of the overlapping grid approach to a variety of different problems. These include the solution of incompressible fluid flows with moving geometry, the solution of high-speed compressible reactive flow with moving rigid bodies using adaptive mesh refinement, and the solution of the time-domain Maxwell's equations of electromagnetism.

1. Introduction

We give an overview of our work on overlapping grids and describe its application to the solution of a variety of partial differential equations (PDEs). Our intent is to provide a flavour of the types of problems that the technique has been applied to and provide some details on the discrete approximations used. Our approach is based on the use composite overlapping grids to represent the problem domain as a collection of structured curvilinear grids. This method, as discussed in Chesshire and Henshaw (1990), allows complex domains to be represented with smooth grids that can be aligned with the boundaries. The use of smooth grids is particularly important for obtaining accurate approximations to PDEs and boundary conditions. The majority of an overlapping grid often consists of Cartesian grid cells so that the speed and low memory usage inherent with such grids is retained. Overlapping grids, also known as Chimera or overset grids have been used successfully for the numerical solution of a wide variety of problems, see for example, Meakin (1999); Henshaw and Schwendeman (2008), and the references therein.

Solving partial differential equations on overlapping grids with moving geometry and adaptive mesh refinement (AMR) involves considerable programming complexity due to the multiple grids and the curvilinear geometries. In addition, there is a need for specialized component grid generation and overlapping grid generation algorithms. We have developed a freely available software framework called Overture that provides support for the solution of PDEs on overlapping grids. We have also developed a set of composite grid solvers that

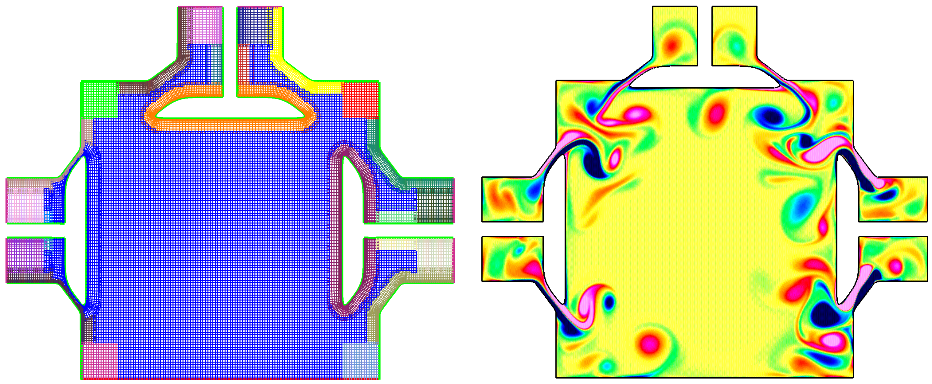

Figure 1. Left: an overlapping grid for three moving valves. Right: contours of the vorticity at some instant in time computed from the solution to the incompressible Navier-Stokes equations. The valves move at each time step according to a specified motion.

are available with the CG software[1]. These include solvers for incompressible and compressible fluid flow as well as Maxwell's equations, as described further in subsequent sections.

2. Incompressible Flows

We solve the incompressible Navier-Stokes (INS) equations with a pressure-velocity formulation and a split-step method where the pressure is solved as a separate step. For a given domain Ω, with boundary $\partial\Omega$, the equations are given by

$$\begin{aligned} \mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \nu\Delta\mathbf{u} - \mathbf{f} &= 0, \qquad t>0, \quad \mathbf{x}\in\Omega \\ \Delta p + \nabla\mathbf{u} : \nabla\mathbf{u} - \alpha\nabla\cdot\mathbf{u} - \nabla\cdot\mathbf{f} &= 0, \qquad t>0, \quad \mathbf{x}\in\Omega \end{aligned}$$

with some appropriate initial and boundary conditions,

$$\begin{aligned} \mathbf{u}(\mathbf{x},0) &= \mathbf{u}_I(\mathbf{x}), \qquad t=0, \quad \mathbf{x}\in\Omega, \\ \mathcal{B}^F(\mathbf{u},p) &= 0, \qquad t>0, \quad \mathbf{x}\in\partial\Omega\ . \end{aligned}$$

Here $\mathbf{u} = \mathbf{u}(\mathbf{x},t)$ is the velocity, p the pressure and ν the kinematic viscosity. The term $\alpha\nabla\cdot\mathbf{u}$ in the pressure equation is important to add to the discrete approximation as it acts as a damping term on the divergence of the velocity. A second-order accurate and fourth-order accurate scheme have been developed to solve these equations on overlapping grids, see Henshaw (1994); Henshaw *et al.* (1994); Henshaw and Petersson (2003) for more details. There has been some controversy as to the appropriate boundary conditions to use for the pressure at no-slip walls. For a no-slip wall we use the following physical boundary

[1]Overture and CG are available at www.llnl.gov/casc/Overture

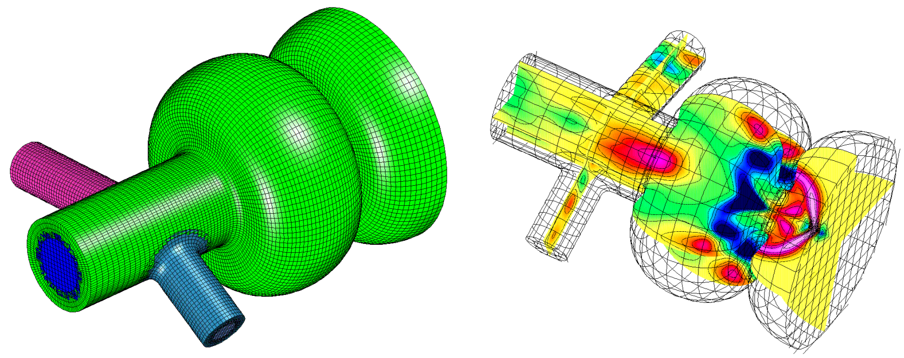

Figure 2. An overlapping grid for the end section of an accelerator cavity and the computed solution (E_z) for a moving source charge.

conditions (i.e. conditions required by the continuous equations to define a well-posed problem),

$$\mathbf{u} = 0, \quad \nabla \cdot \mathbf{u} = 0, \quad \mathbf{x} \in \partial\Omega,$$

as well as the numerical boundary conditions (i.e. conditions required by the discrete scheme to define an accurate and stable approximation),

$$\begin{aligned} &p_n = -\mathbf{n} \cdot (\nu \nabla \times \nabla \times \mathbf{u} + \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u}), \\ &\text{extrapolate } \mathbf{t}_m \cdot \mathbf{u}, \end{aligned}$$

where $\mathbf{n}$ is the outward-normal and $\mathbf{t}_m$, $m = 1, 2$ are linearly independent tangent vectors at the boundary. See Petersson (2001); Henshaw and Petersson (2003) for a discussion of this boundary condition and the benefits gained from using the curl-curl operator $\nabla \times \nabla \times \mathbf{u}$, instead of $\Delta \mathbf{u}$, for implicit time-stepping.

The INS equations can be solved on domains with moving boundaries. Figure 1 shows the overlapping grid and solution from a moving valve computation. At each time-step the component grids associated with the valves are moved and the interpolation points are re-computed. The equations on each grid are solved in the moving coordinate frame associated with the grid. As the grids move there will be some hidden, unused grid-points that become exposed and active. Values for these exposed points are interpolated from other valid values as discussed in Henshaw and Schwendeman (2006).

3. Electromagnetics

The overlapping grid approach has been applied to the solution of Maxwell's equations. We solve the time-domain equations in second-order form,

$$\begin{aligned} \epsilon\mu \; \partial_t^2 \mathbf{E} &= \Delta \mathbf{E} + \nabla\Big(\nabla \ln \epsilon \;\cdot \mathbf{E}\Big) + \nabla \ln \mu \times \Big(\nabla \times \mathbf{E}\Big) - \nabla(\frac{1}{\epsilon}\rho) - \mu \partial_t \mathbf{J}, \\ \epsilon\mu \; \partial_t^2 \mathbf{H} &= \Delta \mathbf{H} + \nabla\Big(\nabla \ln \mu \;\cdot \mathbf{H}\Big) + \nabla \ln \epsilon \times \Big(\nabla \times \mathbf{H}\Big) + \epsilon \nabla \times (\frac{1}{\epsilon}\mathbf{J}). \end{aligned}$$

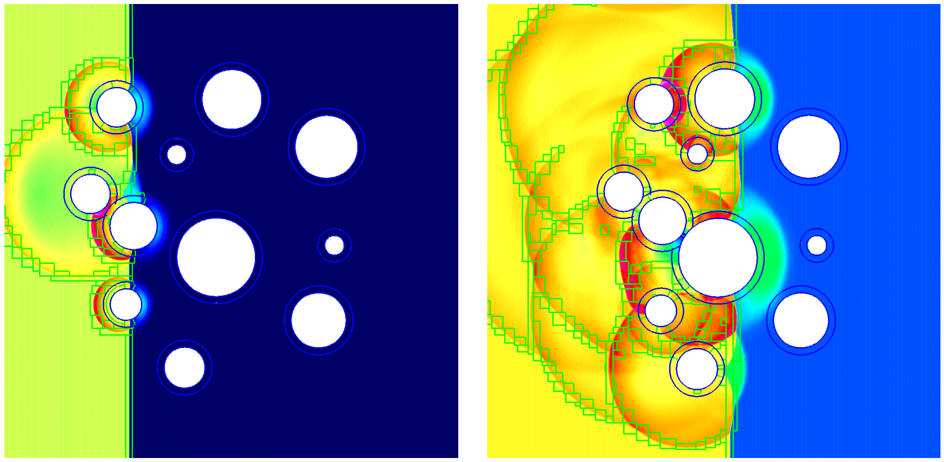

Figure 3. A shock hitting a collection of moving cylinders. Contours of the density are shown along with the boundaries of the base grids (in blue) and the AMR grids (in green). The annular grids around each cylinder can move at each time step. The AMR grids are recomputed every few time steps based on a estimate of the error.

A fully fourth-order accurate in space and time approximation has been developed, Henshaw (2006). The advantage of using the second-order form is that there is no need to use a staggered grid. In addition, in many cases only the **E** field need be solved for. The spatial approximation uses efficient high-order accurate finite-difference approximations on Cartesian grids and some newly devised high-order accurate symmetric finite-volume approximations for curvilinear grids. The *modified-equation* time-stepping method is used which provides fourth-order accuracy in time while using only three levels in time. In addition, unlike most higher-order time-stepping approaches which require a smaller time-step for stability as the order increases, the time step for the modified-equation scheme does not decrease as the order increases. A key component of the discrete scheme for Maxwell's equations was the development of accurate and stable approximations for boundary conditions and material interfaces. We use high-order *centered* approximations at boundaries and interfaces that are derived from the governing equations.

Figure 2 shows results from a computation of a charge source moving through a section of an accelerator cavity. The overlapping grid for this geometry was constructed with the aid of the geometry, CAD, and grid generation capabilities in Overture.

4. Compressible Flows and Adaptive Mesh Refinement

We have developed capabilities to solve the compressible Navier-Stokes equations and reactive-Euler equations on overlapping grids. The later equations are given by

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x_1}\mathbf{F}_1(\mathbf{u}) + \frac{\partial}{\partial x_2}\mathbf{F}_2(\mathbf{u}) + \frac{\partial}{\partial x_3}\mathbf{F}_3(\mathbf{u}) = \mathbf{H}(\mathbf{u}),$$

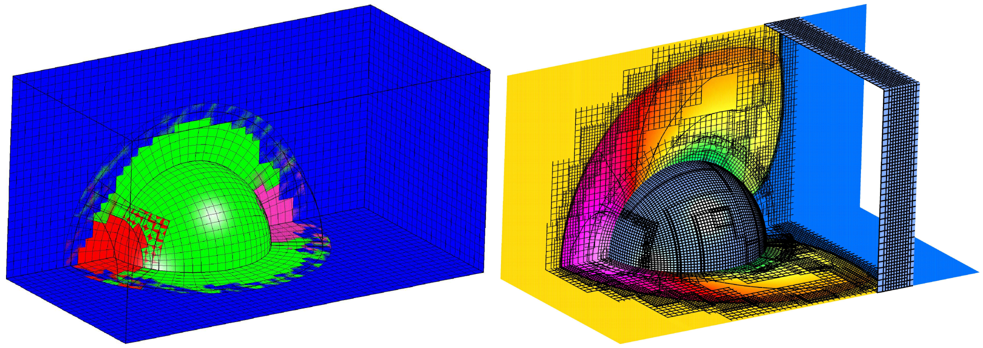

Figure 4. Left: the overlapping grid for the quarter-sphere problem consists of four component grids. Orthographic patches are used at the poles of the sphere to remove the coordinate singularities. Right: contours of the density along with the adaptive mesh refinement grids. An incident shock moving from left to right has diffracted around most of the sphere. A reflected shock is also shown. The grid shown is coarsened by a factor of 4.

where

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho\mathbf{v} \\ E \\ \rho\mathbf{Y} \end{bmatrix}, \qquad \mathbf{F}_n = \begin{bmatrix} \rho v_n \\ \rho v_n \mathbf{v} + p\mathbf{e}_n \\ v_n(E+p) \\ \rho v_n \mathbf{Y} \end{bmatrix}, \qquad \mathbf{H} = \begin{bmatrix} 0 \\ \mathbf{0} \\ 0 \\ \rho\mathbf{R} \end{bmatrix}.$$

Here ρ is density, $\mathbf{v} = (v_1, v_2, v_3)$ is velocity, p is pressure, E the total energy and $\mathbf{Y}$ the species mass fractions. These equations are discretized with a higher-order accurate extension of Godunov's method as described in Henshaw and Schwendeman (2003). Adaptive mesh refinement (AMR) is used to add resolution near sharp features. The approach has been applied to the solution of problems with moving geometry and the motion of rigid bodies as discussed in Henshaw and Schwendeman (2006), as well as multi-material flows, Banks *et al.* (2007) and detonations, Banks *et al.* (2008). Figure 3 shows results from a computation of a shock hitting a collection of rigid cylinders. The figure shows the density of the gas along with the boundaries of the grids at two different times. Each cylinder is evolved by solving the Newton-Euler equations for rigid-body motion with the pressure from the fluid providing the force on the boundaries. An annular grid surrounds each cylinder and this annular grid can move at each time step. The AMR grids are also shown in the figure. AMR grids are constructed in the parameter space of each annular grid as well as on the Cartesian background grid. The locations of the AMR grids are recomputed every few time steps based on an estimate of the error.

The solution approach for compressible flows has been extended to three-dimensions and parallel, see Henshaw and Schwendeman (2008). Figure 4 shows results from a parallel AMR computation of a shock diffracting from a quarter-sphere. The overlapping base grids and refinement grids are also shown. Notice that by using overlapping grids, there are no small cells near the poles of the sphere. On parallel distributed memory computers, each grid (base grid or AMR grid) can be distributed over one or more processors. A modified bin-packing algorithm is used to load-balance and distribute the grids over the processors. The approach was carefully validated using the method of analytic solutions and by estimating the L_1- and L_2-norm self-convergence rates by solving a given problem on a sequence of increasingly finer grids.

5. Conclusions

We have given a brief overview of our work on solving PDEs on overlapping grids. We have shown some of the advantages of this approach for the solution of problems with complex geometry and for problems with moving boundaries. Smooth boundary fitted curvilinear grids and Cartesian background grids enable accurate and efficient finite-difference and finite volume approximations. We have described the solution of the incompressible Navier-Stokes equations using a pressure-velocity formulation. An example solving an incompressible flow problem with moving valves was shown. The overlapping grid approach has also been applied to the solution of Maxwell's equations. We solve the time-domain equations in second-order form using an efficient fourth-order accurate method. We use some new high-order accurate and symmetric finite-volume approximations as well as high-order accurate centered approximations at boundaries and material interfaces. We have solved high-speed reactive flow problems using adaptive mesh refinement and moving grids. A high-order accurate extension of Godunov's method is used to discretize the reactive Euler equations. An example of a shock hitting a collection of rigid moving cylinders was shown. The AMR approach runs in parallel on distributed memory computers.

In extensions of this work we are developing new approaches for treating multi-domain, multi-physics applications, such as conjugate-heat-transfer and fluid-structure problems, where different PDEs are solved in different domains.

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