Computational Fluid Dynamics and Combustion Dynamics

Progress Report

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Marsha J. Berger
Courant Institute

This is a summary of the research at the Courant Institute, which is part of the HPCC Grand Challenge Project on Computational Fluid Dynamics and Combustion Dynamics. Our research efforts this year concentrated on two fronts: (1) automatic geometry definition for Cartesian grid calculations in 3D, including a CAD interface, and (2) development of a parallel compressible adaptive AMR in a data parallel environment also in 3D. We are also still working on investigating conservative interface conditions for overlapping meshes.

Geometry Representation It is well known the grid generation part of solving a problem can take an order of magnitude more time than the flow simulation itself. We have been developing an approach for representing realistic engineering geometries using a Cartesian mesh representation of the boundary. Part of the benefit of Cartesian grids is the simplicity of the grid generation. We have developed an automatic Cartesian grid generator about arbitrary geometries that uses both conventional and CAD/CAM surface geometry descriptions. This is work with my PhD student John Melton, who is also an employee at NASA Ames Research Center. Using algorithms from computational geometry, and aided by a package of routines called DTNURBS (from the David Taylor Research Laboratory), the geometry quantities that describe the intersection of a Cartesian cell with a multi-faceted object can be computed [1]. We are in the process of generalizing the procedure to handle component based geometry definition. This does away with the "natural" NURBS criteria (where the NURB surfaces must meet along a common intersection curve), and is the more common way a CAD system is maintained. As an example of the tremendous utility of this approach we have been able to compute the flow around a C17 configuration with wing, fuselage, engines and pylons from start to finish within a day. Our Cartesian grid approach will enable rapid prototyping of engineering design options, for example, locations of splitter plates, etc. in a fluid flow, which are simply not possible if the grid generation process is not automated.

Several aspects of this work are still under development. Foremost, we need to further develop the flow solver, in particular, develop the algorithms for use at the non-body-fitted cells that intersect the body geometry. We are investigating several algorithms, and conducting convergence studies to determine their accuracy on irregular grids. Second, we are still developing criteria on which to base the geometric refinement used in describing an object itself. Our rules so far are based on curvature; we need to do more testing to see if that is sufficient or something else is needed to supplement it.

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A related project to this one is the development of a numerical method for compressible flow which will have improved multigrid performance. It is well-known that multigrid for hyperbolic problems exhibits convergence rates well below the level for elliptic problems. Unfortunately, it has previously been shown (by Spekrijse) that Gauss-Seidel sweeps on second order limited schemes is unstable (in the scalar two dimensional case). For steady state calculations in the compressible case, a postdoc (David Sidilkover) has developed a numerical scheme which is stable with Gauss Seidel, is second order at steady state. To accomplish this requires the development of a so-called truly multidimensional finite volume scheme. However, unlike previous efforts along these lines he does not try to represent the physics of the flow by a finite number of simple waves each with an associated advection equation (the wave modelling approach) [2]. He is investigating the performance of this new scheme with multigrid. One of the terms in the new scheme looks very much like a divergence equation (even in the compressible case), suggesting a very interesting connection between the compressible and incompressible cases that are also under investigation.

For more complicated geometries where a more accurate representation of solid boundaries is required, an alternative to the use of Cartesian grids is overlapping composite grids. One of the difficulties with this approach is deriving conservative interface conditions for use at the overlapping mesh boundaries. We are developing algorithms for this problem and trying to determine their stability region and overall behavior.

Parallel Algorithms Since there is still a lot of uncertainty in parallel architectures, as part of this HPCC project we are investigating the performance of several different types of parallel computers, including shared memory and distributed memory in both MIMD and SIMD mode. We are also investigating the use of parallel programming tools for these kinds of applications, since the software development effort is still prohibitive.

One type of architecture we are investigating in particular is the CM-5, which supports a data parallel programming model. We have developed a three-dimensional implementation of adaptive mesh refinement for hyperbolic systems of equations. We have previously developed a 2D AMR implementation for the CM-2 [3,4]. Although the CM-5 architecture took a bit of a different turn much of the work remained useful in the extension to 3D. We have finished our 3D implementation, and are now at the point of experimentation and tuning for optimal performance. To our knowledge, this is the first data parallel implementation of a structured adaptive mesh refinement scheme. We have made certain tradeoffs to keep the calculation load balanced and to keep the communication overhead between approximately 10 and 20 %. The key idea in this work was a data layout scheme that preserves locality between dynamically changing adaptively placed fine grids. The key performance metrics are single grid integrator performance and overhead for regridding and interpolation. With the current implementation we observe over 10 megaflops per node using 64 nodes on the CM-5. Although this work is finding usefulness in its own right, the next step in this line of research is to investigate the parallelization of a Cartesian mesh algorithm.

This complicates the load balancing problem, since cells near a solid body use a different difference scheme with a varying amount of computational work. After that are extensions to incompressible flow and the Navier-Stokes equations, where the substantial complication of solving a system of equations must be tackled.

[1] "3D Automatic Cartesian Grid Generation for Euler Flows", by J. Melton, F. Enomoto, M. Berger. AIAA Paper 93-3386, 11th AIAA Computational Fluid Dynamics Conference, Orlando, Fla., July, 1993.

[2] "A Genuinely Two-Dimensional Scheme for the Compressible Euler Equations", by David Sidilkover. In preparation.

[3] "Structured Adaptive Mesh Refinement on the Connection Machine", by M. Berger and J. Saltzman. Proc. 6th SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, Va., March, 1993.

[4] "AMR on the CM-2", by M. Berger and J. Saltzman. RIACS Report No. 92-16. Proc. Workshop on Adaptive Computational Methods for Partial Differential Equations, RPI, May, 1992. To appear, Applied Num. Math.

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