Numerical modeling and verification - overview

The numerical modeling and verification group of the 2008 summer program involved four projects and fifteen participants. While the specific topics were diverse, all groups shared the common theme of developing and assessing new algorithms for the accurate prediction of complex turbulent flows.

In the project of Hickel and Larsson, the implicit LES methodology developed previously by the first author and collaborators for incompressible flows is extended to the compressible flow equations. In the implicit LES methodology, the turbulence closure problem and the problem of numerical errors present particularly at high wavenumber are in a sense merged: the numerical error present in the discretization is used as an implicit subgrid scale model. An important distinction of this work from other implicit LES approaches is that the present discretization is not fixed, but instead involves free parameters that can be selected to control the nature of the truncation error and thus control the effect of the implicit subgrid scale model. In the present project, homogeneous isotropic turbulence (HIT) was used to calibrate these free parameters by solving an optimization problem. Using these calibrated parameter values, very favorable comparisons of decay rates and spectra are reported for other HIT cases.

In the project of Domino, a powerful verification technique called the method of manufactured solutions is applied to verify the accuracy of a coupled algorithm for the incompressible Navier-Stokes equations with variable density. With the ultimate goal of developing accurate solvers for low-Mach number multi-physics flow problems in complex geometry, Domino argues that the splitting error present in segregated approaches to solving these equations can be in conflict with the stabilization "errors" required inherently by collocation of velocity and pressure. While the decision to solve the equations in a fully coupled manner requires the solution of a large, non-linear system in each time step, Domino describes a computational framework developed at Sandia National Laboratory that helps simplify this process, including the construction of analytic Jacobians. Manufactured solutions are presented that verify the second-order spatial accuracy of the coupled discretization.

In the project of Duchaine, Mendez, Nicoud, Corpron, Moureau, and Poinsot, a method for conjugate heat transfer (CHT) is developed for simulations involving turbulent reacting flows with conductive walls. In this project, the requirements for CHT capability are developed in terms of both simulation infrastructure and numerical algorithms. For the infrastructure, the authors pursued the approach of using two separate parallel solvers for the flow and heat transfer parts, respectively, with boundary data exchanged by a third code called a coupler. Algorithmically a nominally first-order in time approach was considered, characterized by the periodic exchange of heat fluxes from the fluid to the thermal solver, and surface temperatures from the thermal to the fluid solver. One-dimensional problems were considered to investigate the accuracy of the results to the coupling time scale, and it was concluded that coupling exchanges must occur on a time-scale that is of the order of the smallest time scale in the problem, generally the flow time scale. Finally a simulation of a hot flow interacting with a cooled turbine blade was performed both with and without CHT, illustrating how CHT tends to reduce the wall temperature compared to the adiabatic case.

Finally, in the project of Bewley, Cessna, Colburn, Ham, Iaccarino, and Wang, a completely different but equally important aspect of the "prediction" problem was considered in the context of turbulent flows. While the previous three projects focused on improving the details of the simulation tool to perform (supposedly) better individual simulations, this project applied a new data-assimilation algorithm to a fixed simulation tool to improve its predictive capability. Data-assimilation algorithms already play a central role in many important problems where forecasting is required, including short-term weather prediction for hurricanes, contaminant plume forecasting in urban environments, and climate change. In this project a new data-assimilation algorithm called Ensemble/Variational Estimation (EnVE) is presented as a consistent hybrid of the ensemble Kalman filtering and the space/time variational (4DVar) methods. An object-oriented framework is described that separates the data assimilation from the model simulation, such that the EnVE implementation is easily adapted to complex legacy codes. This was demonstrated by performing predictions of velocity field and scalar transport around a bluff body using Stanford's unstructured solver, CDP.

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