Predictive science - overview

The Predictive Science group was the largest of the summer program, resulting in 15 papers on topics ranging from numerical analysis of unstructured finite volume methods to the analysis of massive spectral DNS databases looking for evidence of self-sustained Keplerian turbulence. In all cases, however, these projects shared the common goal of using numerical simulation to better understand and predict turbulent flow phenomena. In past summer programs, these projects would have been divided along the lines of "Numerical Methods", "RANS", and "LES/DNS". The decision to join them was made in recognition of their common motivation of "Prediction", a topic whose formalism is of great importance to the turbulence simulation community, and one where clearly the methods, models, and theory, along with large-scale computing all play important roles.

The first five papers of this section involve the use of large-scale simulation – often DNS – in a "discovery" mode. In the paper of Jiminez *et al.*, a massive simulation database of rotating sheared turbulence is interrogated for evidence of non-linear growth. The database was generated earlier this year using 6 days $\times$ 65,536 processors of Lawrence Livermore's BlueGene/L computer. In the paper of Zaki *et al.*, a DNS of flow through a linear compressor cascade is analyzed to understand the role of freestream turbulence on transition. The pressure surface boundary layer is shown to remain attached due to bypass transition associated with the freestream forcing. On the suction surface, however, the boundary layer is shown to separate independent of the freestream condition. In the paper of Duraisamy and Lele, DNS of isolated turbulent Batchelor vortices is used to further our understanding of the growth and decay mechanisms in coherent trailing vortices associated with airplane wings and helicopter blades. In the paper of Stemmer *et al.*, DNS is used to study the behavior of harmonic waves passing through a strong shock in the presence of chemical reactions and thermal non-equilibrium. The broad objective of their work is to develop a predictive capability for the transition process during hypersonic re-entry from low-earth orbit, and their current results highlight the first-order influence of non-equilibrium effects on the hypersonic transition process. In the paper of Mendez *et al.*, wall-resolved LES of turbulent flow around a perforated plate are performed to investigate the flow structure characteristic of the multi-perforated walls used in gas turbine combustion chambers. Results show the jet angle departs from the hole angle with a strong recirculation region on the downstream side.

The next seven papers fall under the broad category of turbulence modeling. In the context of RANS turbulence models, the paper of Revell *et al.* assesses the performance of a new three-equation model suitable for wingtip trailing vortices which accounts for the stress-strain misalignment present in these flows. Their new approach is validated for the NACA0012 half wing, and is shown to inherit the stability advantages of the less accurate two equation eddy-viscosity models. In the context of subgrid-scale modeling for LES, the paper of Toschi *et al.* tests the validity of the Shear Improved Smagorinsky Model in the turbulent backward facing step flow. Their model is shown to give accurate results, comparable with those achieved using the dynamic Smagorinsky model. The model has the advantage of extra computational simplicity relative to the dynamic model, although computing a meaningful local mean shear in non-stationary flows remains an open issue. In the paper of Novikov and Bodony, a multi-scale modeling approach for the subgrid-scale stress based on coupling the SGS fluctuations to the resolved field with a dynamically-determined constant is investigated for isotropic decaying turbulence. Their multi-scale approach is shown to perform well for this flow, even when the energy-containing eddies are in the SGS part of the spectrum. In the paper of Miesch *et al.*, Smagorinsky and dynamic Smagorinsky subgrid-scale models are developed for global solar simulations using the anelastic spherical harmonic (ASH) code. Preliminary results show the largest scales are less viscous than in previous models and power is spread over a wider range of wavenumbers for a given spatial resolution, however some issues with long-time stability of the calculations must be resolved. In the paper of Hickel *et al.*, an implicit subgrid-scale modeling approach is developed and tested for passive scalar transport. In their implicit approach, the truncation error of the numerical discretization functions as the subgrid-scale model. Their results validate their implicit approach over a wide range of Schmidt numbers for both isotropic turbulence and turbulent channel flow. In the paper of Vasilyev *et al.* two subgrid-scale models are developed and evaluated in the context of the Stochastic Coherent Large Eddy Simulation (SCALES) methodology. For the freely decaying homogeneous turbulence case investigated, SCALES is shown to more accurately predict the DNS energy spectra compared to traditional grid-based LES with similar field compression. In the paper of Piomelli *et al.* grid discontinuities are artificially introduced into large-eddy simulations of plane channel flow to study their effect. This work is motivated by the broader objective of developing the LES methodology for complex geometries, where grid and potentially filter discontinuities will invariably occur. Their investigation distinguishes substantially different behavior for flow interfaces parallel or perpendicular to the mean advection direction. In the later case, the transition results in a decrease in resolved Reynolds stresses across the interface that none of the models investigated is capable of compensating for.

The final three papers deal specifically with the development of numerical methods for complex geometries and/or complex flow physics. In the paper of Domino, the errors associated with a class of time-accurate collocated finite volume methods are identified as splitting and stabilization errors, and a new projection method that circumvents the stabilization error is proposed. The method is implemented within the SIERRA/Fuego framework of Sandia National Laboritories and tested using the method of manufactured solutions, however the additional Poisson solve required in each time step increases the cost significantly, making it non-competive with other approaches. In the paper of Schluter, the CHIMPS coupling software developed at Stanford's ASC center is used to integrate RANS and LES flow solvers in an attempt to relax the strict resolution requirements that turbulent boundary layers impose on wall-resolved LES. In an overlap region near the wall, virtual body forces are applied to the LES solution to drive the LES mean to the RANS solution. This hybrid method is shown to significantly improve the mean predicted by under-resolved LES alone with a near-wall spacing of $\Delta y^+ \approx 100$. In the final paper, Wray *et al.* compare the accuracy and efficiency of the multi-group and multi-bin methods for handling the complex frequency dependence in solving radiation transport for the Apollo AS-501 re-entry. Their comparison shows that the multi-bin method, specifically the Opacity Distribution Function (ODF) method, allows a huge reduction in cost for comparable accuracy. As noted in the paper, this approach is commonly used by astrophysicists for solar calculations.

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