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Abstracts of Papers to Appear

A Stochastic Projection Method for Fluid Flow. II. Random Process. Olivier P. Le Maître,* Matthew T. Reagan,† Habib N. Najm,† Roger G. Ghanem,‡ and Omar M. Knio.§ *Centre d'Etudes de Mécanique d'Ile de France, Université d'Evry Val d'Essone, 40 rue du Pelvoux, 91020 Evry cedex, France; †Combustion Research Facility, Sandia National Laboratories, Livermore, California 94550; ‡Department of Civil Engineering, The Johns Hopkins University, Baltimore, Maryland 21218-2686; and §Department of Mechanical Engineering, The Johns Hopkins University, Baltimore, Maryland 21218-2686.

An uncertainty quantification scheme is developed for the simulation of stochastic thermofluid processes. The scheme relies on spectral representation of uncertainty using the polynomial chaos (PC) system. The solver combines a Galerkin procedure for the determination of PC coefficients with a projection method for efficiently simulating the resulting system of coupled transport equations. Implementation of the numerical scheme is illustrated through simulations of natural convection in a 2D square cavity with stochastic temperature distribution at the cold wall. The properties of the uncertainty representation scheme are analyzed, and the predictions are contrasted with results obtained using a Monte Carlo approach.

On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes. Miguel R.Visbal and Datta V. Gaitonde. Computational Sciences Branch, Aeronautical Sciences Division, Air Force Research Laboratory, Wright-Patterson AFB, Ohio 45433.

This study enables the use of very high-order finite-difference schemes for the solution of conservation laws on stretched, curvilinear, and deforming meshes. To illustrate these procedures, we focus on up to 6th-order Pade-type spatial discretizations coupled with up to 10th-order low-pass filters. These are combined with explicit and implicit time integration methods to examine wave propagation and wall-bounded flows described by the Navier–Stokes equations. It is shown that without the incorporation of the filter, application of the high-order compact scheme to nonsmooth meshes results in spurious oscillations which inhibit their applicability. Inclusion of the discriminating low-pass high-order filter restores the advantages of high-order approach even in the presence of large grid discontinuities. When three-dimensional curvilinear meshes are employed, the use of standard metric evaluation procedures significantly degrades accuracy since freestream preservation is violated. To overcome this problem, a simple technique is adopted which ensures metric cancellation and thus ensures freestream preservation even on highly distorted curvilinear meshes. For dynamically deforming grids, an effective numerical treatment is described to evaluate expressions containing the time-varying transformation metrics. With these techniques, metric cancellation is guaranteed regardless of the manner in which grid speeds are defined. The efficacy of the new procedures is demonstrated by solving several model problems as well as by application to flow past a rapidly pitching airfoil and past a flexible panel.

Nodal High-Order Methods on Unstructured Grids. I. Time-Domain Solution of Maxwell's Equations. J. S. Hesthaven and T. Warburton. Division of Applied Mathematics, Brown University, Box F, Providence, Rhode Island 02912.

We present a convergent high-order accurate scheme for the solution of linear conservation laws in geometrically complex domains. As our main example we include a detailed development and analysis of a scheme for the time-domain solution of Maxwell's equations in a three-dimensional domain. The fully unstructured spatial discretization is made possible by the use of a high-order nodal basis, employing multivariate Lagrange polynomials

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defined on the triangles and tetrahedra. Careful choice of the unstructured nodal grid points ensures high-order accuracy, while the equations themselves are satisfied in a discontinuous Galerkin form with the boundary conditions being enforced weakly through a penalty term. Accuracy, stability, and convergence of the semidiscrete approximation to Maxwell's equations is established rigorously and bounds on the growth of the global divergence error are provided. Concerns related to efficient implementations are discussed in detail. This sets the stage for the presentation of examples, verifying the theoretical results, and illustrating the versatility, flexibility, and robustness for solving two- and three-dimensional benchmark problems in computational electromagnetics. Pure scattering as well as penetration is discussed and high parallel performance of the scheme is demonstrated.

A Coupled Schrödinger Drift-Diffusion Model for Quantum Semiconductor Device Simulations. P. Degond* and A. El Ayyadi.† *MIP, UMR 5640 (CNRS-UPS-INSA), Université Paul Sabatier, 118, Route de Narbonne, 31062 Toulouse Cedex, France; and †MIP, UMR 5640 (CNRS-UPS-INSA), INSA, 135, Avenue de Rangueil, 31077 Toulouse Cedex, France.

In this paper, we derive a coupled Schrödinger drift–diffusion self-consistent stationary model for quantum semiconductor device simulations. The device is decomposed into a quantum zone (where quantum effects are expected to be large) and a classical zone (where they are supposed negligible). The Schrödinger equation is solved for scattering states in the quantum zone while a drift–diffusion model is used in the classical zone. The two models are coupled through interface conditions which are derived from those of N. Ben Abdallah (1998, *J. Stat. Phys.* **90**, 627) through a diffusion approximation. Numerical tests in the case of a resonant tunneling diode illustrate the validity of the method.

Direct Simulation of the Motion of Neutrally Buoyant Circular Cylinders in Plane Poiseuille Flow. Tsorng-Whay Pan and Roland Glowinski. Department of Mathematics, University of Houston, Houston, Texas 77204-3476.

In this article we discuss the generalization of a Lagrange multiplier-based fictitious domain method to the simulation of the motion of neutrally buoyant particles in a Newtonian fluid. Then we apply it to study the migration of neutrally buoyant circular cylinders in plane Poiseuille flow of a Newtonian fluid by direct numerical simulation. The Segré–Silberberg effect is found for the cases with one and several circular cylinders. In general, it is believed that the migration away from the center of the channel is due to an effect of the curvature of velocity profile. Via direct numerical simulation, we find that this effect is not weakened by the presence of many particles, but by the collisions among the particles. Experiments and simulations for hundreds of circular cylinder cases show that particles concentrate in the central region where the shear rate is low. A power law associated with the horizontal velocity of the mixture of fluid/particles is also presented.