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COUPLING BOLTZMANN AND NAVIER–STOKES EQUATIONS BY HALF FLUXES. Patrick Le Tallec*,† and François Mallinger.† **Université Paris-Dauphine; *,†INRIA, Domaine de Voluceau, Rocquencourt, B.P. 105, Le Chesnay Cedex, France.*

We introduce an adaptative coupling of the Boltzmann and Navier–Stokes equations to compute hypersonic flows around a vehicle at high altitude. The coupling is achieved by matching half fluxes at the interface of the Boltzmann and Navier–Stokes domains. The domains are determined automatically by computing local kinetic residuals on a preliminary Navier–Stokes solution. Our method is developed here for monoatomic gases. Different numerical results illustrate its validity and limits.

A NUMERICAL METHOD USING UPWIND SCHEMES FOR THE RESOLUTION OF TWO-PHASE FLOWS. F. Coquel,* K. El Amine,*,† E. Godlewski,* B. Perthame,* and P. Rascle.† **Laboratoire d'Analyse Numérique-Tour 55-65 5ème étage, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris cedex 05, France; †E.D.F./D.E.R./R.N.E./Ph.R., 1 avenue du Général de Gaulle, 92141 Clamart Cedex, France.*

This work is devoted to the numerical approximation of two-fluid flow models described by six balance equations. We introduce an original splitting technique which is especially derived to allow a straightforward extension to various and detailed exchange source terms. When based on suitable kinetic upwind schemes, the whole scheme preserves the positivity of all the thermodynamic variables under a fairly unrestrictive CFL-like condition. Several stiff numerical tests, including phase separation, are displayed in order to highlight the efficiency of the method we propose.

COMPENSATING MASS MATRIX POTENTIAL FOR CONSTRAINED MOLECULAR DYNAMICS. Abhinandan Jain. *Jet Propulsion Laboratory/California Institute of Technology, 4800 Oak Grove Drive, Pasadena, California 91109.*

Rigid internal constraints are used in molecular models to speed up molecular dynamics (MD) simulations. It is well recognized that statistical averages from such constrained MD simulations differ by a metric tensor-dependent term from similar averages computed using conventional unconstrained MD simulations. Fixman proposed augmenting the standard potential with a compensating term which depends on the metric tensor to nullify the effects of this bias term. However, in the absence of tractable algorithms to compute this compensating tensor potential and its gradient its use has been impractical. This paper derives a new algorithm for computing the compensating potential, as well as its gradient for tree topology molecular systems. The algorithm is quite straightforward and is an extension of the spatial operators based $O(\mathcal{N})$ algorithm that has been recently proposed for constrained dynamics. Indeed, the compensating potential is closely related and computed from the articulated body inertia quantities available from this $O(\mathcal{N})$ algorithm.

SPH AND RIEMANN SOLVERS. J. J. Monaghan. *Department of Mathematics, Monash University, Clayton, Victoria 3168, Australia.*

Smooth particle hydrodynamics (SPH) is usually based on equations derived from the momentum and thermal energy equations of fluid dynamics. Artificial viscosity is added to these equations to handle shocks. In this paper we show how the equations may be formulated using the specific energy equation instead of the thermal energy equation. The resulting equations are very similar to the equations constructed for Riemann solutions of compressible gas dynamics. In particular the artificial viscosity is analogous to terms constructed from signal velocities and jumps in variables across characteristics. When applied to shock tubes, blast waves, wall shocks, and the Roberts and Sjögreen problems the new equations give very good results. They also provide the basis for the generalization of SPH to relativistic flows.

HYBRID SIMULATIONS OF THE EFFECTS OF ENERGETIC PARTICLES ON LOW-FREQUENCY MHD WAVES. E. V. Belova,* R. E. Denton,* and A. A. Chan.† **Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire 03755; †Rice University, Houston, Texas 77251.*

A hybrid MHD-gyrokinetic simulation model is presented which is suitable for self-consistent study of the interaction of energetic particles with low-frequency MHD waves. Fully electromagnetic gyrokinetic equations are used to describe the energetic particles, while the cold background plasma is treated as a fluid, using nonlinear one-fluid MHD equations. Based on this model a hybrid MHD-gyrokinetic particle code has been developed. A δf algorithm has been implemented in the code for $\beta \sim 1$ electromagnetic perturbations. The gyrokinetic description enables us to remove the restriction on the particle time step dictated by the gyromotion, while the δf algorithm strongly reduces the simulation numerical noise level. Therefore, considerably larger time steps and a smaller number of particles can be used in the simulations as compared to conventional methods. The conservation properties of the model and corresponding δf scheme have been investigated. Representative two-dimensional simulations of the mirror instability and the temperature gradient driven instability of the compressional mode were performed, and the simulation results are in very good agreement with linear theory.

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