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Abstracts of Papers to Appear

VORTEX METHODS WITH SPATIALLY VARYING CORES. Georges-Henri Cottet,* Petros Koumoutsakos,† and Mohamed Lemine Ould Salihi.* **LMC-IMAG, Université Joseph Fourier, Grenoble, France; and †Institut für Fluiddynamik, ETH, Zürich, Switzerland, and CTR, NASA Ames 202A-1, Moffett Field, California 94035.*

The accuracy of vortex methods employing smooth vortex particles/blobs is determined by the blob size, which can be viewed as a mollifier of the vorticity field. For computational efficiency, this core size needs to be spatially variable as particles are used to discretize different parts of the flow field, such as the boundary layer and the wake in bluff body flows. We derive here a consistent approximation for the viscous Navier–Stokes equations using variable size vortex particles. This derivation is based on the implementation of mappings that allow the consistent formulation of the diffusion and convection operators of the Navier–Stokes equations in the context of vortex methods. Several local mappings can be combined giving the capability of "mesh-embedding" to vortex methods. It is shown that the proposed variable method offers significant improvement on the computational efficiency of constant-core-size methods while maintaining the adaptive character of the method. The method is ideally suited to flows such as wakes and shear layers and the validity of the approach is illustrated by showing results from cylinder flows and wall–vortex interactions. Using this scheme, previously unattainable simulations of cylinders undergoing rotary oscillations at high Reynolds numbers reveal an interesting mechanism for drastic drag reduction.

SIMULATED ANNEALING CLUSTERIZATION ALGORITHM FOR STUDYING MULTIFRAGMENTATION. Rajeev K. Puri and Joerg Aichelin. *SUBATECH, Laboratoire de Physique Subatomique et des Technologies Associees, UMR Universite de Nantes, IN2P3/CNRS, Ecole des Mines de Nantes, 4 rue Alfred Kastler, F-44070 Nantes, France.*

We here present the details of the numerical realization of a recently advanced algorithm developed to identify fragmentation in heavy ion reactions. This new algorithm is based on the simulated annealing method and is dubbed the simulated annealing clusterization algorithm [SACA]. We discuss the different parameters used in the simulated annealing method and present an economical set of parameters which is based on extensive analysis of central and peripheral collisions of Au–Au, Nb–Nb, and Pb–Pb. These parameters are crucial for the success of the algorithm. Our set of optimized parameters gives the same results as the most conservative choice, but is very fast. We also discuss the nucleon and fragment exchange processes, which are very important for energy minimization, and finally present an analysis of the reaction dynamics using the new algorithm. This algorithm can be applied whenever one wants to identify which of a given number of constituents form bound objects.

DEVELOPMENT OF HIGH-ORDER TAYLOR–GALERKIN SCHEMES FOR LES. Olivier Colin* and Michael Rudgyard.† **AEROSPATIALE MATRA MISSILES/CERFACS, France; and †Oxford University Computing Laboratory, Oxford, United Kingdom.*

In this paper we describe the implementation and development of a new Taylor–Galerkin finite-element scheme within an unstructured/hybrid parallel solver. The scheme has been specifically conceived for unsteady LES: it is third-order in space and time and has a low dissipative error. Minimal additional CPU costs are achieved by using a new approximation of the finite-element integrals and a simple iterative method for the approximate inversion of the modified mass matrix. Basic convective tests are carried out in two and three dimensions for arbitrary elements. Numerical estimates of the order of convergence are presented on regular and perturbed grids. Finally, test cases

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that are relevant to LES are carried out, and these clearly demonstrate the important improvements that our new scheme offers relative to a selection of existing methods.

EFFICIENT METHODS FOR HANDLING LONG-RANGE FORCES IN PARTICLE-PARTICLE SIMULATIONS. Hans Fangohr,*,† Andrew R. Price,† Simon J. Cox,† Peter A. J. de Groot,* and Geoffrey J. Daniell.* **Department of Physics and Astronomy and †Department of Electronics and Computer Science, University of Southampton, Southampton SO17 1BJ, United Kingdom.*

A number of problems arise when long-range forces, such as those governed by Bessel functions, are used in particle–particle simulations. If a simple cut-off is used for the interaction, the system may find an equilibrium configuration at zero temperature that is not a regular lattice yet has an energy lower than the theoretically predicted minimum for the physical system. We demostrate two methods for overcoming these problems in Monte Carlo and molecular dynamics simulations. The first uses a smoothed potential to truncate the interaction in a single unit cell; this is appropriate for phenomenological characterizations, but may be applied to any potential. The second is a new method for summing the unmodified potential in an infinitely tiled periodic system, which is in excess of 20,000 times faster than previous naïve methods which add periodic images in shells of increasing radius: this is suitable for quantitative studies. Finally we show that numerical experiments which do not handle the long-range force carefully may give misleading results; both of our proposed methods overcome this problem.