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Abstracts of Papers to Appear in Future Issues

NUMERICALLY IMPLEMENTED PERTURBATION METHOD FOR THE NONLINEAR MAGNETIC MOMENT OF AN ANISOTROPIC SUPERCONDUCTOR. Igor Žutić and Oriol T. Valls. *School of Physics and Astronomy and Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, Minnesota 55455-0149.*

We present a method to compute the magnetic moment of a bulk, finite-size, three-dimensional, anisotropic superconductor. Our numerically implemented perturbative procedure is based on a solution of the nonlinear Maxwell–London electrodynamic equations, where we include the nonlinear relation between current and gauge invariant velocity. The method exploits the small ratio of the finite penetration depths to the sample size. We show how to treat the open boundary conditions over an infinite domain and the continuity requirement at the interface. We demonstrate how our method substantially reduces the computational work required and discuss its implementation to an oblate spheroid. The numerical solution is obtained from a finite-difference method. We briefly discuss the relevance of this work to similar problems in other fields.

COMMON MOLECULAR DYNAMICS ALGORITHMS REVISITED: ACCURACY AND OPTIMAL TIME STEPS OF STÖRMER–LEAPFROG INTEGRATORS. Alexey K. Mazur. *Laboratoire de Biochimie Théorique, CNRS UPR9080 Institut de Biologie Physico-Chimique 13, rue Pierre et Marie Curie, Paris, 75005, France.*

The Störmer–Verlet–leapfrog group of integrators commonly used in molecular dynamics simulations has long become a textbook subject and seems to have been studied exhaustively. There are, however, a few striking effects in the performance of algorithms which are well known but have not received adequate attention in the literature. A closer view of these unclear observations results in unexpected conclusions. It is shown here that contrary to the conventional point of view, the leapfrog scheme is distinguished in this group both in terms of the order of truncation errors and the conservation of the total energy. In this case the characteristic square growth of fluctuations of the total energy with the step size, commonly measured in numerical tests, results from additional interpolation errors with no relation to the accuracy of the computed trajectory. An alternative procedure is described for checking energy conservation of leapfrog-like algorithms which is free from interpolation errors. Preliminary tests on a representative model system suggest that standard step size values used at present are lower than necessary for accurate sampling.

A DOMAIN DECOMPOSITION METHOD FOR THE HELMHOLTZ EQUATION AND RELATED OPTIMAL CONTROL PROBLEMS. Jean-David Benamou,* and Bruno Desprès†. **Domaine de Voluceau, INRIA, B. P. 105, 78153 Le Chesnay Cedex, France; †Commissariat à l'Energie Atomique, 94195 Villeneuve Saint Georges Cedex, France.*

We present an iterative domain decomposition method to solve the Helmholtz equation and related optimal control problems. The proof of convergence of this method relies on energy techniques. This method leads to efficient algorithms for the numerical resolution of harmonic wave propagation problems in homogeneous and heterogeneous media.

A PDE SENSITIVITY EQUATION METHOD FOR OPTIMAL AERODYNAMIC DESIGN. Jeff Borggaard and John Burns. *Interdisciplinary Center for Applied Mathematics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061-0531.*

The use of gradient-based optimization algorithms in inverse design is well established as a practical approach to aerodynamic design. A typical procedure uses a simulation scheme to evaluate the objective function (from the approximate states) and its gradient, then passes this information to an optimization algorithm. Once the simulation scheme (CFD flow solver) has been selected and used to provide approximate function evaluations, there are several possible approaches to the problem of computing gradients. One popular method is to differentiate the simulation scheme and compute design sensitivities that are then used to obtain gradients. Although this black-box approach has many advantages in shape optimization problems, one must compute mesh sensitivities in order to compute the design sensitivity. In this paper, we present an alternative approach using the PDE sensitivity equation to develop algorithms for computing gradients. This approach has the advantage that mesh sensitivities need not be computed. Moreover, when it is possible to use the CFD scheme for both the forward problem and the sensitivity equation, then there are computational advantages. An apparent disadvantage of this approach is that it does not always produce consistent derivatives. However, for a proper combination of discretization schemes, one can show *asymptotic consistency* under mesh refinement, which is often sufficient to guarantee convergence of the optimal design algorithm. In particular, we show that when asymptotically consistent schemes are combined with a trust-region optimization algorithm, the resulting optimal design method converges. We denote this approach as the *sensitivity equation method*. The sensitivity equation method is presented, convergence results are given, and the approach is illustrated on two optimal design problems involving shocks.

OPTIMAL CONTROL OF TWO- AND THREE-DIMENSIONAL INCOMPRESSIBLE NAVIER–STOKES FLOWS. Omar Ghattas and Jai-Hyeong Bark. *Computational Mechanics Laboratory, Department of Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213.*

The focus of this work is on the development of large-scale numerical optimization methods for optimal control of steady incompressible Navier–Stokes flows. The control is affected by the suction or injection of fluid on portions of the boundary, and the objective function represents the rate at which energy is dissipated in the fluid. We develop reduced Hessian sequential quadratic programming methods that avoid converging the flow equations at each iteration. Both quasi-Newton and Newton variants are developed and compared to the approach of eliminating the flow equations and variables, which is effectively the generalized reduced gradient method. Optimal control problems are solved for two-dimensional flow around a cylinder and three-dimensional flow around a sphere. The examples demonstrate at least an order-of-magnitude reduction in time taken, allowing the optimal solution of flow control problems in as little as half an hour on a desktop workstation.

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