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Abstracts of Papers to Appear

THE ORIGIN AND NATURE OF SPURIOUS EIGENVALUES IN THE SPECTRAL TAU METHOD. Paul T. Dawkins,* Steven R. Dunbar,* and Rod W. Douglass.† **Department of Mathematics and Statistics, University of Nebraska-Lincoln, Lincoln, Nebraska 68588-0323; †Computational Mechanics, Idaho National Engineering Laboratory, Idaho Falls, Idaho 83415-3808.* E-mail: pdawkins, sdunbar@math.unl.edu, rxd@inel.gov.

The Chebyshev–tau spectral method for approximating eigenvalues of boundary value problems may produce spurious eigenvalues with large positive real parts, even when all true eigenvalues of the problem are known to have a negative real part. We explain the origin and nature of the "spurious eigenvalues" in an example problem. The explanation will demonstrate that the large positive eigenvalues are an approximation of infinite eigenvalues in a nearby generalized eigenvalue problem.

A DENSITY PERTURBATION METHOD TO STUDY THE EIGENSTRUCTURE OF TWO-PHASE FLOW EQUATION SYSTEMS. J. Cortes,* A. Debussche,† and I. Tuomi.‡ **French Atomic Energy Commission (CEA) Centre d'Etudes de Cadarache, DEC/SECA, bat.216, Saint-Paul les Durance, 13108, France; †University of Orsay Paris XI and CNRS, Laboratoire d'Analyse Numerique, bat.425, Orsay, 91405, France; ‡French Atomic Energy Commission (CEA) Centre d'Etudes de Saclay, DMT/SERMA, bat.470, Gif-sur-Yvette, 91191, France.*

Many interesting and challenging physical mechanisms are concerned with the mathematical notion of eigenstructure. In two-fluid models, complex phasic interactions yield a complex eigenstructure which may raise numerous problems in numerical simulations. In this paper, we develop a perturbation method to examine the eigenvalues and eigenvectors of two-fluid models. This original method, based on the stiffness of the density ratio, provides a convenient tool to study the relevance of pressure momentum interactions and allows us to get precise approximations of the whole flow eigendecomposition for minor requirements. Roe scheme is successfully implemented and some numerical tests are presented.

MODELING ARTERIOLAR FLOW AND MASS TRANSPORT USING THE IMMERSED BOUNDARY METHOD. Kayne M. Arthurs,* Leon C. Moore,† Charles S. Peskin,‡ E. Bruce Pitman,§ and H. E. Layton.* **Department of Mathematics, Duke University, Durham, North Carolina 27708-0320; †Department of Physiology and Biophysics, State University of New York, Stony Brook, New York 11794-8661; ‡Courant Institute of Mathematical Sciences, New York University, New York, New York 10012; §Department of Mathematics, State University of New York, Buffalo, New York 14214-3093.* E-mail: ksmith@math.duke.edu, moore@physiology.pnb.sunnysb.edu, peskin@cims.nyu.edu, pitman@sand.math.buffalo, edu, layton@math.duke.edu.

Flow in arterioles is determined by a number of interacting factors, including perfusion pressure, neural stimulation, vasoactive substances, the intrinsic contractility of arteriolar walls, and wall shear stress. We have developed a two-dimensional model of arteriolar fluid flow and mass transport. The model includes a phenomenological representation of the myogenic response of the arteriolar wall, in which an increase in perfusion pressure stimulates vasoconstriction. The model also includes the release, advection, diffusion, degradation, and dilatory action of nitric oxide (NO), a potent, but short-lived, vasodilatory agent. Parameters for the model were taken primarily from the experimental literature of the rat renal afferent arteriole. The incompressible Navier–Stokes equations are computed by means of a splitting that uses upwind differencing for the inertial term and a spectral method for the viscous term and incompressibility condition. The immersed boundary method is used to include the forces arising from the arteriolar walls. The advection of NO was computed by means of a high-order flux-corrected

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transport scheme; the diffusion of NO was computed by a spectral solver. Simulations demonstrated the efficacy of the numerical methods employed, and grid refinement studies confirmed the anticipated first-order temporal convergence and demonstrated second-order spatial convergence in key quantities. By providing information about the effective width of the immersed boundary and sheer stress magnitude near that boundary, the grid refinement studies indicate the degree of spatial refinement required for quantitatively reliable simulations. Owing to the dominating effect of advection, relative to degradation and diffusion, simulations indicate that NO has the capacity to produce dilation along the entire length of the arteriole.

AN ITERATIVE METHOD FOR THE INVERSION OF THE TWO-DIMENSIONAL WAVE EQUATION WITH A POTENTIAL. Guanquan Zhang* and Yu Zhang.† *_State Key Laboratory of Scientific and Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences, Beijing, 100080 People's Republic of China; †Institute of Computational Mathematics and Scientific/Engineering Computing, Chinese Academy of Sciences._

A numerical method for a nonlinear inversion problem for the 2D wave equation with a potential is discussed. In order to avoid the ill-posedness, we substitute a coupled system of one-way wave equations for the original wave equation. An iterative algorithm is constructed to improve the accuracy of the inversion. Numerical experiments are performed on several examples to examine the effectiveness of this method.

COMBINING DISSIPATIVE PARTICLE DYNAMICS AND MONTE CARLO TECHNIQUES. S. M. Willemsen, T. J. H. Vlugt, H. C. J. Hoefsloot, and B. Smit. _Department of Chemical Engineering, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands._ E-mail: sanderw@chemeng.chem.uva.nl, tampert@ct-cr6.chem.uva.nl, huubh@chemeng.chem.uva.nl, smit@chemeng.chem.uva.nl.

Dissipative particle dynamics (DPD) has been introduced as a method for simulating complex fluids at hydrodynamic time scales. In this work we investigate the possibilities to combine this DPD method with advanced Monte Carlo techniques. We show that this combined approach results in a more efficient sampling scheme to compute thermodynamic properties. We illustrate these advantages by computing a phase diagram of two liquids that de-mix and the calculation of the chemical potential of a polymer in solution.