Journal of Computational Physics **171,** 851–852 (2001)
doi:10.1006/jcph.2001.6868, available online at http://www.idealibrary.com on IDEAL®

Abstracts of Papers to Appear

Separable and Non-separable Multi-Wavelets in Multi-Dimensions. C. J. Tymczak, Anders M. N. Niklasson, and Heinrich Röder. Los Alamos National Laboratory, Theoretical Division, MS B221, Los Alamos NM 87545.

We report on a method of constructing multi-dimensional bi-orthogonal interpolating multi-wavelets. The approach is based upon polynomial interpolation in $\mathbf{R}^d$ [C. de Boor and A. Ron, Math Comp. **58**, 198 (1997)] and an extension of the lifting scheme [J. Kovačević and W. Sweldens, IEEE Trans Image Proc. **9**(3), 480 (2000)]. The constructed wavelets have compact support, are nearly isotropic and retain partial scale invariance leading to a fast and efficient multi-dimensional wavelet transform. We demonstrate an implementation for these wavelets of variable polynomial order up to four dimensions. Finally, we show that these wavelets have a much sparser representation of discontinuous functions as compared to tensor product wavelets, which allows for a more compact and efficient representation.

Modeling Quantum Structures with the Boundary Element Method. F. Gelbard and K. J. Malloy. Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87131.

A detailed analysis of the boundary element formulation of the electronic states of quantum structures is presented. Techniques for minimizing computation time by reducing the number of boundary integrals, utilizing the repetitive nature of embedded multiple quantum structures, and eliminating boundary elements for modeling the effects of quantum wells that contain quantum structures are discussed. Boundary element solutions for isolated and coupled quantum wires and pyramidal quantum dots are presented. The results for the coupling of such quantum structures clearly show the splitting of ground and excited states into "bonding" and "antibonding" states for both wires and dots. The numerical algorithm is shown to accurately capture these symmetry properties of a system of quantum structures if the boundary element and quadrature points are properly organized. For an asymmetric system of quantum dots the resulting electric dipole is shown to have either a positive or negative value depending on the energy level. Results are also presented showing the increase in energy levels due to the additional confinement arising from placing quantum dots into a quantum well.

The Construction of Projection Vectors for a Deflated ICCG *Method Applied to Problems with Extreme Contrasts in the Coefficients.* C. Vuik,* A. Segal,* J. A. Meijerink,† and G. T. Wijma.* *Delft University of Technology, Faculty of Information Technology and Systems, Department of Applied Mathematical Analysis, Mekelweg 4, 2628 CD Delft, The Netherlands; and †Shell International Exploration and Production, P.O. Box 60, 2280 AB Rijswijk, The Netherlands.

To predict the presence of oil and natural gas in a reservoir, it is important to know the fluid pressure in the rock formations. A mathematical model for the prediction of the fluid pressure history is given by a time-dependent diffusion equation. Application of the finite-element method leads to systems of linear equations. A complication is that the underground consists of layers with very large contrasts in permeability. This implies that the symmetric and positive definite coefficient matrix has a very large condition number. Bad convergence behavior of the ICCG method has been observed, and a classical termination criterion is not valid in this problem. In [19] we have shown that the number of small eigenvalues of the diagonally scaled matrix is equal to the number of high-permeability domains, which are not connected to a Dirichlet boundary. In this paper the proof is extended to an Incomplete Cholesky decomposition. To annihilate the bad effect of these small eigenvalues on the convergence, the Deflated ICCG method is used. In [19] we have shown how to construct a deflation subspace for the case of a set of more or

0021-9991/01 $35.00

less parallel layers. That subspace proved to be a good approximation of the span of the "small" eigenvectors. As a result of this, the convergence of DICCG is independent of the contrasts in the permeabilities. In this paper it is shown how to construct deflation vectors even in the case of very irregular shaped layers, and layers with so-called inclusions. A theoretical investigation and numerical experiments show that the DICCG method is not sensitive to small perturbations of the deflation vectors. The efficiency of the DICCG method is illustrated by numerical experiments.

Osculatory Interpolation in the Method of Fundamental Solution for Nonlinear Poisson Problems. Karthik Balakrishnan and Palghat A. Ramachandran. Department of Chemical Engineering, Washington University, St. Louis, Missouri 63130.

The Method of Fundamental Solution (also known as the F-Trefftz method or the singularity method) is an efficient numerical method for the solution of Laplace equation for both two- and three-dimensional problems. In recent years, the method has also been applied for the solution of Poisson equations by finding the particular solution to the nonhomogeneous terms. In general, approximate particular solutions are constructed using the interpolation of the nonhomogeneous terms by the radial basis functions. The method has been validated in recent papers. This paper presents an improvement of the solution procedure for such problems. The improvement is achieved by using radial basis functions called osculatory radial basis functions. Such functions make use of the normal gradient at boundary to obtain improved interpolation. The efficacy of the method is demonstrated for some prototypical nonlinear Poisson problems and for multiple Poisson equations.

A Novel Gauge Invariant Multistate Smearing Technique. P. Boyle. Department of Physics and Astronomy, University of Edinburgh, Edinburgh.

We present an investigation of a gauge invariant smearing technique that allows the construction of smearing functions with arbitrary radial behavior, by foresaking the space-filling nature of traditional smearing techniques. This is applied to both heavy–heavy, heavy–light, and light–light systems with one particular choice of radial "wavefunction"—the hydrogenic solutions—and we find good stability for both fitted masses and amplitudes of the radially excited states. The dependence of the amplitudes on the smearing radius is demonstrated to be well understood, while near optimal smearing radii may be found with extremely low statistics using a property of the smeared-local correlator. The smearing technique is inexpensive since it is noniterative, achieves a good signal-to-noise ratio, and can be altered to use wavefunctions from, say, potential models or the Bethe–Salpether equations in future simulations.