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A Fast Direct Solver for a Class of 3-D Elliptic Partial Differential Equation with Variable Coefficient

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Abstract. We propose a direct solver for the three-dimensional Poisson equation with a variable coefficient, and an algorithm to directly solve the associated sparse linear systems that exploits the sparsity pattern of the coefficient matrix. Introducing some appropriate finite difference operators, we derive a second-order scheme for the solver, and then two suitable high-order compact schemes are also discussed. For a cube containing N nodes, the solver requires $\mathcal{O}(N^{3/2}\log^2 N)$ arithmetic operations and $\mathcal{O}(N\log N)$ memory to store the necessary information. Its efficiency is illustrated with examples, and the numerical results are analysed.

AMS subject classifications: 15A15, 15A09, 15A23

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1 Introduction

In dealing with sparse linear algebraic systems that arise in the discretization of elliptic partial differential equations, iterative solvers require the pre-handling of ill-conditioned matrices, e.g., the Conjugate Gradient and Generalized Minimum Residual methods. On the other hand, compared with the iterative solvers using direct elimination can always get result easier when dealing with poorly conditioned coefficient matrices usually.

In a typical direct solver, there is usually an initial ordering step to reorder the rows and columns, so that the transformed coefficient matrix has some special structure such

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as block-triangular form. The internal structure of the dense matrices may also be exploited, to reduce the computational cost [4,5]. For example, a spiral pattern of the orderings that arise from a 2-D elliptic PDE can render the linear system in a block-tridiagonal form [1]; and it has also been shown that a sweeping ordering efficiently solves a 2-D discrete system arising from a moving perfectly matching layer (PML), using banded LU-factorization [2]. Another technique for dimension-reduction, with a much simpler format to deal with such structured matrices [1], has influenced us in designing our direct solver. It combines a similar dimension-reduction technique with fast algorithms for the spiral pattern, to solve the resulting sequence of sparse coefficient matrices.

Our main application is to a Poisson equation with variable coefficient, which arises in many areas including electric or electromagnetic field theory and heat conduction, i.e.,

$$\nabla\cdot\rho\nabla u = f. \tag{1.1}$$

For example, Eq. (1.1) applies in the theory of electrolyte solutions, where the distribution of counterion density strongly depends on the dielectric coefficients [7,8]. Changes in the dielectric coefficient for the electrolyte solution (from 10 to 25, 40, 60, and 78.5 within the first 7.4 Angströms at the surface of DNA) substantially increase the calculated surface concentration of counterions of all sizes. In a contoured lattice model involving a dielectric boundary and Boltzmann equation for the charge density, the Poisson equation

$$-\nabla\cdot[\varepsilon(r)\nabla\phi(r)] = \rho(r)/\varepsilon_0$$

of form similar to (1.1) can be approximated by the finite element representation

$$\sum_j [(\phi_i-\phi_j)\varepsilon_{ij}] = \rho_i h^2/\varepsilon_0,$$

where ε_{ij} is the arithmetic average of the dielectric coefficients (for the elements i and j) and ρ_i denotes the relevant value of the charge distribution. Yet another example arises in diffusion-reaction processes [9], where

$$\begin{aligned}&\frac{\partial p^i(r,t)}{\partial t} = \nabla\cdot\Big\{D^i(r)e^{-\beta V^i(r,t)}\nabla\big(e^{\beta V^i(r)}p^i(r,t)\big)\Big\} + \alpha^i(r)p^i(r,t),\\ &\nabla\cdot\epsilon\nabla\phi(r,t) = -\rho^f(r) - \sum_i q^i p^i(r,t)\end{aligned}$$

involves the density distribution function $p^i(r,t)$ of the diffusing particles of the ith species with diffusion coefficient $D^i(r)$ and charge q^i, the fixed source charge distribution ρ^f, the inverse Boltzmann energy β, the dielectric coefficient ϵ, the potential V^i that imposes driving forces on the ith diffusing species, and the intrinsic reaction rate $\alpha^i(r)$. The dielectric coefficient actually depends in a complicated way on the pressure, temperature and material density, but for simplicity it was argued that one may adopt the linear form

$$\epsilon = \epsilon_p + \frac{p^w}{p_0^w} * (\epsilon_w - \epsilon_p), \tag{1.2}$$