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Massively Parallel Iterative Methods:
Multiscale Preconditioners and Implicit Methods

Final Report

Grant Period: 6/17/91 - 6/16/94. No cost extension to: 9/30/94.

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Faculty: Tony F. Chan, Tarek Mathew, Beth Ong, Barry Smith, Panayot Vassilevski.

Postdoctoral fellow: Patrick Ciarlet, Jr., Francoise Lamour, Jun Zou

Graduate students: Jennifer Y.C. Chang (Ph.D. 92), Jianping Shao (Ph.D. 93), Tedd Szeto (Ph.D. 94).

2 Description of Research:

Nonlinear and linear systems of equations often arise in scientific computation, for example in implicit methods in Computational Fluid Dynamics (CFD). It is important to find cost-effective and accurate methods to solve such systems. Iterative methods are among those widely used, especially for 3D problems. In this project, we consider iterative methods which are especially suited to massively parallel architectures.

To accelerate convergence of these iterative methods, preconditioners are often used. Good preconditioners reduce the number of iterations and involves few arithmetic operations per iteration. Effective parallel preconditioners must account for the global coupling inherent in elliptic problems. On the other hand, efficient parallel implementation often favors local computations. Multiscale iterative methods represent a good compromise between these two conflicting goals. We focused our attention on two classes of multiscale preconditioners: multilevel basis preconditioners and domain decomposition preconditioners.

Domain decomposition methods are techniques which solve a boundary value problem posed on a general domain by patching together solutions on small subdomains, usually in an iterative fashion. They seem ideally suited for coarse grain parallel machines, with each subdomain assigned to a single processor. We derived efficient methods in this class, for overlapping and nonoverlapping subdomains, for convection-diffusion problems, for unstructured meshes and for partitioning meshes.

For the successful application of preconditioned iterative methods, in addition to efficient preconditioners, robust and efficient convergence acceleration and stabilization methods are also needed. We investigated ways to construct conjugate gradient like methods for nonsymmetric systems which possess some of the following desirable properties: short recurrences, transpose-free, no breakdowns, smooth convergence and efficient use of matrix-vector multiplies. We have developed a simple technique called *composite step*, which can overcome one kind of breakdowns in BCG methods. We also give one of the first convergence proofs of the BCG method by analyzing as a Petrov-Galerkin method defined on Krylov subspaces and use the theory of Babuska and Azis. Moreover, we have now extended this composite step technique to stabilize other product methods derived from BCG, such as CGS, BiCGSTAB and several other variants.

Finally, we also studied some basic linear algebra problems, including rank-revealing QR factorizations and stable Toeplitz solvers, which have applications to signal and image processing.

3 Summary of Most Important Results

1. We extended existing domain decomposition and multigrid algorithms for elliptic problems to unstructured grids. The key issues are how to decompose the grid into subgrids, and how to construct the coarse grid. We proved convergence without assuming the space of coarse grid functions are nested within the fine grid function spaces and we also allow the coarse grid's boundary to not match that of the fine grid.

2. We proved that the "Recursive Spectral Bisection" method for partitioning unstructured mesh is *optimal* in the sense that it computes the nearest discrete feasible solution to the optimal solution of a continuous form of the discrete graph optimization problem (which is computed by solving an eigenvalue problem). Based on this result, we developed a more efficient variant of the algorithm based on using the sign of the eigenfunction instead of its median.

3. We developed "boundary probing" interfacial preconditioners in domain decomposition, which adapts to the coefficients of the differential operator

and the geometry of the subdomains. We extended this to derive a more efficient version of the vertex space method of Smith and Widlund.

4. We have developed a simple technique called *composite step*, which can overcome one kind of breakdowns in BCG methods. We also give one of the first convergence proofs of the BCG method by analyzing as a Petrov-Galerkin method defined on Krylov subspaces and use the theory of Babuska and Azis. Moreover, we have now extended this composite step technique to stabilize other product methods derived from BCG, such as CGS, BiCGSTAB and several other variants.

5. Using a result on the relationship between the overlapping and nonoverlapping methods in domain decomposition, we proved that many domain decomposition algorithms have convergence rates that are independent of the aspect ratios of the subdomains or the amount of overlap.

6. We developed a block–ILU factorization technique for block–tridiagonal discretization matrices that need not necessarily be M-matrices. It is based on combining the multigrid idea with the block ILU factorization. We proved the existence of the factorization and derived estimates for the spectral equivalence relation between the original matrix and the proposed preconditioner.

7. Developed look-ahead Levinson algorithms which are stable for a much more general class of Toeplitz systems, including indefinite ones, while retaining the efficiency of the classical algorithm. Fortran and MATLAB codes have been developed also.

8. Developed rank-revealing QR factorization algorithms, which can be viewed as inexpensive alternatives to the singular value decomposition. We developed applications to total least squares, subset selection, rank-deficient least squares.

4 List of papers/reports supported by this contract

4.1 Ph.D. Thesis

1. Jennifer Yu-Chung Chang, *Comparison of Finite Difference and the Pseudo-Spectral Approximations for Hyperbolic Equations and Implementation Analysis on Parallel Computer CM-2,* UCLA CAM 92-02, January 1992. Ph.D. thesis.

2. *Domain decomposition algorithms*, J.P. Shao, UCLA CAM report 93-38, Oct. 1993. Ph.D. thesis.

3. *Composite step conjugate gradient methods for solving nonsymmetric linear systems*, Tedd Szeto, UCLA CAM report 94-19, June 1994. Ph.D. thesis.

4.2 Papers in domain decomposition and multigrid methods

1. Tony F. Chan, Tarek P. Mathew, and Jian-Ping Shao, *Efficient Variants of the Vertex Space Domain Decomposition Algorithm*, Siam J. Sci. Comp., 15.6, 1994, 1349-1374.

2. *The interface probing technique in domain decomposition*, by T. Chan and T. Mathew, SIAM J. Matrix Anal., 13, pp. 212-238, 1992,

3. *Fourier and Probe Variants of the Vertex Space Domain Decomposition Algorithm*, by T.F. Chan, T.P. Mathew and J.P. Shao, in Proc. of 5th Int'l Symp. on Domain Decomposition Methods, D.E. Keyes (eds.), SIAM, Philadelphia, 1992, pp. 236-249.

4. *Domain Decomposition Preconditioners for Convection-Diffusion Problems*, by T.F. Chan and T.P. Mathew, Contemporary Math., 157, 1994, 157-175. Proc. of the 6th Int'l Symp. on Domain Decomposition Methods, Como, Italy, June 1992.

5. *Preconditioning Non-Symmetric and Indefinite Capacitance Matrix Problems in Domain Imbedding*, by Wlodek Proskurowski and Panayot S. Vassilevski, December 1992.

6. *A Framework for Block-ILU Factorizations Using Block–size Reduction*, by Tony F. Chan and Panayot S. Vassilevski, CAM 92-29, Accepted in final form to appear in Math. Comp.

7. *The application of a domain decomposition method to solving singular Neumann boundary problems*, by J.P. Shao, UCLA CAM repoprt 93-09.

8. *Optimal coarse grid size in domain decomposition*, by T.F. Chan and J.P. Shao, UCLA CAM report 93-24.

9. *Optimal coarse grid size in domain decomposition,* by T.F. Chan and J.P. Shao, J. Comp. Math. 12.4, 1994, 291-297.

10. *Parallel complexity of domain decomposition methods and optimal coarse grid size*, by T.F. Chan and J.P. Shao, UCLA CAM Report 941-5, 1994. To appear in Parallel Computing.

11. *Additive Schwarz domain decomposition methods for elliptic problems on unstructured meshes*, by T.F. Chan and J. Zou, Numer. Alg. 8, 329-346, 1994.

12. *Domain decomposition and multigrid algorithms for elliptic problems on unstructured meshes,* by T.F. Chan and B. Smith, In Proc. of 7th Int'l Conf. on Domain Decomposition, Penn State Univ., Oct. 93, Contemporary Math., Vol. 180, AMS, pp. 175-189, 1994. Also appeared in slightly modified form in Elec. Trans. Numer. Anal., 171-182, Vol. 2, 1994.

13. *Multigrid and domain decomposition methods for unstructured meshes,* by T.F. Chan, B. Smith and J. Zou, in "Numerical Methods and Applications", Proc. of 3rd Int'l Conf., August 1994, Sofia, Bulgaria.

14. *Domain decomposition algorithms for nonsymmetric parabolic problems on unstructured meshes,* by T.F. Chan and J. Zou, UCLA CAM Report 94-22.

15. *Overlapping Schwarz methods on unstructured meshes using non-matching coarse grids,* by T.F. Chan, B. Smith and J. Zou, UCLA CAM Report 94-8, 1994.

16. *Domain decomposition algorithms*, by T.F. Chan and Tarek Mathew, Acta Numerica, 1994, 61-143.

5 Papers in Mesh Partitioning

1. *On the optimality of the median cut spectral bisection graph partitioning method*, by T.F. Chan, P. Ciarlet Jr. and W. Szeto, UCLA CAM 93-14. To appear in SIAM J. Sci. Comp.

2. *A sign cut version of the recursive spectral bisection graph partitioning algorithm*, by T.F. Chan and W.K. Szeto, UCLA CAM 94-7. In Proc. of the 5th SIAM Conf. on Applied Lin. Alg., J.G. Lewis (ed.), pp. 562-566, SIAM, Philadelphia, 1994.

3. *An efficient low cost greedy graph partition heuristic,* by P. Ciarlet, Jr. and F. Lamour, UCLA CAM Report 94-1.

4. *Recursive partitioning methods and greedy partitioning methods: A comparison on finite element graphs,* by P. Ciarlet, Jr. and F. Lamour, UCLA CAM Report 94-9.

5. *On the influence of the partitioning schemes on the efficiency of overlapping domain decomposition methods,* by P. Ciarlet, Jr., F. Lamour and B.F. Smith, UCLA CAM Report 94-23. To appear in Proc. of Frontiers of Massively Parallel Computations Conf., Feb. 1995.

6. *On the validity of a front-oriented approach to partitioning large sparse graph with a connectivity constraint,* by P. Ciarlet, Jr. and F. Lamour, UCLA CAM Report 94-37.

5.1 Papers in Nonsymmetric Krylov subspace methods

1. *A Quasi Minimal Residual Variant of the Bi-CGSTAB Algorithm for Nonsymmetric Systems*, by T.F. Chan, E. Gallopoulos, V. Simoncini, T. Szeto and C.H. Tong, CAM 92-26, accepted in final form to appear in SIAM J. Sci. Comp., 15.2, 1994, 338-347.

2. *Composite step product methods for solving nonsymmetric linear systems*, by T.F. Chan and T. Szeto, CAM Report 94-18, talk presented at Colorado Conf. on Iter. Meth. April, 1994.

3. *A composite step bi-conjugate gradient algorithm for nonsymmetric linear systems*, by R.E. Bank and T.F. Chan, Numer. Alg. 7, 1994, 1-16.

4. *An Analysis of the Composite Step BiConjugate Gradient Method*, by R.E. Bank and T.F. Chan, November, 1992. Numer. Math. 66, 295-319, 1993.

5. *A composite step conjugate gradient squared algorithm for solving nonsymmetric linear systems*, by T.F. Chan and Tedd Szeto, Numer. Alg. 7, 1994, 17-32.

6. *The composite step family of nonsymmetric conjugate gradient methods*, by T.F. Chan and T. Szeto, In Proc. of PCG'94, Keio Univ., Yokahama, Japan. T. Nodera (ed.), Keio Univ. Press, 1994.

7. *Analysis of projection methods for solving linear systems with multiple right hand sides*, by T.F. Chan and W.L. Wan, UCLA CAM Report 94-26, 1994.

8. *Linear system solvers: sparse iterative methods*, by H. van der Vorst and T.F. Chan, UCLA CAM Report 94-28, 1994. A chapter in the Proc. of the IACSE/LaRC Workshop on Parallel Numerical Algorithms, May 23-25, 1994.

9. *Approximate and incomplete factorizations*, by H. van der Vorst and T.F. Chan, UCLA CAM Report 94-27, 1994. A chapter in the Proc. of the IACSE/LaRC Workshop on Parallel Numerical Algorithms, May 23-25, 1994.

5.2 Other papers

1. Tony F. Chan and Julia Olkin, *Circulant Preconditioners for Toeplitz-Block Matrices*, Numer. Alg., 6, 1994, 89-101.

2. *Performance Modelling for High Order Finite Difference Methods on the Connection Machine CM-2*, by Y.C. Chang and T.F. Chan, UCLA CAM report 93-04. Accepted to appear in J. Supercomputer Applic.

3. *Weighted Essentially Non-oscillatory Schemes*, by X.D. Liu, S. Osher and T.F. Chan, J. Comp. Phys., Vol. 115, 1994, 200-212.