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PARALLEL IMPLICIT ALGORITHMS FOR CFD

By
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FINAL REPORT
For the period ended September 30, 1998

December 1998

Final Report on NASA Grant NAGI-1692 (ODURF Reference Number 151671): *Parallel Implicit Algorithms for CFD*

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1 Project Overview

The main goal of this project was efficient distributed parallel and workstation cluster implementations of Newton-Krylov-Schwarz (NKS) solvers for implicit CFD. "Newton" refers to a quadratically convergent nonlinear iteration using gradient information based on the true residual, "Krylov" to an inner linear iteration that accesses the Jacobian matrix only through highly parallelizable sparse matrix-vector products, and "Schwarz" to a domain decomposition form of preconditioning the inner Krylov iterations with primarily neighbor-only exchange of data between the processors. Prior experience has established that Newton-Krylov methods are competitive solvers in the CFD context and that Krylov-Schwarz methods port well to distributed memory computers. The combination of the techniques into Newton-Krylov-Schwarz was implemented on 2D and 3D unstructured Euler codes on the parallel testbeds that used to be at LaRC and on several other parallel computers operated by other agencies or made available by the vendors. Early implementations were made directly in MPI with parallel solvers we adapted from legacy NASA codes and enhanced for full NKS functionality. Later implementations were made in the framework of the PETSc library from Argonne National Laboratory, which now includes pseudo-transient continuation Newton-Krylov-Schwarz solver capability (as a result of demands we made upon PETSc during our early porting experiences).

A secondary project pursued with funding from this contract was parallel implicit solvers in acoustics, specifically in the Helmholtz formulation. A 2D acoustic inverse problem has been solved in parallel within the PETSc framework.

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2 Papers and Book Chapters Supported In Part by the Contract

Details on the specifics of the research accomplished under partial sponsorship of this contract have been widely published, including in the following archival publications, listed in reverse chronological order. (The first four of these are available on the WWW in advance of publication.)

1. *Trends in Algorithms for Nonuniform Applications on Hierarchical Distributed Architectures*, D. E. Keyes, 1998, in "Computational Aerosciences in the 21st Century" (M. D. Salas, et al. eds.), Kluwer, Dordrecht (to appear).

2. *How Scalable is Domain Decomposition in Practice?*, D. E. Keyes, 1998 (under review for Proceedings of the 11th International Symposium on Domain Decomposition Methods).

3. *Newton-Krylov-Schwarz Methods for Aerodynamics Problems: Compressible and Incompressible Flows on Unstructured Grids*, D. K. Kaushik, D. E. Keyes and B. F. Smith, 1998 (under review for Proceedings of the 11th International Symposium on Domain Decomposition Methods).

4. *Globalized Newton-Krylov-Schwarz Algorithms and Software for Parallel Implicit CFD*, W. D. Gropp, D. E. Keyes, L. C. McInnes and M. D. Tidriri, 1998, ICASE Technical Report 98-24 (under review for International Journal of Supercomputer Applications).

5. *Parallel Newton-Krylov-Schwarz Algorithms for the Transonic Full Potential Equation*, X.-C. Cai, W. D. Gropp, D. E. Keyes, R. G. Melvin & D. P. Young, 1998, SIAM J. Sci. Comp. 19:246–265.

6. *Convergence Analysis of Pseudo-Transient Continuation*, C. T. Kelley & D. E. Keyes, 1998, SIAM J. Num. Anal. 35:508–523.

7. *Additive Schwarz Methods for Hyperbolic Equations*, Y. Wu, X.-C. Cai & D. E. Keyes, 1998, in "Proceedings of the 10th International Conference on Domain Decomposition Methods" (J. Mandel et al., eds.), AMS, Providence, pp. 513–521.

8. *On the Interaction of Architecture and Algorithm in the Domain-Based Parallelization of an Unstructured Grid Incompressible Flow Code*, D. K. Kaushik, D. E. Keyes & B. F. Smith, 1998, in "Proceedings of the 10th International Conference on Domain Decomposition Methods" (J. Mandel et al., eds.), AMS, Providence, pp. 311–319.

9. *Parallel Implicit PDE Computations: Algorithms and Software*, W. D. Gropp, D. E. Keyes, L. C. McInnes & M. D. Tidriri, 1997, in "Proceedings of Parallel CFD '97" (A. Ecer et al., eds.), North Holland, Amsterdam, pp. 333–344.

10. *Prospects for CFD on Petaflops Systems*, D. E. Keyes, D. K. Kaushik & B. F. Smith, 1997, in "CFD Review" (M. Hafez et. al., eds.), Wiley, New York (to appear).

11. *Newton-Krylov-Schwarz: An Implicit Solver for CFD*, X.-C. Cai, D. E. Keyes & V. Venkatakrishnan, 1997, in "Proceedings of the Eighth International Conference on Domain Decomposition Methods" (R. Glowinski et al., eds.), Wiley, Chichester, pp. 387–402.

12. *Newton-Krylov-Schwarz Methods: Interfacing Sparse Linear Solvers with Nonlinear Applications*, D. E. Keyes & V. Venkatakrishnan, 1996, Zeitschr. Angew. Math. **76**(Suppl. 1):147–150.

13. *Application of Newton-Krylov Methodology to a Three-Dimensional Unstructured Euler Code*, E. J. Nielsen, R. W. Walters, W. K. Anderson & D. E. Keyes, 1995, in "Proceedings of the 12th AIAA Computational Fluid Dynamics Conference" (San Diego, June 1995), AIAA Paper 95-1733.

3 Presentations Crediting NASA Support

Results from the project have been featured, with credits to NASA, in presentations at the following conferences and workshops, as well as in NASA Langley presentations and many departmental seminars:

1. Eleventh International Conference on Domain Decomposition Methods, Greenwich, England, July 1998.

2. Workshop in Honor of Professor V. S. Ryaben'kii, ICOSAHOM'98, Tel Aviv, Israel, June 1998.

3. Petaflops Systems Operations Review (POWR) Workshop, Bodega Bay, CA, June 1998.

4. Computational Aerosciences in the 21st Century, NASA-Langley, Hampton, VA, April 1998.

5. Workshop on Adaptive Methods for Differential Equations, Royal Institute of Technology (KTH), Stockholm, Sweden, March 1998.

6. Numerical Analysis Conference in Honor of Olof B. Widlund on the Occasion of his 60th Birthday, Courant Institute, NY, January 1998.

7. Tenth International Conference on Domain Decomposition Methods, Boulder, CO, August 1997.

8. SIAM Annual Meeting, Stanford, CA, July 1997.

9. Workshop on the Future of High Performance Computing, Bergen, Norway, May 1997.

10. Workshop on Algorithms for Petaflops Computing, Williamsburg, VA, April 1997.

11. Eighth SIAM Conference on Parallel Processing for Scientific Computing, Minneapolis, MN, March 1997.

12. Workshop on Computational Heat Transfer, Las Vegas, NV, March 1997.

13. Workshop on Structured Adaptive Mesh Refinement, Institute for Mathematics and its Applications (IMA), Minneapolis, MN, March 1997.

14. Ninth International Conference on Domain Decomposition Methods in Science and Engineering, Bergen, Norway, June 1996.

15. Workshop on Iterative Methods, International Linear Algebra Year, CERFACS, Toulouse, France, June 1996.

16. Conference on Iterative Methods, Copper Mountain, CO, April 1996.

17. SIAM Annual Meeting, Charlotte, NC, October 1995.

18. Iterative Methods for Large Scale Nonlinear Problems, Utah State University, Logan, UT, September 1995.

19. ICIAM '95, Hamburg, Germany, July 1995.

20. Eighth International Conference on Domain Decomposition Methods in Science and Engineering, Beijing, China, May 1995.

# 4 Personnel Supported by the Contract

1. Satish Balay, M.S. in Computer Science, 1995, Old Dominion University

2. Kumar Kareti, M.S. in Computer Science, 1995, Old Dominion University

3. Dinesh Kaushik, currently Ph.D. candidate

4. Jay Morris, currently Ph.D. candidate

5. Yunhai Wu, post-doctoral fellow in Computer Science, Old Dominion University

5 Project Highlight

The project has demonstrated the feasibility of scaling important implicit external aerodynamics problems to the thousand-processor regime, permitting large grids (in the millions of vertices) to be employed in structured and unstructured discretizations, in incompressible and compressible regimes.

A recently achieved "high water mark" stemming from the algorithmic and software efforts undertaken under this contract is presented in histogram form

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below. The performance data is for steady incompressible Euler flow over an
ONERA M6 Wing, converged ten orders of magnitude in residual norm from
a uniform initial field, on a tetrahedral grid of 2,761,744 vertices, based on
a KMeTiS-PETSc implementation of NASA code FUN3D run on up to 1024
processors of a 600 MHz T3E made available courtesy of SGI-Cray. The im-
plementation was principally performed by Dinesh Kaushik, an ODU doctoral
candidate supported in part by this grant, under the guidance of David Keyes
of ODU and ICASE and Barry Smith of Argonne National Laboratory.
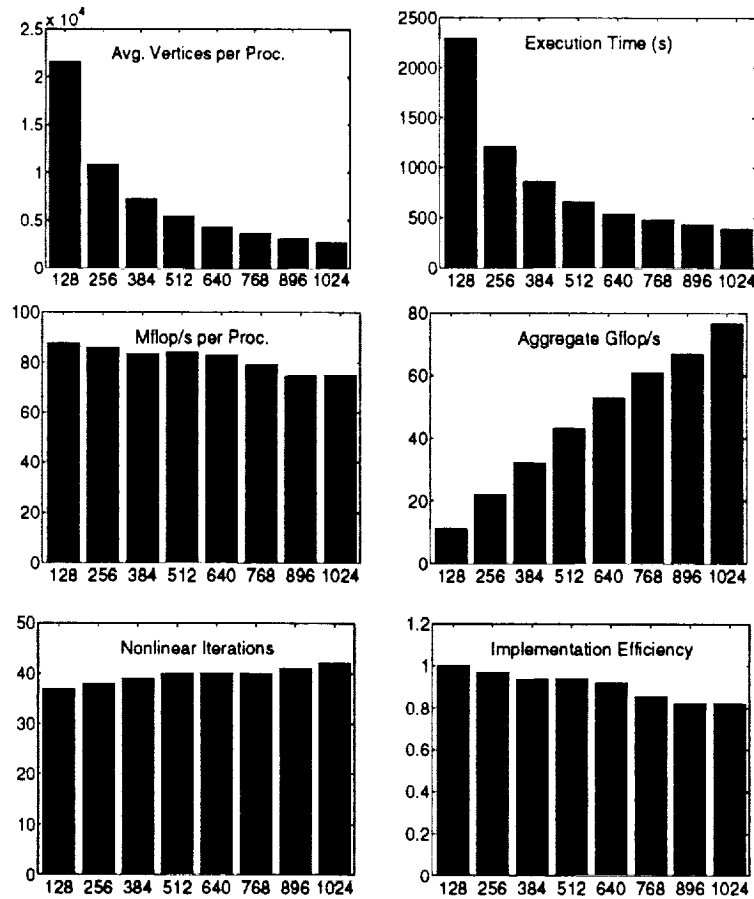
The fixed-problem-size scaling study shows reductions in wallclock execution
time that closely follow the number of vertices per processor, as processors are
varied from 128 in number to 1024. The lower end of the range is limited by per-
node memory capacity; the upper end is not intrinsically limited, but marginal
efficiency is beginning to be defeated by subdomain surface-to-volume ratio.

The middle row of figures shows that the computational rate per processor
remains nearly level as problem size per processor varies over a range of 8.

Therefore the aggregate computational grows rate nearly linearly in processor number, to nearly 80 Gflop/s.

The bottom row shows that there is only a small degradation in convergence rate as the number of processors is increased and the Schwarz preconditioner is divided into finer diagonal blocks. The final figure shows implementation efficiency (speedup per processor on a per-iteration basis) in excess of 80% over a range of 8-fold in processor number.

6   Leveraged Activities

The research undertaken pursuant to this contract has been aided by the following other grants and contracts awarded to the same principal investigator at Old Dominion University. The process of obtaining some of these other grants was significantly enhanced by the credibility of the original contract from NASA, which predated all of them. Hence, the funds from NASA were effectively employed as seed funds to accomplish work of importance to NASA, as well as to three other federal agencies.

1. *Parallel PDE Algorithms for the Accelerated Strategic Computing Initiative.* LLNL (DOE), 10/97 – 9/98.

2. *Development and Application of the Portable Extensible Toolkit for Scientific Computing.* ANL (DOE), 9/97 – 10/97.

3. *A Numerical Laboratory for Multi-Model Multi-Domain Computational Methods in Aerodynamics and Acoustics.* NSF, 10/95 – 9/98.

4. *Graduate Fellowships in Computer Science* (GAANN). U. S. Dept. of Education, 9/95 – 8/98.

5. *Solution-Adaptive Grid Partitioning and Variable Ordering for PDEs.* NSF, 7/95 – 6/98.