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RNR NAS, NASA AMES RESEARCH CENTER, GRANT NAG 2-827
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CHARBEL FARHAT

*Department of Aerospace Engineering Sciences
Center for Aerospace Structures
University of Colorado at Boulder
Boulder, CO 80309-0429*

SUMMARY

This is a final report on the research work supported by the RNR NAS at NASA Ames Research Center under Grant NAG 2-827, **Massively Parallel and Scalable Implicit Time Integration Algorithms for Structural Dynamics**.

1. Motivations and research plan

Explicit codes are often used to simulate the nonlinear dynamics of large-scale structural systems, even for low frequency response, because the storage and CPU requirements entailed by the repeated factorizations traditionally found in implicit codes rapidly overwhelm the available computing resources. With the advent of parallel processing, this trend is accelerating because of the following additional facts: (a) explicit schemes are easier to parallelize than implicit ones, and (b) explicit schemes induce short range inter-processor communications that are relatively inexpensive, while the factorization methods used in most implicit schemes induce long range interprocessor communications that often ruin the sought-after speed-up. However, the time step restriction imposed by the Courant stability condition on all explicit schemes cannot yet be offset by the speed of the currently available parallel hardware. Therefore, it is essential to develop efficient alternatives to direct methods that are also amenable to massively parallel processing because implicit codes using unconditionally stable time-integration algorithms are computationally more efficient when simulating the low-frequency dynamics of aerospace structures.

We have proposed to develop, under the NASA Research Announcement NRA2-35250(JLB), a massively parallel scalable methodology for large-scale implicit transient

computations in structural mechanics that requires significantly less storage than factorization algorithms, that is several times faster than other popular direct and iterative solvers, which can be easily implemented on both shared and local memory parallel processors, and which is both computationally and communication-wise efficient. The key ingredients of this methodology will be: (a) a novel unconditionally stable time integration algorithm for hybrid substructuring methods, (b) a domain decomposition method based on a hybrid variational principle and featuring a massively parallel and numerically efficient preconditioner, and (c) a mesh partitioning algorithm for implicit computations that optimizes a compromise between load balancing and communication costs.

More specifically, we have proposed three tasks to be completed during a three-years research program:

- TASK 1: the design of an unconditionally stable and second order accurate parallel implicit time-integration scheme that is based on the FETI domain decomposition methodology developed by the PI.
- TASK 2: the development of a scalable parallel preconditioner for problems with a large number of subdomains; for these problems, the spectrum of the interface operator with the “lumped” preconditioner previously developed is such that superconvergence conditions are not met.
- TASK 3: the development of a two-level mesh partitioning strategy that would allow controlling the growth of the condition number of the interface problem by keeping the number of subdomains relatively small — and therefore, the subdomain aspect ratio close to unity —, without reducing the degree of parallelism of the domain decomposition method. Toward the end of the first funding year, we have found that the same objectives could be better achieved via the design of a coarsening operator for dynamics problems that would propagate the error globally, control the condition number associated with fine mesh partitions, and therefore accelerate convergence.

After several discussions with our first grant monitor, Dr. Eddy Pramono, the following two tasks were added:

- TASK 4: the tuning of the parallel domain decomposition method for problems with multiple and/or repeated right hand sides in order to solve efficiently linear transient problems such as those encountered in aeroelastic dynamic computations.
- TASK 5: the improvement of the performance of the FETI domain decomposition method for heterogeneous plate and shell substructures such as those encountered in stiffened aircraft wings.

2. Progress history

2.1. TASK 1

TASK 1 was completed during the first year of the grant.

2.2. TASK 2

During the first funding year, we have developed a scalable parallel preconditioner based on a force/displacement interpretation of the FETI methodology, and have implemented it on the iPSC-860 parallel processor. This preconditioner is optimal in the sense that it ensures a performance that is independent of the mesh size. However, it is more expensive than the original lumped preconditioner and requires more storage. The relative performance of both preconditioners is problem dependent, and machine dependent in the sense that memory can be a limitation for the optimal preconditioner. However, both preconditioners outperform a direct skyline solver.

During the second funding year, we have coupled both lumped and optimal preconditioners with the coarse grid operator developed for dynamic problems to ensure a performance that is independent of the number of subdomains. We have also analyzed the effect of the subdomain aspect ratio on the convergence rate of the preconditioned FETI method and developed a fast optimization algorithm for improving the aspect ratio of existing mesh partitions. We have shown that the new optimization algorithm can improve the solution time of the FETI method factors greater than 1.6.

During the third funding year, we have improved both lumped and optimal preconditioners to solve efficiently heterogeneous plate and shell structures.

2.3. TASK 3

During the second and third funding years, we have developed a new efficient and scalable domain decomposition method for solving implicitly linear and nonlinear time-dependent problems in computational mechanics. The method is derived by adding a coarse problem to the transient FETI substructuring algorithm developed during the first funding year in order to propagate the error globally and accelerate convergence. We have proved that in the limit for large time steps, the new method converges toward the FETI algorithm for time-independent problems. We have reported computational results that confirm that the optimal convergence properties of the time-independent FETI method are preserved in the time-dependent case. We have also presented an iterative scheme for solving efficiently the coarse problem on massively parallel processors, and demonstrated the effective scalability of the new transient FETI method with the large-scale finite element dynamic analysis on the Paragon XP/S system of several diffraction grating finite element structural models. We have shown that for sufficiently large problems and/or fine mesh partitions, the new domain decomposition method outperforms both the original one and the popular direct skyline solver.

2.4. TASK 4

During the second funding year, we have also developed a methodology for extending the range of applications of domain decomposition methods to problems with multiple or repeated right hand sides. Such problems arise, for example, in multiple load static analyses, in implicit linear dynamics computations, in the solution of nonlinear problems via a quasi-Newton scheme, in various structural eigenvalue problems, and in the iterative solution of the FETI coarse grid problems. Basically, we have formulated the overall problem as a series of minimization problems over K -orthogonal and supplementary subspaces, and tailored the preconditioned conjugate gradient algorithm to solve them efficiently. The resulting solution method is scalable, whereas direct factorization schemes and forward and backward substitution algorithms are not. We have illustrated the proposed methodology with the solution structural dynamic problems, and highlighted its potential to outperform forward and backward substitutions on the iPSC-860 and Paragon XP/S computers. Of particular importance is the impact of this methodology on the scalable parallel solution of coarse grid problems.

During the third funding year, we have extensively benchmarked the new transient FETI solver resulting from TASK 3 and TASK 4 and applied it to the massively parallel solution of realistic aeroelastic simulations. We have also transferred this technology to several aerospace companies and finite element software houses including Lockheed and Centrics.

2.5. TASK 5

Numerical experiments have shown us that for stiffened shell problems such as those encountered in aircraft wing structures, and/or problems with heterogeneous substructures (jumps in the material properties), the FETI method does not perform as well as for smoother problems. Indeed, shell problems are related to the biharmonic operator, and therefore are more ill-conditioned than elasticity problems which are related to the Laplacian operator. Moreover, jumps in the material properties across the substructure interfaces require a different redistribution of the interface tractions and jumps than currently done in the FETI method. Addressing both issues would improve the performance of the FETI method for extremely difficult problems and enhance its robustness.

During the second and third years of funding, we have addressed mainly the heterogeneous substructures problem; we have devised a smoothing operator for the FETI method that improves its convergence rate when applied to these difficult problems encountered in wing-box structures. This smoothing operator has been validated for model problems. During the third year of funding, we have further developed this smoother for realistic structural models and initiated its integration in the full FETI code. Finally, we have also augmented the FETI method with corner modes in order to handle more efficiently plate and shell problems.

3. Publications that have resulted from the three years of support

1. C. Farhat, P. S. Chen and F. X. Roux, "The Two-Level FETI Method - Part II: Extension to Shell Problems, Parallel Implementation and Performance Results," *Computer Methods in Applied Mechanics and Engineering*, (in press)
2. C. Farhat and J. Mandel, "The Two-Level FETI Method for Static and Dynamic Plate Problems - Part I: an Optimal Iterative Solver for Biharmonic Systems," *Computer Methods in Applied Mechanics and Engineering*, (in press)
3. D. Rixen and C. Farhat, "Preconditioning the FETI and Balancing Domain Decomposition Methods for Problems with Intra- and Inter-subdomain Coefficient Jumps," *Domain Decomposition Methods for Partial Differential Equations*, ed. by P. Bjorstad, M. Espedal, and D. Keyes, Wiley and sons, (in press)
4. C. Farhat, M. Lesoinne, P. Stern and S. Lantéri, "High Performance Solution of Three-Dimensional Nonlinear Aeroelastic Problems Via Parallel Partitioned Algorithms: Methodology and Preliminary Results," *Advances in Engineering Software*, Vol. 28, pp. 43-61 (1997)
5. D. Vanderstraeten, C. Farhat, P. S. Chen, R. Keunings and O. Zone, "A Retrofit and Contraction Based Methodology for the Fast Generation and Optimization of Mesh Partitions: Beyond the Minimum Interface Size Criterion," *Computer Methods in Applied Mechanics and Engineering*, Vol. 133, pp. 25-45 (1996)
6. C. Farhat, S. Lantéri and H. D. Simon, "TOP/DOMDEC, A Software Tool for Mesh Partitioning and Parallel Processing," *Journal of Computing Systems in Engineering*, Vol. 6, No. 1, pp. 13-26 (1995)
7. C. Farhat, L. Crivelli and M. Geradin, "Implicit Time Integration of a Class of Constrained Hybrid Formulations - Part I: Spectral Stability Theory and Linear Applications," *Computer Methods in Applied Mechanics and Engineering*, Vol. 125, pp. 71-107 (1995)
8. C. Farhat, N. Maman and G. Brown, "Mesh Partitioning for Implicit Computations via Iterative Domain Decomposition: Impact and Optimization of the Subdomain Aspect Ratio," *International Journal for Numerical Methods in Engineering*, *International Journal for Numerical Methods in Engineering*, Vol. 38, pp. 989-1000 (1995)
9. C. Farhat, P. S. Chen and P. Stern, "Towards the Ultimate Iterative Substructuring Method: Combined Numerical and Parallel Scalability, and Multiple Load Cases," *Journal of Computing Systems in Engineering*, Vol. 5, No. 4-6, pp. 337-350 (1995)
10. C. Farhat, "Optimizing Substructuring Methods for Repeated Right Hand Sides, Scalable Parallel Coarse Solvers, and Global/Local Analysis," *Domain-Based Parallelism and Problem Decomposition Methods in Computational Science and Engineering*, ed. by D. Keyes, Y. Saad and D. G. Truhlar, SIAM, pp. 141-160 (1995)
11. C. Farhat, P. S. Chen and J. Mandel, "A Scalable Lagrange Multiplier Based Domain Decomposition Method for Implicit Time-Dependent Problems," *International Journal of Numerical Methods in Engineering*, Vol. 38, pp. XX-XX (1995)

12. C. Farhat, F. Hemez, and J. Mandel "Improving the Convergence Rate of a Transient Substructuring Iterative Method Using the Rigid Body Modes of its Static Equivalent," *AIAA Paper 95-1271, AIAA 36th Structural Dynamics Meeting*, New Orleans, Louisiana April 10-13 (1995)
13. C. Farhat, L. Crivelli and F. X. Roux, "A Transient FETI Methodology for Large-Scale Parallel Implicit Computations in Structural Mechanics," *International Journal for Numerical Methods in Engineering*, Vol. 37, pp. 1945-1975 (1994)
14. C. Farhat, L. Crivelli and F. X. Roux, "Extending Substructure Based Iterative Solvers to Multiple Load and Repeated Analyses," *Computer Methods in Applied Mechanics and Engineering*, Vol. 117, pp. 195-209 (1994)
15. C. Farhat and P. S. Chen, "Tailoring Domain Decomposition Methods for Efficient Parallel Coarse Grid Solution and for Systems with Many Right Hand Sides," *Contemporary Mathematics*, Vol. 180, pp. 401-406 (1994)

4. Technology transfert

4.1. TOP/DOMDEC

The TOP/DOMDEC software package for mesh partitioning and parallel processing is currently used in many places in both industry and government laboratories including IBM, SGI, Lockheed, Ford Motors, Centrics, the Livermore National Laboratories, and MCNC.

4.2. FETI

The FETI solvers have been implemented in production codes at Lockheed and Ford Motors, and are currently being examined by commercial finite element software houses.

4.3. Projection based preconditioners

The projection based preconditioners and techniques for solving iteratively systems with multiple/repeated right hand sides have found their way in the Spectrum code of Centrics.

