

PARTITIONING ALGORITHMS AND THEIR APPLICATION TO MASSIVELY PARALLEL COMPUTATIONS OF MULTI-PHASE FLUID FLOWS IN POROUS MEDIA

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I. Summary of the Overall Progress

In agreement with the research plan, during the second year we have concentrated our efforts and achieved good progress in the following interrelated groups of problems:

- (1) Local error estimators and refinement strategies;
- (2) Algorithms for partitioning and load balancing;
- (3) Nonconforming domain decomposition methods and mortar approximations;
- (4) Domain decomposition structure for parallel computations in fluid flow modeling;
- (5) Finite volume element methods for reactive flows in porous media.

1. Local error estimators and refinement strategies

We have tested our 2-dimensional code for adaptive grid refinement to the problem of flows in presence wells and used the technique of multilevel grid refinement. We have experimentally studied applications of this code to bio-screen problem (see some of the particular numerical experiments on our website <http://www.isc.tamu.edu/EPA/parallelcomp.html>). It provides a useful and efficient tool in the simulation of two-dimensional models of reactive flows in porous media.

We have concentrated our research on the problem of adaptive local grid refinement for 3-dimensional problems. This effort was very time consuming and related to search and installation of reliable 3-D mesh generator, connection with a partitioner of the mesh based on our previous research and design and implementation of a suitable data structure for the adaptive computations.

We have theoretically address problems of local refinement in the finite volume element method and implemented our findings into the 2-D code. We have implemented fully auto-

matic adaptive grid refinement strategy in the 2-D code on general grids. See some examples on our website <http://www.isc.tamu.edu/EPA/parallelcomp.html>.

2. Algorithms for partitioning and load balancing

We have concentrated our efforts on implementation issues, working on two versions of our partitioning algorithms. The first implementation uses a simpler strategy for searching the graph based on the levels of a breadth-first search combined with recursive bisection. In addition, separators that give better ratio of component to boundary sizes were given higher priority than those that give a better balance. The second implementation is of an algorithm that exploits the planarity of the mesh and divides the graph directly into p parts, instead of recursively subdividing.

This algorithm works better for triangulations of high aspect ratios. Our work on dynamic separators focused on the use of amortization and average case analysis in order to improve the average query time.

3. Nonconforming domain decomposition methods and mortar approximations

In the recent years there has been growing interest in the finite volume method (called also control-volume method or box-schemes). This interest is mostly due to the desire of having discretizations which are locally conservative. This is a discrete variant of the property of the continuous model which expresses conservation of certain quantity (mass, heat, momentum, etc). In the early stages, such methods were based on finite differences on rectangular meshes with quite complicated treatment of the coefficients and the right-hand side. therein).

Recently, the finite volume approach has been combined with the technique of the finite element method in a new development which is capable of producing accurate approximations on general triangular and quadrilateral grids.

The main advantages of the method are compactness of the discretization stencil, good accuracy, and discrete local conservation, which for many applications is the most desirable feature of the approximation. In particular, this technique is very suitable for groundwater simulations by several reasons. First, it gives a flexibility of mesh the domain independently and in parallel, so that multi block approach highly recommended and widely used by the group of M. Wheeler can be implemented in a natural way. Secondly, it allows a independent coarsening and refining in the subdomains so efficient solution methods can be employed. And finally, it gives a possibility of sliding meshes and moving grids whenever this is necessary in presence of faults.

We have extended the mortar technique to the finite volume methods in two ways. First, following the traditional mortar approach we have used finite volume element approximations only on the subdomains and finite element on the interfaces for Lagrange multipliers. Second,

we have proposed numerical schemes using finite volume element on both the subdomains and on the interfaces. It has been shown on various numerical examples that the latter scheme converge much fast (5-8 times) than the former. This resulted in the works [proc-ell], [proc-lpv], [TR-coupl], and [TR-klpv].

4. Implementation of the domain decomposition structure on parallel computers

We have completed our 2-D code development and currently we have a running code for finite element approximations to steady-state and transient second order problems on our Intel-Paragon. They model single phase and two-phase Richard's flows in porous media. Currently we are running 2-D test problems on bio-screen model with one concentration and 2-D reservoirs with one and two wells.

We have investigated also a new and very promising technique for domain decomposition computations using non-matching grids using non-matching grids. A multi-grid technique for uniformly preconditioning linear systems arising from a mortar finite element discretization of second order elliptic boundary value problems has been introduced and analyzed.

5. Finite volume element methods for reactive flows in porous media

We have studied finite volume element methods for one-dimensional and two-dimensional problems of nonlocal reactive transport in underground water flows in porous media. The developed general framework for obtaining finite volume element approximations and studying their error analysis included linear elements and L -splines and very detailed study of the properties and the error in various norms. All developed schemes are locally conservative and have optimal approximation properties in both 1-D and 2-D problems. Our next goal is to exploit the theory in order to simulate efficiently multidimensional time-dependent problems. For more detail about the developed theory we refer to [jour-ell1] and [jour-ell2].

II. A Brief Summary of Plans for the Final Year

We intend to continue the work initiated during the first three years. The problems we list here either emerged during our work during this phase, or are natural extensions and improvements of results reported in Section 1 of this report. This list is in close correspondence with the original plan of our project.

1. Local error estimators and adaptive grid refinement

We shall continue our research from the previous years. Firstly, we plan to theoretically address problems of local refinement and well models and implement these strategies in our codes. We plan to implement 3-D grid refinement algorithms based on the analysis of the singular behavior of the solution in the vicinity of any singularity in the general framework of multilevel grid refinement.

Secondly, we shall design and implement an adaptive error estimates and the error indicators for designing adaptive strategies for finite volume element approximations based on a posteriori error estimates.

Our goal will be fully automatic adaptive grid refinement strategy implemented in a 2-D code on general grids.

2. Algorithms for partitioning and load balancing

We plan to continue our implementation efforts by adding more algorithms and combining several strategies (e.g., multilevel partitioning, spectral partitioning, and Kernighan-Lin). We will also do some experimental work by running our algorithms on very large meshes and comparing the speed and the quality of the resulting partitions with those of other approaches. On the problem of partitioning weighted graphs, we plan to continue our study on three dimensional meshes. We expect that the ideas of our algorithm for two dimensions could be generalized to 3-d.

3. Using separators for adaptive mesh partitioning and refinement

We plan to continue our ongoing work, by studying how the springs method works for smoothing three dimensional meshes. Next we will examine the more difficult problem of adapting the ideas for producing a new algorithm for mesh generation. We expect that such a generalization will not be straightforward, but feel that there are useful properties of our approach that should be further exploited for the mesh generation problem.

4. Implementation of the domain decomposition structure on parallel computers

Our goal for the final year is to have a running parallel code on SGI Origin 2000 and investigate various refinement strategies and methods for grid partitioning with load balancing. We shall to put together the results in optimal graph partitioning and grid refinement to experimentally study the performance of the method and for computer simulations of ground-flow computations. Examples of such flows are bio-screens, water reservoirs, and petroleum reservoirs.

Another step in our research will be to consider mortar domain methods for gluing together approximations on non-matching grids. Finally, we shall explore and implement grid refinement strategies for 3-D problems and implement highly efficient iterative techniques based on the BPS and BEPS-like preconditioners. We plan to apply these schemes for contaminant transport in groundwater reservoirs.

5. Finite volume approximations for steady-state and transient flows

We intend to study finite volume methods that will lead to more accurate locally conservative approximations. Based on this new method and hierarchical presentation of the basis, we shall develop a strategy of a posteriori error analysis and algorithms for grid refinement. Here

we shall include also strategies for adaptive grids to nonlocal in time transient problems. This class of methods are more expensive in terms of memory and adaptivity will need special consideration on the integral term, since the grid will change in time.

III. Publications Resulted from the Support of the Grant

Accepted or published in journals

- jour-jg H. N. Djidjev, J.R. Gilbert, Separators in graphs with negative or multiple vertex weights, (accepted in *Algorithmica*).
- jour-ell1 R. Ewing, R. Lazarov, and Y. Lin, Finite volume element approximations of nonlocal in time one-dimensional flows in porous media, (accepted to *Computing*).
- jour-ell2 R. Ewing, R. Lazarov, and Y. Lin, Finite volume element approximations of nonlocal reactive transport in porous media in 2-D (accepted to *Numer. Meth. PDEs*).
- jour-gp J. Gopalakrishnan and J. Pasciak), Multigrid for the mortar finite element method, (to appear in *SIAM J. Numer. Anal.*).
- jour-elp R. Ewing, R. Lazarov, S. Lyons, D. Papavassiliou, and J. Pasciak, Numerical well models for non-Darcy flows, (to appear in *Computational Geosciences*).

Invited presentation and presentations at refereed conferences

- proc-AMS R. Lazarov, J. Pasciak, and P. Vassilevski, Locally conservative discretizations on non-matching grids, 948-th AMS Meeting, October 8-10, 1999, University of Texas, Austin, Texas.
- proc-aj L.G. Aleksandrov, H.N. Djidjev, Maintaining Partitions of Dynamic Planar Meshes, *Proceedings of Canadian Conference on Computational Geometry (CCCG'98)*, in print.
- proc-alms L. Aleksandrov, M. Lanthier, A. Maheshvari, J.-R. Sack, An ε -approximation algorithm for weighted shortest paths on polyhedral surfaces, *Proceedings of Scandinavian Workshop of Algorithmic Theory (SWAT'98)*, in print.
- proc-ell R. Ewing, R. Lazarov, Y. Lin, Finite volume element approximations of integro-differential parabolic problems, *Recent Advances in Numerical Methods and Applications* (O. Iliev, M. Kaschiev, S. Margenov, Bl. Sendov, P. Vassilevski, Eds.), 1998, World Scientific, 1999, 3–15.
- proc-elll R. Ewing, R. Lazarov, T. Lin, and Y. Lin, Domain decomposition capabilities for the mortar finite volume element methods, to appear in *Proc. Eleventh Conference on Domain Decomposition Methods*, London, 1998.

- proc-fkvv Feigenbaum, J., Kannan, S., Vardi, M.Y., Viswanathan, M.: Complexity of Problems on Graphs Represented by OBDDs, *Proc. 15th Symp. on Theoretical Aspects of Computer Science*, Springer-Verlag, Lecture Notes in Computer Science 1373, (1998), 216–226.
- proc-lpt R. Lazarov, J. Pasciak, and S. Tomov, Multilevel grid refinement based on a posteriori error control for second order elliptic problems, to appear in *Analytical and Numerical Methods for Singularly Perturbed Problems*, Nuova Science Publishing House, USA, Proc. Workshop on Solution Methods for Singularly Perturbed Problems held August 26-31, 1998, Lozenetz, Bulgaria .
- proc-lpv R. Lazarov, J. Pasciak, and P. Vassilevski, Coupling mixed and finite volume discretizations of convection-diffusion-reaction equations on non-matching grids, in *Finite Volumes for Complex Applications II. Problems and Perspectives*, R. Vilsmeier, F. Benkhaldoun, and D. Hanel eds, Hermes Science Publications, Paris, 1999, pp. 51- 68.
- proc-lv R. Lazarov and P. Vassilevski, Least-squares streamline diffusion finite element approximations to singularly perturbed convection-diffusion problems, to appear in *Analytical and Numerical Methods for Singularly Perturbed Problems*, Nuova Science Publishing House, USA, Proc. Workshop on Solution Methods for Singularly Perturbed Problems held on August 26-31, 1998, Lozenetz, Bulgaria.

Submitted to journals

- jour-j1 H. Djidjev, Partitioning planar graphs with vertex costs: algorithms and applications, submitted to *Algorithmica*.
- jour-lpv R. Lazarov, J. Pasciak, and P. Vassilevski, Iterative solution of a combined mixed and standard Galerkin discretization method for elliptic problems, (submitted to *Numer. Linear Algebra Appl.*)

Technical reports

- TR-elp R. Ewing, R. Lazarov, S. Lyons, D. Papavassiliou, and J. Pasciak, Numerical well models for non-Darcy flows, *Technical Report ISC-98-05-MATH*.
- TR-gp J. Gopalakrishnan and J. Pasciak, Multigrid for the mortar finite element method, *Technical Report ISC-98-04-MATH*.
- TR-lpt R. Lazarov, J. Pasciak, and S. Tomov, Multilevel grid refinement based on a posteriori error control for second order elliptic problems, *Technical Report ISC-98-06-MATH*.
- TR-klpv C. Kim, R. Lazarov, J. Pasciak, and P. Vassilevski, Multiplier spaces for the mortar finite element method in three dimensions, *Technical Report ISC-99-XX-MATH* (in preparation).

TR-couple R. D. Lazarov, J. E. Pasciak, and P. S. Vassilevski, Coupling mixed and finite volume discretizations of convection-diffusion-reaction equations on non-matching grids
Technical Report ISC-99-07-MATH.