MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 6/1992

Numerical Methods for Parallel Computers

09.02. - 15.02.1992

The conference was chaired by W. Hackbusch (Kiel), R. Rannacher (Heidelberg) and O. Widlund (New York). In 33 lectures the following actual research topics were addressed:

- Parallel algorithms in linear algebra
- Preconditioning methods based on domain decomposition
- Parallelization of multi-level methods
- Parallel methods in flow problems and in oil reservoir simulation
- Parallel time stepping schemes
- Parallelization in BE- and in coupled FE-BE-methods

The discussions concentrated on the efficiency of the proposed parallelization strategies and their effective implementation on existing massively parallel computers. The central question was that of a proper balance between "parallel" efficiency (degree of utilization of the computer) and "computational" efficiency (speed of the algorithm). In parallel *numerical* algorithms the adventage seems to be on the side of the "fast solution methods" which are highly efficient but usually difficult to parallelize. This opens a wide field for further theoretical research which has to be accompanied by intensive numerical experiments. There practical relevance has to be proven through large scale applications which are coming up now with the increasing availability of massively parallel computers. The most prominent and yet unsolved problems are the automatic minimization of the communication overhead and the dynamic load balancing within an adaptive solution procedure.

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Abstracts

O. AXELSSON:

Algebraic multilevel iteration method

A recursive method to construct preconditoners to a symmetric, positive definite matrix is presented using an algebraic multilevel technique based on the partitioning of the matrix in two by two matrix block form, approximating some of these by matrices with more simple sparsity structure and using the corresponding Schur complement as a matrix on the lower level. The quality of the preconditioners for such a matrix sequence is improved by matrix polynomials of special type which recursively connect the preconditioners on every two adjoining levels.
Upper and lower bounds for the degree of the polynomials are derived as conditions for a computational complexity of optimal order for each level and for an optimal rate of convergence, respectively. The method is an extended and more acurate algebraic formulation of a method for nine-point and mixed five- and nine-point difference matrices, presented in some previous papers.

G. BADER:

Parallel solution of a flame sheet model

The numerical solution of flame problems amount to the solution of highly nonlinear, transport dominated systems of partial differential equations. Known domain decomposition methods experience potential convergence difficulties when applied for such problems. We present an alternative parallelization, called "algebraic" domain decompositon, which does not suffer any slow down of convergence speed. Numerical results, obtained on a transputer system, are presented. They demonstrate the high parallel efficiency of this approach.

P. BASTIAN:

Adaptive multigrid solution of unsymmetric and nonlinear problems

A multigrid method with smoothing only in refined regions is presented. The method has been applied to several unsymmetric and nonlinear problems including dominating convection. Some issues of the parallelization of such a method are discussed, especially dynamic load balancing.

C.M. BERGMAN:

CFD on SIMD machines

A 2D multi-block Navier-Stokes solver has been rewritten to take advantage of the data-parallelism employed by the CM-200 and the MasPar MP-1204. The Navier-Stokes equations are discretized in space using central differencing with added artificial dissipation. The resulting system of ODE´s is integrated in time using the explicit Runge-Kutta procedure. For code validation the flow around a NACA 0012 profile was computed. Various grid systems ranging from 1K to 2M points has been used the latter giving a performance of 238 MFLOPS on an 8K' CM-200. Comparisions with a control-parallel version, implemented on a 32 node iPSC/2, will also be given.

P. BJORSTAD:

Parallel solution of 3-d elliptic equations

The talk will present computational results using a massively parallel SIMD computer when implementing on additive Schwarz algorithm in two and three dimensions.

J. BURMEISTER:

Time-parallel multigrid method

An iterative solution procedure for time- and space-dependent problems has been discussed. In opposite to the usual way of solving time-dependent problem in a sequential manner, a set of $k > 1$ timesteps is solved simultaneously. The iterative solver is a multigrid method consisting of a smoothing procedure and a coarse-grid-correction. Convergence results for the one-dimensional heat equation are derived. The main result is: We have a norm estimate for the iteration matrix which guarantees monotone convergence. The bound is independent of the discretization parameters h and Δt and of the number of timesteps k to be solved simultaneously.

XIAO-CHUAN CAI:

Overlapping domin decomposition methods for nonsymmetric problems

We discuss several overlapping domain decomposition algorithms for the solution of the linear systems of equations arising from the finte element discretization of elliptic or parabolic problems in two- and three-dimensional spaces. More precisely, we introduce some multiplicative versions of the Schwarz methods and show that they are convergent and the convergence rates are optimal, independent of the mesh parameter h, coarse mesh size H, and the number of levels in the case of multilevel methods. For parabolic problems we show that the algorithms remain to be optimal even if the coarse mesh space is dropped.

T.F. CHAN:

On the choice of coarse grid size for some domain decomposition algorithms

In this talk, we consider the problem of choosing the size of the coarse grid in order to minimize the computational cost of certain domain decomposition algorithms. Specifically, we consider a Fourier approximation based variant of Smith's vertex space algorithm and study how the optimal coarse grid size depends on the complexity of the subdomain and coarse grid solvers.

C. DAWSON:

Application of domain decomposition techniques in reservoir simulation

The talk consists of two parts. First, explicit/implicit domain decomposition methods for time-dependent problems are discussed. In these methods, boundary information on subdomain interfaces are approximated explicitly, then implicit subdomain problems are solved in parallel. Error estimates and numerical results for different versions of this algorthm are presented.
The next part of this talk is on the application of domain decomposition techniques in a reservoir simulator. We will discuss the application of the Glowinski-Wheeler algorithm for mixed finite element methods to the solution of the pressure equation in the UTCHEM simulator.

M. DRYJA:

Additive Schwarz methods for finite elliptic problems

Finite element approximations of second order elliptic problems with discontinuous coefficients defined in 3-d region are considered. For solving of arising systems additive Schwarz methods are presented with rate of convergence independent of jumps of the coefficients. For analysis of these methods a general framework of additive Schwarz method is used.
The presented results have been obtained jointly with Olaf Widlund.

R. EWING:

Parallel methods for reservoir simulation problems

Although vectorization techniques have proved to be extremely effective for large-scale reservoir simulations, parallel capabilities hold even greater potential for these enormous problems. Domain decomposition methods can allow the physical problem to be devided and addressed in parallel. These techniques also allow efficient application of local grid refinement to resolve important local phenomena that may govern the flow process. Eulerian-Lagrangian methods that follow the flow can also profit extensively from parallel treatment of the characteristics of the flow. Nodal bases with Labatto quadrature for mixed finite element methods also enhance parallel implementation. The effectiveness of these techniques will be demonstrated on research codes and illustrative applications.

A. FROMMER:

Calculating enclosures with asynchronous iterations

Asynchronous iterations arise naturally on shared memory computers if processors are allowed to proceed totally independently from each other, without waiting for other processors having completed certain tasks. Asynchronous iterations can also be implemented on local memory machines. Their potential attractiveness is that they tend to minimize communicational delays. We present convergence results for enclosure methods using asynchronous iterations via both- classical "real" and interval arithmetic calculations. In the latter case, the conditions for convergence are essentially equivalent to those for the synchronous iteration. Numerical examples on a 26 processor Sequent Symmetry (at Argonne National Lab) are given and show the poptential of the asynchronous scheme.

D. HÄNEL:

Parallel algorithms for the Navier-Stokes equations

The paper is concerned with the solution of the Navier-Stokes equations for multi-dimensional, compressible flow. A brief discussion is given about the major solution concepts and about the requirements for grid resolution and computer capacity.
Parallel solutions of two different explicit Navier-Stokes solvers on a PARSYTEC SC 256 (RWTH Aachen) are presented. Measured performances are shown and compared with other computers.

G. HORTON:

Time-parallel methods for the solution of partial differential equations on multi-processors

We consider the problem of the solution of partial differential equations on MIMD machines. Standard methods proceed by solving the time-steps sequentially with an iterative method when an implicit discretization is used. This is true even for parallel methods, which accelerate the solution procedure at each time-step. The parallel computation time is, however, still proportional to the length of the time interval to be integrated. We consider a new approach, known as time-parallelism, whereby the parallelization is performed across the time direction, rather than in the space directions. Using this approach, different processors are allocated successive time-steps and solve these simultaneously. Thus it becomes possible to obtain parallel computation times which are essentially independent of the number of time steps to be solved. The critical factors affecting the performance of a time-parallel method are identified and discussed. Experimental numerical results obtained with various time-parallel schemes are used to demonstrate to what degree these criteria can be met in practice. Results obtained for the heat equation and for the Navier-Stokes equations demonstrate the high efficiencies obtainable by time-parallel schemes. The time-parallel approach is contrasted to standard grid-partitioning and domain-decomposition parallelization strategies, whereby it is shown that the methods differ considerably in several important respects.

D. KEYES:

Domain decomposition methods in computational fluid dynamics

Domain decomposition extends the usefulness of numerical techniques for certain special partial differential equation problems to those of more general structure. Geometrical features of operator inhomogeneities that inhibit the global application of basic algorithms often suggest natural decompo-sitions of problem domains into subdomains of simpler structure on which existing solvers are effective. An obvious hurdle to this approach is the specification of boundary conditions on the artificially introduced interfaces between subdomains, upon possession of which the subdomains trivially decouple. Rarely is a direct derivation of these auxiliary conditions from the differential or algebraic formulations of the problem the most economical way to proceed. Instead, the local solvers are employed as components of a global approximate inverse. For solvers whose complexity grows faster than linearly in the number of degrees of freedom, large problem size alone motivates decompo-sition and renders affordable the iteration required to enforce consistency at the artificial subdomain boundaries. As a parallelization paradigm, domain decomposition is often more natural than operator decomposition, and readily integrates local adaptivity.
Though domain decomposition is conceptually as old as the analysis of engineering systems, the last decade has provided significant theoretical underpinning for model problems and heuristics for practical problems. The speaker will review recent developments, and their application to problems in fluid dynamics.

J. MANDEL:

Balancing preconditioner with unstructured subdomains

The Neumann-Neumann algorithm is coupled with a coarse problem consisting of constants on each subdomain and averages on interfaces. The algorithm is interpreted in terms of global balancing and local solves, and condition bound of $\log^2(H/h)$ proved. The method can be also interpreted as a two-grid variational multigrid method.

V. MEHRMANN:

Numerical solution of nonsymmetric block linear systems on a transputer network

We discuss the numerical solution of block linear systems that arise for example in finite volume approaches for Navier-Stokes and Euler equations. We use parallel divide and conquer methods for the computation of block tridiagonal preconditioners or for block incomplete LU decompositions and compute the solution then with iterative methods like conjugate gradient or splitting methods. The methods are implemented on a 64 processor transputer system.

A. MEYER:

The parallel realization of PCGM for finite element splitting of the stiffness matrix and parallel preconditioners

If nonoverlapping DD-ideas for the linear system solvers are embedded in more complex finite element packages, one can observe a very low data communication on MIMD parallel computers, if the natural finite element splitting of the stiffness matrix $K = \Sigma_S A_S^T K_S A_S$ into subdomain parts K_S (belonging to subdomain Ω_S, stored in processor P_S) is consequently used in the conjugate gradient iteration. Especially the parallel distribution of the large vectors has to be done in the following way: All vectors containing inner products (right hand side $b_i = \langle f_i,\varphi_i \rangle$, residuum $r_i = a(u-u^*,\varphi_i)$ ...) are calculated and stored locally, i.e. $b = \Sigma_S A_S^T b_S$, whereas vectors containing nodal values get the right values on the subdomain Ω_S, so $u_S = A_S u$. We demonstrate that PCGM on a message-passing-MIMD-machine requires exactly one data-transfer step for data exchange over coupling boundaries per iteration step, when the DD-preconditioners (B.P.S. for Schur complement) and the hierarchical Yserentant and B.P.X. preconditioners are used.

Y.A. KUZNETSOV:

Multilevel domain decomposition / Fictitious domain preconditioners

At present it becomes clear that the problem of constructing optimal numerical algorithms for the solution of systems of grid equations may be solved via combining different approaches such as domain decomposition, fictitious domain and multigrid methods. This report presents examples of combining domain decomposition and fictitious domain methods to construct optimal preconditioners for a number of specific applied problems of fluid mechanics and electrodynamics.

U. LANGER:

Parallel iterative solvers for coupled DD-FE-BE equations

The use of the FEM and BEM in different subdomains of a non-overlapping Domain Decomposition (DD) and their coupling over the coupling boundaries (interfaces) brings about several advantages in many practical applications. The resulting coupled FE-BE-DD equations can be reformulated as a system of linear algebraic equations with a symmetric, but indefinite system matrix. This paper provides a parallelization and a preconditioning of Bramble/Pasciak's CG (1988) applied to the symmetric, indefinite coupled FE-BE-DD equations. Both the parallelization and the preconditioning are essentially based on the domain decomposition approach. The parallelized algorithm presented is well suited for computations on MIMD computers with local memory and message passing principle. The hypercube seems to be the most suitable architecture for the implementation, at least, on a reasonable number of processors.

S. NEPOMNYASCHIKH:

Domain decomposition method for elliptic problems with jumps in the coefficients

Boundary value problems for elliptic differential equations with jumps in the coefficients are considered. The original domain consists of subdomains where the coefficients of the elliptic equation are constants. The main purpose of the paper is the construction of a preconditioning operator for the system of grid equations. It is shown, that the rate of convergence of the corresponding conjugate gradient method is independent of both the grid size and the jumps in the coefficients.

P. OSWALD:

Norm equivalencies and multilevel additive Schwarz methods

Recent work by Widlund et. al. on the theory of additive Schwarz methods has shown the crucial role of certain splitted norms with respect to the underlying subspace decomposition. In case the decomposition is of multilevel type, estimates for those norms can be obtained in a rather standard way. We discuss certain applications to triangular and rectangular finite element schemes for the biharmonic problem. The main result are sharp condition number estimates for the hierarchical basis resp. for BPX-like preconditioners.

J.E. PASCIAK:

A multigrid method for a Fredholm equation of the first kind

I will consider a multigrid method for solving certain Fredholm equations of the first kind. Specifically, I will consider the problem of finding to solution x to

$$Ax = y,$$

where A is a pseudo differential operator of order minus one. Multigrid methods are developed using base inner product spaces corresponding to a negative Sobolev index. Regularity free etimates are then provided by applying results from "Convergence estimates for multigrid algorithms without regularity assumptions" by Bramble, Pasciak, Wang and Xu.

The resulting algorithms are effective on computers with parallel architecture. Parallelization can be achieved over the grid levels by using the additive form of the multigrid algorithm. Additional parallelism can be obtained by parallelizing the computations performed on each level.

J. PERIAUX:

Fictitious domain method for the incompressible Navier Stokes equations

In this lecture, we discuss a fictitious domain method for the numerical solution of the Navier Stokes equations modelling incompressible viscous flow. The methodology takes a systematic advantage of time discretization by operator splitting in order to treat separately advection and incompressiblility; it seems well suited to moving boundary flow problems. Due to the decoupling, fast elliptic solvers can be used to treat the incompressibility condition. Even if the orgional problem is taking place on a non regular geometry. Preliminary numerical results show that this new method looks quite promising.

F. SCHIEWECK:

Palallel solution of the stationary incompressible Navier Stokes equations with a multigrid algorithm on a transputer system

We compare a sequential and a parallel version of a multigird algorithm which is based on a blockstructured grid. In the parallel version each processor works only for one grid block, exchanges its boundary informations with the processors of the neighbouring blocks and performs global communication with all processors for controlling the multigrid algorithm and for solving the coarsest grid problem on the whole domain. We study communication overhead and parallel efficiency for different numbers of processors and different numbers of multigrid levels.

B.F. SMITH:

Parallel solution of PDE's using domain decomposition

On modern distributed memory parallel computers the choice of the layout of the data across the memories has a large impact on the computational performance. For the numerical solution of PDE's, the most natural distribution is by domain decomposition. The domain is decomposed into subdomains and the data for each subdomain, or group of subdomains, is stored in a single processor node. The distribution of data does not, however, determine the iterative method used. Multigrid, incomplete factorization, or domain decomposition iterative solvers may all be used, for instance.

We will discuss BlockComm, a simple programming language for the transfer of data between grids. BlockComm is built on top of the primative message passing facilities of the Intel iPSC/860 and the portable message passing package P4. We will also discuss the use of an object oriented approach to programming interative solvers and sparse matrix routines in a data structure neutral manner.

E. STEIN:

Concepts for the parallelization of coupled FE- and BE methods

Problems in solid and structural mechanics are governed by a big variety of geometrical and physical phenomena which are modeled usually according to the leading effects, respectively. The differential operators are linear or nonlinear elliptic, parabolic or even locally hyperbolic.

The numerical methods based on finite domain and finite boundary element discretizations (FEM and BEM) should be self-adaptive within the considered model (k-,k-p-adaptivity). Furthermore, dimensional and model adaptivity can be necessary in order to get reliable overall results. Corresponding algorithms for MIMD-computers, e.g. using nested approximation spaces and multigrid iterative solvers, are compared for different strategies, namely additive Schwarz domain decomposition methods (ASM) and algebraic decomposition methods for the total systems in the sequence of adaptive meshes.

In the ASM, overlapping domains are necessary especially due to the fact that the finite element nodes from both sides don't conincide due to local adaptivity or partial plastic deformations. A smoothing process is needed in the overlapping domain, e.g., using polynomials.

Therefore, algebraic decomposition methods are prefered in order to get optimal load balancing but taking into account a higher amount of global communications. This can be realized with some computer types with high speed communication properties.

C.W. UEBEHUBER:

Architecture adaptive algorithms

Portable programs that run efficiently on different parallel systems are only possible if they can adjust themselves to fit the respective computer system they run on. The essence of such programs are algorithms which are able to adapt themselfs to different computer architectures: Architecture Adaptive Algorithms. Environment Enquiries are defined which provide information about the available processors, communication channels, memory hierarchies, etc. By taking this information into account, a portable parallel algorithm can adapt its behavior to environment characteristics and thus increase its efficiency significantly.

M.F. WHEELER:

Parallel algorithms for flow in porous media

Transport of contaminants in groundwater is frequently described by convective-diffusion equations. Numerical procedures based on the coupling of characteristic methods with Galerkin finite elements treating the diffusion have been applied with much success. One of the main advantages of these approaches is that large time steps may be employed for a given accuracy. Disadvantages of these schemes include difficulties of implementation in three dimensions and nonconservation.
Here we formulate and analyze in three spatial dimensions a conservative mixed characteristic algorithm for linear advection problems. In our presentation we will discuss parallel implementation with emphasis on application to contaminant tranport.

W. WENDLAND (zus. mit B. KHAROMSKIJ):

Spectrally equivalent preconditioners for boundary equations in substructuring

We introduce a preconditioning technique for the iterative solution of boundary integral equations. These arise as a natural reduction to the boundary for the elliptic boundary value problems when domain decomposition is used. For two- and three-dimensional problems we construct a family of easily invertible preconditioners on Sobolev spaces on the sceleton using some "artificial" boundary integral operators on a set of canonical domains in combination with appropriate bi-Lipschitz mappings. The proposed algorithm is highly parallelizable.

P. WESSELING:

On Mulder's parallel multigrid method

W.A. Mulder (J.Comp.Phys. 83, 303-323, 1989) has proposed a parallel multigrid method for hyperbolic problems using multiple coarse grids per level. Although good for hyperbolic problems, the method is found not to work well for elliptic problems. N.H. Naik and J. Van Rosendale (ICASE Report 91-70, 1991) have introduced a modification that makes the method effective for elliptic equations. Due to the use of multiple coarse grids per level, simple smoothing methods suffice, allowing the choice of smoothing methods that easily allow massive parallelism. Due to the large number of coarse grid points per level, no processor needs to remain idle during coarse grid correction.

G. WITTUM:

On parallel frequency filtering methods

In the first part of the talk we present frequency filtering decompositions, which are useful to construct a new class of fast solvers for large systems of equations. A smoothing-correction method based on these frequency filtering decompositions is closely related to the multi-grid idea, i.e. successively filtering out certain frequencies from the error, but without using coarse grids. The corresponding method has asymptotic complexity of $O(n \log(n))$. On grids of intermediate size, however, it is quite efficient and compares well with multi-grid. After presenting the algorithms we give a convergence proof and several examples on the performance of the method applied to linear and
non-linear equations.
The second part of the talk deals with the parallelization of this new method. It is possible to connect the frequency filtering ideas with a Schur-Complement DD method. We present algorithms and recent numerical results.

Ch. ZENGER:

Adaptive multidimensional numerical integration

A new algorithm for the numerical integration in multidimensional spaces is presented, which combines the following important properties:
- The algorithm is fully adaptive.
- The complexity does not grow exponentially with the dimension of the underlying space.
We present this algorithm as a case study for the development of algorithms in a functional programming style allowing a well structured transparent program fully exploiting the inherent parallelism of the algorithm. It is demonstrated that this is not possible if we use the conventional imperative programming style.

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