Sparse Days at CERFACS

June 18-19th, 2009

CERFACS, Toulouse, France

Thursday, June 18th 2009

9.30 - 10.00 Registration and coffee break

Session I

10.00 - 10.30 *Augmented backward stability of Lanczos's symmetric matrix tridiagonalization process*
C. Paige

10.30 - 11.00 *Mixing direct and iterative methods for the solution of large linear systems*
D. Nuentsa Wakam

11.00 - 11.15 Break

11.15 - 11.45 *A DAG-based sparse Cholesky solver for multicore architecture*
J. Scott

11.45 - 12.15 *Efficient and scalable parallel graph partitioning and static mapping*
J.-H. Her

Lunch

Session II

14.00 - 14.30 *Stopping criteria for the iterative solution of linear least squares problems*
D. Titley-Peloquin

14.30 - 15.00 *Statistical stopping criteria for regression problems*
M. Arioli

15.00 - 15.30 *A parallel hybrid multigrid/direct method for large systems arising from finite element discretization of high frequency Maxwell problems*
M. Chanaud

15.30 - 16.00 Coffee break

Session III

16.00 - 16.30 *Acyclic and star colorings of joins of graphs and an algorithm for cographs*
A. Lyons

16.30 - 17.00 *Load flow with FDLF preconditioned GMRES*
R. Idema

17.00 - 17.30 *The optimization test environment*
M. Fuchs

20.00 - 23.00 Banquet at the restaurant "Le Pôvre Yves" in Toulouse.

Friday, June 19th 2009

Session IV

9.00 - 9.30 *On the semidefinite B-Arnoldi method*
G. W. Stewart

9.30 - 10.00 *Dynamic scheduling for sparse direct solver on NUMA and multicores architectures*
M. Faverge

10.00 - 10.30 Coffee break

Session V

10.30 - 11.00 *Proper Generalized Decomposition within the LATIN domain decomposition method*
J.-C. Passieux

11.00 - 11.30 *Comparison of algorithms to build an efficient Schur complement preconditioner in HIPS*
J. Gaidamour

11.30 - 12.00 *Parallel preconditioning of linear systems based on ILUPACK for multithreaded architectures*
A. Martin

Lunch

Session VI

13.30 - 14.00 *On the efficiency of Spectral Clustering : interpretation and results*
S. Mouysset

14.00 - 14.30 *Massively parallel linear solver for large 3D problems*
A. Haidar

14.30 - 15.00 *A stable variant of Simpler GMRES and GCR*
P. Jiranek

Closure and Coffee break

1 Session I

Augmented backward stability of Lanczos's symmetric matrix tridiagonalization process

C. Paige (School of Computer Science, McGill University, Canada). It has been found that any good implementation of Lanczos's symmetric matrix tridiagonalization process [C. Lanczos, J. Res. Nat. Bur. Standards, 45 (1950), pp. 255-282] produces a tridiagonal matrix that is numerically backward stable for a strange augmented problem. This will be referred to as the "augmented backward stability" of the process. Since the process is not stable in the standard sense, this augmented stability result cannot be transformed to prove standard stability. However it is hoped that it will lead to an increased understanding of the Lanczos tridiagonalization process, and eventually be used to analyze many applications of the process to large sparse matrix problems such as the solution of the eigenproblem, compatible linear systems, least squares, and the singular value decomposition. If this is so, then it might eventually provide standard results on the convergence and accuracy of the many applications of the Lanczos process. This augmented backward stability result appears to be an important resource for future use. Research supported by NSERC of Canada grant OGP0009236.

Mixing direct and iterative methods for the solution of large linear systems

D. Nuentsa Wakam (INRIA Centre de Rennes – Bretagne Atlantique) joint work with J. Erhel (INRIA Centre de Rennes – Bretagne Atlantique) and E. Canot (INRIA Centre de Rennes – Bretagne Atlantique). We consider the solution of a set of large systems arising from fluid dynamics simulation. The linearized form can be written as:

$$Ax = b \tag{1}$$

where $A \in \mathbb{R}^{n \times n}$ is a real and unsymmetric sparse matrix, x, $b \in \mathbb{R}^n$ are respectively solution and right hand side vectors. Although the solvers suitable for the system (1) are based either on sparse direct or iterative methods, the separation between these two classes is tight. Presently, techniques from the first class are used as preconditioners into the second class. Even in the second class, there are a variety of techniques based on Krylov subspace methods or multilevel methods (Multigrid, Domain decomposition).

We first consider the solution with two distributed direct solvers, namely SuperLU_DIST [1] and MUMPS [2]. Even with an out-of-core factorization available in MUMPS, we see that the price to pay, in terms of memory requirements is still too high. In SuperLU_DIST, the accuracy in the final solution of some systems is not guaranteed probably due to the static pivoting used to enhance the scalability. Then, we consider domain decomposition preconditioners based on Schwarz methods in which direct methods are used to solve the local systems. We give a short comparative study between additive Schwarz preconditioner available in PETSc and the recently proposed multiplicative Schwarz preconditioner [3].

References

[1] X. S. Li and J. W. Demmel. SuperLU_DIST : A Scalable Distributed-Memory Sparse Direct Solver for Unsymmetric Linear Systems *ACM Trans. Mathematical Software*, 29(2):110-140, 2003.

[2] P. Amestoy, I. Duff, J.-Y. L'Excellent, J. Koster, A fully asynchronous multifrontal solver using distributed dynamic scheduling, *SIAM J. on Matrix Analysis and Applications,* 23(1):15-41, 2001.

[3] G.-A. Atenekeng Kahou, E. Kamgnia, B. Philippe. An explicit formulation of the multiplicative Schwarz preconditioner. *Applied Numerical Mathematics*, 57:1197-1213, 2007.

A DAG-based sparse Cholesky solver for multicore architecture

J. Scott (Rutherford Appleton Laboratory (RAL, UK)) joint work with J. Hogg (RAL, UK) and J. Reid (RAL, UK). Recent research by Buttari et al. [1, 2] and Hogg [3] into efficiently solving dense linear systems of equations on multicore architectures has shown that directed acyclic graphs (DAGs) can be used to obtain significant parallel speedups. We explain how the DAG approach may be adapted for sparse linear systems. In particular, we describe the design and development of a new sparse Cholesky code `HSL_MA87` [4]. Using problems arising from a range of practical applications, we demonstrate that `HSL_MA87` obtains good serial and parallel times on an 8-core machine and its performance compares very favourably with other well-known parallel sparse symmetric solvers, notably MUMPS and the Intel MKL version of PARDISO.

References

[1] A. Buttari, J. Dongarra, J. Kurzak, J. Langou, P. Luszczek, and S. Tomov, *The impact of multicore on math software*, in Proceedings of Workshop on State-of-the-art in Scientific and Parallel Computing (Para06), 2006.

[2] A. Buttari, J. Langou, J. Kurzak, and J. Dongarra, *A class of parallel tiled linear algebra algorithms for multicore architectures*, Technical Report UT-CS-07-600, ICL, 2007. Also LAPACK Working Note 191.

[3] J. Hogg, *A DAG-based parallel Cholesky factorization for multicore systems*, Technical Report RAL-TR-2008-029, Rutherford Appleton Laboratory, 2008.

[4] J. Hogg, J. Reid and J. Scott, *A DAG-based sparse Cholesky solver for multicore architectures*, Technical Report RAL-TR-2009-004, Rutherford Appleton Laboratory, 2009.

Efficient and scalable parallel graph partitioning and static mapping

J-H Her (INRIA Bordeaux - Sud-Ouest- LaBRI) joint work with F. Pellegrini (INRIA Bordeaux - Sud-Ouest- LaBRI). Graph partitioning is the combinatorial problem aiming at finding a small vertex separator or edge cut in a given (possibly weighted) graph such that the separator or cut can disconnect the graph into a prescribed number of parts of roughly equivalent sizes or weights. In the scientific computing field, such graph partitioning tools are commonly used to compute domain decompositions for parallel iterative linear system solvers. However, as recent parallel computing architectures are characterized by ever increasing numbers of processors and heavily heterogeneous communication subsystems, taking into account the underlying topology of the target machine is essential to effective minimization of running time. Static mapping is the corresponding combinatorial problem, which aims at assigning statically parallel processes onto physical processors so as to reduce realistic message congestion. In this talk, we will describe the current parallel graph partitioning features of PT-Scotch, and present some experimental results, including a comparison with ParMeTiS. We will also introduce ongoing work on parallel static mapping, to be included in the forthcoming version of PT-Scotch.

2 Session II

Stopping criteria for the iterative solution of linear least squares problems

D. Titley-Peloquin (School of Computer Science, McGill University, Canada) joint work with Xiao-Wen Chang (School of Computer Science, McGill University, Canada) and Chris Paige (School of Computer Science, McGill University, Canada). Given $A \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m$, the linear least squares (LS) problem is

$$\min_x \|b - Ax\|_2.$$

Iterative methods for the solution of large sparse LS problems produce a sequence of iterates $x_k \in \mathbb{R}^n$ (for $k = 1, 2, \dots$) which hopefully converge to the true LS solution. One important question to ask when using an iterative method is when to stop the iteration, in other words for which k is the approximate solution x_k "good enough"?

We first define what we mean by an *acceptable LS solution* and a *backward stable LS solution.* We then explain an interesting property of minimum residual iterative methods for the solution of LS problems. Our analysis demonstrates that the stopping criteria commonly used with these methods can in some situations be too conservative, causing any chosen method to perform too many iterations or even fail to detect that an acceptable iterate has been obtained. We propose a less conservative criterion to determine if a given iterate is an acceptable LS solution. This is merely a sufficient condition, but it approaches a necessary condition in the limit as the given iterate approaches the exact LS solution. We also propose a necessary and sufficient condition to determine if a given approximate LS solution is an acceptable LS solution, based on recent results on backward perturbation analysis of the LS problem. Although both of the above new conditions use quantities that are too expensive to compute directly in practical situations, we suggest potential approaches for estimating some of these quantities efficiently. We illustrate our results with several numerical examples. Research supported by the Natural Sciences and Engineering Research Council of Canada (NSERC).

Statistical stopping criteria for regression problems

Mario Arioli (Rutherford Appleton Laboratory (RAL, UK)) joint work with Serge Gratton (CNES-CERFACS). The Preconditioned Conjugate Gradient method can be successfully used in solving the normal equations obtained from least-squares problems in linear estimation. Taking into account recent results, which make it possible to approximate the energy norm of the error during the conjugate gradient iterative process, we adapt an existing stopping criterion introduced in the framework of partial differential equations. We show how the energy norm of the error is related to statistical properties of the least-squares problem and to the $\chi 2$ and the Fisher-Snedecor distributions. Finally, we present the results of several numerical tests that experimentally validate the effectiveness of our stopping criteria.

A parallel hybrid multigrid/direct method for large systems arising from finite element discretization of high frequency Maxwell problems

M. Chanaud (INRIA Bordeaux Sud-Ouest and LaBRI) joint work with D. Goudin and J.J. Pesqué (CEA/DAM/CESTA) and J. Roman (INRIA Bordeaux Sud-Ouest and LaBRI, Université de Bordeaux). We propose a methodology based on a multigrid method driven by a direct solver to solve large linear systems arising from Maxwell equations discretized with first-order Nédélec elements. From this idea, a new parallel solver is developed. This solver combines the PaStiX parallel direct solver and full-multigrid cycles. The goal of the proposed method is to compute a solution on fine irregular meshes given an unique coarse input mesh. The considered problem is the electromagnetic behaviour simulation of 3D objects in the frequency domain. This method allows us to perform multiple solves, each one involving a different frequency, on an object using an unique input mesh describing the geometry. The usual Maxwell problem

wavelength restriction is automatically met by the method's successive refinements.

The particularity of that solver is that it is totally driven by direct solve : the data distribution is computed once (during the first solve), and then is conserved during the whole process. Given that the refinement involved in multigrid is homogeneous, both load balancing and communication scheme are preserved.

The method can be divided in three main phases leading to the following algorithm : direct factorization and solve on the coarse level, solution interpolation over the automatically refined mesh, multigrid V-cycles to improve interpolated result. Once the fine mesh solution is computed, it can be interpolated on an even finer mesh using the prolongation operator, and so on.

As a remainder, the 2 grid multigrid V-cycle involving fine mesh h and coarse mesh $2h$ and solving $A.x = b$ is described in following algorithm :

$$\begin{aligned}
x_h &\leftarrow \text{smooth}(A_h, x_h, b_h), \\
r_h &\leftarrow b_h - (A_h.x_h), \\
r_{2h} &\leftarrow R_h^{2h}.r_h \ (\textbf{restriction}), \\
e_{2h} &\leftarrow A_{2h}^{-1}.r_{2h}, \\
e_h &\leftarrow P_{2h}^{h}.e_{2h} \ (\textbf{prolongation}), \\
x_h &\leftarrow x_h + e_h, \\
x_h &\leftarrow \text{smooth}(A_h, x_h, b_h).
\end{aligned}$$

In a n grid multigrid V-cycle ($n > 2$), computing e_h is either another multigrid V-cycle or a classical solve. In our case we rely on a multigrid V-cycle until coarsest level is reached, where a direct solve is performed. As the coarse system has already been factorized, it only requires a forward-backward solve phase ($O(nnz)$ complexity), leading to a good error approximation.

As a smoother, we use a matrix-free Jacobi solver for three reasons : it is an easily parallelizable method, got a good smoothing factor and doesn't consume much memory as fine systems are never assembled.

Preliminary results obtained from a sequential version of the solver show that fine grid smoothing and inter-grid correction are quite efficient, leading to an accurate result compared to the exact solution.

3 Session III

Acyclic and star colorings of joins of graphs and an algorithm for cographs

A. Lyons (Argonne National Laboratory, USA). We discuss some graphs coloring problems that are related to the efficient evaluation of sparse derivative matrices. In particular, we consider the problems of finding optimal acyclic and star colorings, which model two different methods for the evaluation of Hessians. Both of these problems are known to be intractable even in severely restricted cases. We present a formula that describes the acyclic and star chromatic numbers of graphs that are decomposable with respect to the join operation, which builds a new graph from a collection of two or more disjoint graphs by adding all possible edges between them. We also show that our results lead to linear time algorithms for finding optimal acyclic and star colorings of cographs, which have the unique property that they are recursively decomposable with respect to the join and disjoint union operations.

Load flow with FDLF preconditioned GMRES

R. Idema (TU Delft, The Netherlands). A power system is the hardware that provides for the generation and transmission of electrical power. The load flow problem, or power flow problem, is the problem of calculating the AC voltages in the entire power system, given the amount of power generated and consumed. The solution of this problem is vital for the planning of construction and operation of power systems. The load flow problem gives rise to a system of non-linear equations, which is generally solved either by Newton-Raphson iterations with a direct solve on the Jacobian system, or by an approximation to the Newton-Raphson method known as the Fast Decoupled Load Flow (FDLF [2]). We focus on deploying Krylov subspace methods to solve load flow problems, to gain efficiency for large problems, and flexibility for the application of load flow calculations as part of more complex power system simulations. We use the Newton-Raphson method to linearise the problem, but also use the knowledge from the FDLF method to aid our goal. The variables solved for, can be split into voltage magnitudes (per unit) and voltage angles. Due to practical restrictions, the magnitudes should generally be between 0.8 and 1.2 p.u., whereas the angles should be between -20 and 20 degrees. As such, from a reasonable starting point, the solution will not vary too much through the Newton-Raphson iterations. Thus if we chose a good preconditioner for our iterative method in the first iteration, it should remain a strong preconditioner throughout all iterations. This motivates the choice of GMRES as iterative method, as the number of iterations needed should remain small, and the minimal residual property outweighs the algorithmic complexity of GMRES. A standard candidate preconditioner for GMRES within a Newton-Raphson method, is the incomplete LU-decomposition (ILU) of the initial Jacobian matrix. However, power system theory also hands us a very interesting canditate through the FDLF method, as was also observed in [1]. For our test cases, GMRES convergence, and spectrum analysis of the preconditioned coefficient matrices, show that FDLF is indeed a very powerful preconditioner, rivalling the performance of direct solves even at small problem sizes. Most current test cases are of such a size, that it is no problem to do a complete LU-decomposition. For larger cases it may be beneficial to use an ILU factorization of the FDLF matrix as preconditioner. Thinking ahead to truely large problems, combining Newton-Rapshon with preconditioned GMRES even gives us the flexibility to use Algebraic Multigrid on FDLF as a preconditioner.

References

[1] A.J. Flueck and H.D. Chiang Solving the nonlinear power flow equations with an inexact Newton method using GMRES *IEEE Transactions on Power Systems*, 13(2):267-273, 1998.

[2] B. Stott and O. Alsac Fast decoupled load flow *IEEE Transactions on Power Apparatus and Systems*, PAS-93(3):859-869, 1974.

The optimization test environment

M. Fuchs (CERFACS, Parallel Algorithms). The TEST ENVIRONMENT is an interface to solve optimization problems efficiently using different solver routines. It is designed as a tool for both developers of solver software and practitioners who just look for the best solver for their specific problem class. The TEST ENVIRONMENT is free to use for research purposes and enables users to:

- Choose and compare diverse solver routines;
- Organize and solve large test problem sets;
- Select interactively subsets of test problem sets;
- Perform exhaustive analysis of the results.

4 Session IV

On the semidefinite B-Arnoldi method

G. W. Stewart (University of Maryland at College Park, USA). The B-Arnoldi method is a variant of the ordinary Arnoldi method in which orthogonalization is done with respect to the inner product generated by a positive definite matrix B. It arises in connection with the generalized eigenvalue problem $Ax = \lambda Bx$, where A is symmetric. When B is semidefinite, the algorithm can proceed formally, with "orthogonalization" taking place in the semi-inner product generated by B. However, it has been observed that components of the Arnoldi vectors lying in the null space of B can grow rapidly. In this talk we examine the source and consequences of this growth.

Dynamic scheduling for sparse direct solver on NUMA and multicores architectures

M. Faverge (INRIA Bordeaux Sud-Ouest and LaBRI) joint work with Pierre Ramet (INRIA Bordeaux Sud-Ouest and LaBRI). Over the past few years, parallel sparse direct solvers have made significant progress. They are now able to solve efficiently real-life three-dimensional problems with several millions of equations. Nevertheless, the need of a large amount of memory is often a bottleneck in these methods. The authors have proposed an hybrid MPI-thread implementation of a direct solver that is well suited for SMP nodes or modern multi-core architectures. Modern multi-processing architectures are commonly based on shared memory systems with a NUMA behavior. These computers are composed of several chip-sets including one or several cores associated to a memory bank. Such an architecture implies hierarchical memory access times from a given core to the different memory banks which do not exist on SMP nodes. Thus, the main data structure of our targeted application have been modified to be more suitable for NUMA architectures. We also introduce a simple way of dynamically schedule an application based on a dependency tree while taking into account NUMA effects. Results obtained with these modifications are illustrated by showing performances of the PaStiX1 solver on different platforms and matrices. Moreover large problems need a 2D distribution scheme to balance the data over the nodes which increases the preprocessing time. We suggest to use the dynamic scheduler inside a shared memory to create more tasks without having the overcost of a full-2D distribution during the preprocessing step. We will present some recent results on large test cases with more than ten millions of unknowns.

5 Session V

Proper Generalized Decomposition within the LATIN domain decomposition method

*J.C. Passieux (ENS Cachan/CNRS/UPMC/PRES UniverSud Paris) joint work with P. Ladevèze (ENS Cachan/CNRS/UPMC/PRES UniverSud Paris and EADS Foundation Chair "*Advanced Computational Structural Mechanics*") and D. Néron (ENS Cachan/CNRS/UPMC/PRES UniverSud Paris).* The simulation of the evolution of complex structures, for instance the study of large structures with local cracking or local buckling, leads to the resolution of large size systems for which parallel computing is required. In [1, 2], a multiscale computational strategy has been proposed for the analysis of structures which are described at a fine scale, both in time and space, compared to the scale of the structure. This strategy, based on the LATIN method [3], can be seen as a non-linear, mixed and multilevel domain decomposition method, including automatic space and time homogenization. An original feature of the LATIN is that the solver operates over the entire time interval at each iteration. As a result, the local problems are time-dependant and the cost of their resolution can become prohibitive.

In this work, a spectral decomposition technique is used to solve these problems. This technique called "radial approximation" belongs to the Proper Generalized Decomposition (PGD [4]) algorithms. It consists in seeking the solution of the coupled space-time problem as a finite sum of products of functions of each variables ; where the families of functions are unknown *a priori*. It can be seen as a *a priori* model reduction method. To solve this kind of approximation, we use techniques inspired from generalized eigenvalue problems, which only involve the resolution of a few time-independant space problems as long as scalar ODE in time.

In practice, one can notice that the construction of the space functions is by far the most expensive. Therefore an adaptive reduced order model is build. In the context of the LATIN method, it consists in storing and reusing the base of space functions from an iteration to another. Each local problem begins by a preliminary phase which consists in updating the time functions corresponding to the base of space functions [4]. Then, if the approximation is not satisfying, the base is enriched automatically.

The capabilities of the method are discussed through 3D numerical illustrations.

References

[1] P. Ladevèze et A. Nouy (2003). On a multiscale computational strategy with time and space homogenization for structural mechanics. *Computer Methods in Applied Mechanics and Engineering*, 192:3061–3087.

[2] P. Ladevèze, D. Néron, and J.-C. Passieux (2009). On multiscale computational mechanics with time-space homogenization. In *Multiscale methods—Bridging the scales in Science and Engineering*. Oxford University Press. Ed. J. Fish.

[3] P. Ladevèze (1999). *Nonlinear Computationnal Structural Mechanics - New Approaches and Non-Incremental Methods of Calculation*. Springer Verlag.

[4] P. Ladevèze, J.-C. Passieux and D. Néron (2009). The LATIN multiscale computational method and the Proper Generalized Decomposition. *Comput. Meth. App. Mech. Eng.* accepted 2009.

Comparison of algorithms to build an efficient Schur complement preconditioner in HIPS

J. Gaidamour (INRIA Bordeaux - Sud-Ouest- LaBRI) joint work with P. Hénon (INRIA Bordeaux - Sud-Ouest- LaBRI). Nowadays, three dimensional numerical simulations often require a tremendous amount of resources. On one hand, direct methods can be mandatory to solve very ill-conditioned systems. But for large 3D simulations, they are constrained by prohibitive memory requirements and they also need a high amount of floating point operations. Iterative methods on the other hand require much less memory and are more scalable in general.

Hybrid methods based on a Schur complement approach try to combine the assets of the two class of methods. An usual method is to use a decomposition of the matrix graph into sub-domains. The matrix part corresponding to the interior unknowns is treated using a direct method and the resolution of the global system is then reduced to the resolution of the Schur complement system. The Schur complement can then be solved using an iterative method.

In the HIPS library (http://hips.gforge.inria.fr/), we have developed such an approach. In our case, we reordered the matrix according to the Hierarchical Interface Decomposition (HID) : it consists in partitioning the set of unknowns of the interface into graph components named "connectors" that are grouped in "levels". A level of connectors plays the role of separators for the immediate inferior level. Based on this ordering, one can construct a robust parallel incomplete factorization of the Schur complement.

In this talk, we will present and compare two ways to compute the incomplete factorization of the Schur complement (apart from the possible choices of fill-in pattern): - The first one consists in building the factorization based on an approximation of the Schur complement. This method aims at reducing the memory needed to store the exact Schur complement. - The second one uses the exact Schur complement to compute the incomplete factorization. This method requires more temporary memory but can dramatically decrease the number of iterations.

We will give the main algorithmic differences and also compare the memory and convergence impact of these methods on large test cases.

Parallel preconditioning of linear systems based on ILUPACK for multithreaded architectures

A. F. Martín (Universidad Jaume I, Spain) joint work with J. I. Aliaga (Universidad Jaume I, Spain), M. Bollhöfer (Institute of Computational Mathematics, TU-Braunschweig, Germany) and E. S. Quintana-Ortí (Universidad Jaume I, Spain). ILUPACK is a numerical serial library for the solution of large-scale sparse linear systems via multilevel inverse-based ILU preconditioned Krylov subspace solvers. In this talk we will review the main design issues which are involved in the development of the parallel version of the ILUPACK library for shared-memory multiprocessors. The approach to parallelization is based on multilevel nested dissection graph partitioning algorithms to split the computation into concurrent tasks, which are then mapped to the processors for the parallel numerical solution steps of the solver. Experimental results for several PDE-based academic applications on a ccNUMA platform with up to 16 processors will reveal that our approach delivers a high degree of concurrence for a moderate number of processors, while inherently preserving the semantics of the preconditioning techniques in ILUPACK.

6 Session VI

On the efficiency of Spectral Clustering : interpretation and results

S. Mouysset (IRIT-ENSEEIHT, University of Toulouse) joint work with J. Noailles (IRIT-ENSEEIHT, University of Toulouse) and D. Ruiz (IRIT-ENSEEIHT, University of Toulouse). Clustering aims to partition a data set by grouping similar elements into subsets. Main problems are, from one hand the choice of similarity criterion and, from the other hand, how to separate clusters one from the other. For many methods based on optimization problems, such as K-means, considering non-convex shapes as clusters becomes out of range. A contrario [1], spectral methods, specially spectral clustering, give better results in many cases including pattern recognition or machine learning fields. Spectral clustering consists in defining a low-dimensional data space in which data points are clustered by selecting dominant eigenvectors of a matrix called affinity matrix in order to define. However, this method involves a free parameter in Gaussian affinity matrix, respectively noted t and A, which has to be properly defined. Numerical experiments [2] show how difficulty and crucial this choice is. For further investigations, we propose an interpretation on how spectral clustering method works. From a sampling of connected components, we want to draw back to original shapes. This leads to formulate spectral clustering algorithm as an eigenvalues problem by assuming data points to nodes of some finite elements discretization and considering A as a representation of Heat kernel. Thus identifying connected component appears to be linked to these eigenfunctions. Then we prove that this property is preserved asymptotically on t when looking at eigenvectors of spectral clustering algorithm. With numerical experiments, we show the efficiency of the spectral clustering method on retrieving groups from several geometrical examples and with various refinements. More precisely, we focus on the behaviour of the method with respect to this new theoretical material.

References

[1] A. Y. Ng, Michael I. Jordan, and YairWeiss On spectral clustering: analysis and an algorithm *Proc. Adv. Neural Info. Processing Systems*, 2002.

[2] S. Mouysset, J. Noailles, and D. Ruiz Using a Global Parameter for Gaussian Affinity Matrices in Spectral Clustering *In High Performance Computing for Computational Science: 8th International Conference, Toulouse, France, June 24-27, 2008.* Revised Selected Papers, page 378. Springer, 2009.

Massively parallel linear solver for large 3D problems

A. Haidar (University of Toulouse, INPT-ENSEEIHT). The main topic of this research work was the study of a numerical technique that had attractive features for an efficient solution of large scale linear systems on large parallel platforms. The goal is to develop a high performance hybrid direct/iterative approach for solving large 3D problems. We focus specifically on the associated domain decomposition techniques for the parallel solution of large linear systems. We have investigated several algebraic preconditioning techniques. The robustness and parallel numerical performance of the solver is reported on large challenging linear systems.

A stable variant of Simpler GMRES and GCR

P. Jiranek (CERFACS, Parallel Algorithms) joint work with M. Rozloznik (Institute of Computer Science, Academy of Sciences of the Czech Republic, Czech Republic). Minimum residual Krylov subspace methods form a popular class of iterative methods for solving large and sparse nonsymmetric systems of linear algebraic equations. Besides the GMRES method [5], other mathematically equivalent implementations like Simpler GMRES [6] and especially GCR [1] are used sometimes in practice. As shown in [6, 4, 3] their numerical behavior depends strongly on

the conditioning of the basis of the generated Krylov subspace, which appears to be directly linked to the convergence of the residual norms. While the basis used in Simpler GMRES is growing with decreasing relative residual norms, fast convergence of the residual norms results in the well-conditioned residual basis of GCR. We propose a stable variant of Simpler GMRES and GCR [2], which is based on the adaptive choice of the Krylov subspace basis at a given iteration step using the intermediate residual norm decrease criterion. The new direction vector is chosen as in the original implementation of Simpler GMRES or it is equal the normalized residual vector as in the GCR method. Such an adaptive strategy leads to a well-conditioned basis of the Krylov subspace, which provides a numerically stable and more robust variant of Simpler GMRES or GCR.

References

[1] S. C. Eisenstat, H. C. Elman, and M. H. Schultz. Variational iterative methods for nonsymmetric systems of linear equations. *SIAM J. Numer. Anal.*, 20(2):345–357, 1983.

[2] P. Jiranek and M. Rozloznik. Adaptive version of Simpler GMRES. Technical Report TR/PA/08/101, CERFACS, Toulouse, France, 2008.

[3] P. Jiranek, M. Rozloznik, and M. H. Gutknecht. How to make Simpler GMRES and GCR more stable. *SIAM J. Matrix Anal. Appl.*, 30(4):1483–1499, 2008.

[4] J. Liesen, M. Rozloznik, and Z. Strakos Least squares residuals and minimal residual methods. *SIAM J. Sci. Stat. Comput.*, 23(5):1503–1525, 2002.

[5] Y. Saad and M. H. Schultz. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.*, 7(3):856–869, 1986.

[6] H. F. Walker and L. Zhou. A simpler GMRES. *Numer. Linear Algebra Appl.*, 1(6):571–581, 1994.