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Survey of Parallel Numerical Analysis Software

RJ Allan YF Hu and P Lockey

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Parallel Application Software on High Performance Computers. Survey of Parallel Numerical Analysis Software. *

R.J. Allan[1], Y.F. Hu[1] and P. Lockey[2]

[1] Computational Science and Engineering Department
CLRC Daresbury Laboratory,
Daresbury, Warrington WA4 4AD, UK

[2] Parallel Applications Centre, University of Southampton,
Highfield, Southampton SO9 5NH, UK

Email: r.j.allan@dl.ac.uk or y.f.hu@dl.ac.uk

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Abstract

This report provides a survey of parallel numerical analysis software packages. The aim of this survey is to serve as a quick reference for users who work on scientific and engineering applications, and who encounter numerical analysis problems which they wish to solve in parallel. Areas covered include iterative and direct linear solvers, eigenvalue solvers, nonlinear equations solvers, optimisation software, PDEs and ODEs solvers. For each package, a brief description is given along with other useful information such as availability, contact addresses and systems supported.

Keywords: parallel computing, numerical analysis, software packages, scientific applications.

*Edition 4: April 1999

Contents

1 Introduction

This report provides a survey of parallel numerical analysis software packages. The aim is to enable scientific parallel computer users to identify whether there exists numerical analysis software for their particular needs without having to wade through the parallel computing literature. It is also hoped that the survey will help prevent the large amount of "re-inventing the wheel" which appears to take place in the field of parallel scientific computing.

Companion reports to this one give more detailed information on parallel diagonalisation packages (eigen-solvers) [1] and serial and parallel FFT routines [2]. Information is not repeated here except in outline form where appropriate.

1.1 Criteria for Inclusion

Packages covered here are those which can be run on either true parallel machines, networked workstations, or on shared-memory systems. In the main we restrict our attention to packages which are based on, or can be used from, FORTRAN77, Fortran 90, C and C++, since these are the most widely used languages for applications and they are also available (or will eventually be available) on most machines.

The main criteria for inclusion is that a package should be of use in a scientific or engineering application. Most of the entries cover packages which are already in existence and available. However, packages which are under construction, or proposed software projects are included if they are thought to be of sufficient interest.

1.2 Individual Entries

The different fields for each package entry should be fairly self explanatory. Names and addresses given are simply somebody who can be contacted about the package; they are not meant to represent the entire cast responsible for the software. For full lists of the organisations and people involved the actual documentation should be consulted.

1.3 Intended Audience and Feedback

The survey is particularly geared towards users of the UK national academic computing facilities and for this reason also has a slight "UK slant". However, the information contained here should also be useful to a wider audience.

It is our intention to keep this report as up to date as possible. To this end, we would be very keen to hear about any packages which are of interest in parallel scientific computing and are not currently included. Corrections and comments are also welcomed. We can be contacted by email as `R.J.Allan@dl.ac.uk` or `Y.F.Hu@dl.ac.uk`.

1.4 Acknowledgements

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2 Parallel Numerical Library Projects

The packages in this report encompass a wide range of functionality. At one end there is single-purpose software. At the other end are packages which provide a large number of higher-level numerical algorithms. There are a number of major efforts represented here: the ScaLAPACK project at the University of Tennessee, the PETSc package from Argonne National Laboratory, the PRISM project, NEOS (ANL and NorthWestern University), the PINEAPL and NAG parallel library (NAG Ltd. and collaborators), and the ParaSol project (CLRC Rutherford-Appleton Laboratory and collaborators). As well as the individual entries for software produced from these projects a brief overview is now given for each one concentrating on the main concepts and philosophies behind the package. Projects are listed roughly according the the apparent effort going into the activity.

2.1 ScaLAPACK

ScaLAPACK (Scalable LAPACK) is an ongoing project aimed at creating a parallel distributed-memory version of the LAPACK (Linear Algebra Package) software. It is a collaborative venture in the USA involving the Oak Ridge National Laboratory and the Universities of Rice, California (Berkeley), California (Los Angeles), Illinois (Champagne-Urbana) and Tennessee (Knoxville). The project is supported by grants from the National Science Foundation, DARPA, the Army Research Office, and DoE.

Part of the ScaLAPACK effort is involved with lower-level packages which provide building blocks for the higher-level numerical routines, but which are also useful packages in their own right. These include BLACS (Basic Linear Algebra Communication Subprograms) and PBLAS (Parallel Basic Linear Algebra Subprograms).

Routines which are currently provided in ScaLAPACK include:

- LU decomposition and solvers;
- QR factorisation and solvers;
- Cholesky factorisation and solvers;
- condition estimation and iterative refinement for LU, QR and Cholesky;
- full-rank linear least squares problems;
- reduction to upper Hessenberg form;
- reduction to tridiagonal or bidiagonal form;
- singular value decomposition.

A number of major research projects have recently amalgamated their efforts under the ScaLAPACK umbrella. Packages in this group include ScaLAPACK itself, BLACS and PBLAS, and LAPACK++, Arpack, PUMMA, ParPre and CAPSS. All the packages are available from Netlib in directory ScaLAPACK, see section 9. Most of the packages have their own specific contacts for feedback, queries etc, but there is also an overall contact at `http://www.netlib.org/scalapack` or `scalapack@cs.utk.edu`.

A users' guide for ScaLAPACK has been published [9]. There are also many LAPACK Working NoteS (LAWNS) some of which cover the design of ScaLAPACK, see `http://www.netlib.org/lapack/lawns` or `http://www.hensa.ac.uk/Subject/num/lawns.html`.

NAG Limited are basing their parallel numerical library on ScaLAPACK, and are active in the ScaLAPACK development team. The numerical Analysis Group at CLRC Rutherford Appleton Laboratory is also involved in the development.

2.2 NAG Parallel and SMP Libraries

The NAG Parallel Library is a numerical library, utilising a message passing paradigm, for dedicated parallel machines and clusters of workstations or PCs. It contains (see `http://www.nag.co.uk`):

- optimisation;
- dense linear algebra (including ScaLAPACK);
- sparse linear algebra;
- random number generators;
- quadrature;
- input/Output, data distribution;
- support/utility routines.

Parallel algorithms are developed in the PINEAPL research project (see below) and migrate into the NAG Parallel Library once user trials have been completed.

A complementary activity is the development of the NAG SMP library (see Web page).

2.3 PINEAPL

PINEAPL (Parallel Industrial NumErical Applications and Portable Libraries) is European Commission funded project in the area of High Performance Computing and Networking (HPCN) [29]. One of the aims of the PINEAPL project is to produce a general-purpose library of parallel numerical software. This library covers the following areas:

- Dense linear algebra: direct methods for solution of linear equations, eigenvalue problems, computing (estimating) condition numbers, banded solvers, tridiagonal solvers;
- Sparse linear algebra: iterative methods for solution of linear equations, preconditioners, black box routines;
- Optimisation: Unconstrained and constrained problems;
- Discrete Fourier Transforms (1,2,3-dimensional FFT);
- Partial Differential Equations (2,3-dimensional): Helmholtz equations, fast Poisson solvers, mesh partitioning, multigrid;
- Others: dynamic load-balancing, data distribution routines (dense and sparse matrices), basic sparse matrix operations (e.g. matrix-vector multiplication, transposed matrix multiplication, etc.)

The project officially finished in January 1999 and the library has been launched by NAG Ltd. Following user trials it will be incorporated in the NAG Parallel Library. See Web page `http://www.nag.co.uk/Projects/Pineapl`.

2.4 PARASOL

PARASOL is an ESPRIT IV long-term research project (number 20160) for "an integrated environment for parallel sparse matrix solvers" [4]. It was active between January 1996 and June 1999. PARASOL provides a library of new parallel algorithms for the solution of sparse systems of linear equations. In order to be able to solve a broad class of problems with this library the most important solver techniques are supported. See Web page `http://www.genias.de/parasol`.

Partners in PARASOL are Apex Technologies, CERFACS, Det Norske Veritas, Genias, GMD (Bonn), INPRO, MacNeal-Schwendler GmbH, ONERA, PALLAS, Polyflow SA, CLRC Rutherford-Appleton Laboratory and Para//ab.

PARASOL is written in Fortran 90 and uses MPI. The final library is in the public domain. Within the project, new parallel algorithms for the direct solution of sparse systems of linear equations, for the iterative solution of such systems based on either multigrid or domain decomposition and for their preconditioning have been developed. Of particular note is the parallel sparse direct solver (MUMPS) based on the multifrontal technique (see separate entry later).

2.5 PETSc

A number of parallel software packages created at the US Argonne National Laboratory have been brought together into a "parallel toolkit" called PETSc (Portable Extensible Tools for Scientific Computation).

PETSc provides clean and effective codes written in C for the various phases of solving PDEs, with a uniform approach for each class of problem. Its design enables easy use and comparison of different algorithms (for example, to experiment with different Krylov subspace methods, preconditioners, or truncated Newton methods). Components enable easy customisation and extension of both algorithms and implementations. The PETSc infrastructure creates a foundation for building portable large-scale applications and extended suites of numerical routines.

Included are:

- the BlockComm package for communication of blocks of distributed arrays;
- the KSP iterative methods package;
- the SLES package which provides a higher level front-end and extensions to KSP;
- the SNEs package for solution of nonlinear systems;
- time stepping;
- preconditioners.

PETSc is supported and actively enhanced. Some of the key ideas behind the toolkit are covered in [20]. The full set of tools is available from `http://www.mcs.anl.gov/petsc` or `ftp://info.mcs.anl.gov/pub/petsc`. There is a user manual [6].

A basic design philosophy behind all the tools is " data-structure-neutrality" – where possible the tools are written in terms of a number of key operations (for example matrix-vector multiply, vector product or vector norm). The users of the tool may provide their own routines for these operations by reverse communication. In this way, the users of the tool are not restricted to any particular data representation or storage scheme. This concept is described further in [18].

The PETSc components function similarly to C++ classes in terms of implementation and use. Each component manipulates a particular family of objects (for instance, vectors) through an abstract interface (simply a set of calling sequences) and one or more implementations using particular data structures.

PETSc was originally written to use the Chameleon message passing harness, but now works directly with MPI and other proprietory systems.

2.6 PRISM

The PRISM (Parallel Research on Invariant Subspace Methods) project is a joint effort of a number of US institutions including the Argonne National Laboratory, Center for Computing Sciences (formerly the Supercomputer Research Center), Duke University, University of California at Berkeley, and University of Kentucky etc. Its overall goal is the development of scaleable, parallel eigensolvers for distributed memory systems.

The two main packages produced so far are:

- SYISDA: A symmetric eigensolver package. It is based on the Invariant Subspace Decomposition Approach (ISDA). This method uses matrix multiplication as its dominant kernel to achieve high performance. The eigensolver can run only on a square logical mesh of processors.
- BiMMER: a package which implements the Broadcast-Multiply-Roll (BMR) algorithm for matrix multiplication. It was developed as a core routine for the SYISDA package, but is available separately since matrix multiplication is an important kernel in many packages. It is meant to be a distributed memory equivalent of DGEMM which is a BLAS-3 routine. It works on any matrix size for an arbitrary number of processors where the processors are treated as a 2D topology.

The PRISM software is based on BLAS and LAPACK for sequential performance. They use the MPI message passing library. Source code and working notes are available from the Web page `http://www-unix.mcs.anl.gov/prism`.

2.7 Japan Center for Promotion of Computational Science and Engineering

The CCSE was established within the Japanese Atomic Energy Research Institute (JAERI) in 1995. It is playing a leading role in the research and development of computational science and engineering in Japan. This is continuing the work started in the Science and Technology Agency (STA) and will continue to satisfy their requirements.

Principal strands of the research and development at CCSE are:

- development of parallel basic software;
- development of parallel algorithms;
- development of parallel processing tools;
- studies of numerical simulations on complex phenomena by particle and continuum methods;

- new computer architectures.

These feed into applications of special interest to the STA laboratories and Japanese Universities and software is available on JAERI and STA computers. Fortran 90 and MPI is used and the software is portable across many platforms including: Intel Paragon, Fujitsu VPP, Hitachi SR2201, Fujitsu AP3000, IBM SP, NEC SX4, Cray T90 etc.

Some specific deliverables relevant to this report include a numerical library (project to finish end of 1999), a matrix precision library and a mesh generator library for both structured and unstructured meshes. The numerical library contains a variety of algorithms including: linear equation solvers, fast Fourier transform, random number generator, least-squares fitting and eigen-solvers. This libary will be in the public domain and down-loadable from the Web site at `http://www.jaeri.go.jp/english/index.cgicomp/comp.html`.

Software from CCSE will also form the basis for applications on the Japan Earth Simulator, which is a national project to tackle very large-scale environmental modelling. The target platform is a very large NEC computer with clusters of SMP vector nodes.

2.8 NEOS

The Optimisation Technology Center (OTC, see `http://www.mcs.anl.gov/home/otc`) is a joint project between the US Argonne National Laboratory and NorthWestern University which started in 1994. The mission of the centre is to widen the community awareness of optimisation techniques and to promote the use of such techniques. The Network-Enabled Optimisation System (NEOS, see `http://www-unix.mcs.anl.gov/neos/Server`) is a WWW interface to the software and computational resources at the OTC. NEOS currently solves usual and stochastic problems and linear network optimisation problems. The home page also points to a decision tree for optimisation problems and software.

2.9 NetSolve

NetSolve [10, 34] uses a client-server-agent software architecture with Condor for its distributed computing management. NetSolve is intended to provide transparent access to a a whole variety of software libraries, highly tuned for the target architecture. This improves maintainability of software and avoids the end user having to download and compile it. It is also of interest in meta-computing applications. This approach has been called a "computational power grid". NetSolve currently has an interface to ScaLAPACK.

Other network software includes PDC (`http://www.pdc.kth.se`), HPC2N (`http://www.hpc2n.umu.se`), Ninf and NetLink. The NetLink [23] project has similar goals fo NetSolve but via the NetLink access agent. The NEOS network package, which is specifically designed for optimisation problems, was described above.

2.10 US Accelerated Strategic Computing Initiative

Whilst it is to be expected that ASCI would contain a project to develop high-performance numerical algorithms there is no clear description of this on the ASCI Web pages. The target application codes are specific to the task of nuclear explosion simulation and stockpile stewardship and are each to be highly optimised for ASCI hardware. Some of the individual application projects are described in `http://www.lanl.gov/asci/applications.html`.

2.11 CLRC Library of Parallel Subroutines

CLIPS [13] is a relatively small project funded by the UK Engineering and Physical Sciences Research Council (EPSRC) partly through its High-Performance Computing Initiative (HPCI). It is intended to gather together a variety of parallel numerical algorithms which were developed partly as a result of funding to the CLRC HPCI Centre since 1994. It currently contains: stabilised conjugate gradient with ILU preconditioner, 3D FFT, sparse matrix ordering, Jacobi eigensolver, parallel optimisation using a genetic algorithm. some modules are mentioned in separate entries below.

2.12 Proprietory Software

A large amount of work is going into the development and optimisation of proprietary parallel software for vender-specific systems. Some examples of which are PESSL (IBM), DXML (Compaq), LibSci (Cray) etc. Many vendor solutions are based on partnership in the projects listed above. Here is a list of Web addresses for further information.

Convex (Hewlett Packard)	http://www.convex.com
DEC	http://www.digital.com/info/hpc/hpc.html
Fujitsu	http://www.fujitsu.co.jp/index-e.html
Hewlett-Packard	http://www.hp.com/home.html
Hitachi	http://www.hitachi.com
IBM	http://lscftp.kgn.ibm.com/pps
Integrated Computing Engines	http://www.iced.com
Intel	http://www.ssd.intel.com/homepage.html
Kuck and Associates	http://www.kai.com
Meiko	http://wqww.meiko.com
NAG	http://www.nag.com
NEC	http://www.nec.co.jp/index_e.html
Parsytec	http://192.166.39.34
Siemens	http://www.sni.com
Silicon Graphics/Cray Research Inc.	http://www.cray.com
SUN SunPerf	http://www.sun.com
Tera	http://www.tera.com/tera.html
Thinking Machines	http://www.think.com

3 Iterative Linear Solvers

3.1 Aztec

Name: Aztec

Description: Aztec is a parallel library of iterative solution methods and preconditioners. Its main aim is to provide tools that facilitate handling the distributed data structures. For this, there is a collection of data transformation tools, as well as query functions of the data structures. It contains CG, GMRES, BiCGstab algorithms, as well as ILUT, ILU(k), BILU(k) and ICC(k) preconditioners.

Systems:	nCUBE 2, IBM SP2 and Intel Paragon, MPI platforms as well as standard serial and vector platforms
Contact:	Ray S. Tuminaro, John N. Shadid, Scott A. Hutchinson, Lydie Prevost and Charles H. Tong Mail Stop 1111, Department 9221 Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185-1111, USA
Email:	`tuminaro@cs.sandia.gov`
URL/FTP:	`http://www.cs.sandia.gov/CRF/aztec1.html`. Available after completing a license agreement on the Web page.
Comments:	Latest version 2.0, 1997.
References:	[24]

3.2 BlockSolve

Name:	BlockSolve
Description:	The BlockSolve package contains iterative routines for solving large sparse symmetric systems of linear equations on massively-parallel distributed memory systems. A number of different preconditioners are also provided.
Systems:	IBM SP series, Cray T3D, Intel Paragon, runs on a variety of parallel architectures including SGI Power Challenge, and networks of Sun, SGI, DEC alpha and HP workstations. Uses the MPI message-passing standard.
Contact:	Mark T. Jones and Paul E. Plassman, Mathematics and Computer Science Division, Argonne National Laboratory, USA.
Email:	`mjones@mcs.anl.gov`, `plassman@mcs.anl.gov`
URL/FTP:	`http://www-unix.mcs.anl.gov/sumaa3d/BlockSolve` `ftp://info.mcs.anl.gov/pub/BlockSolve`
Comments:	BlockSolve can be used with the PETSc package
References:	[25]

3.3 CLIPS

This section to be added later.

3.4 ISIS++

Name:	ISIS++: Iterative Scalable Implicit Solver (in C++)

Description: ISIS++ is a portable, object-oriented framework for solving sparse systems of linear equations. The framework includes implementations of a number of Krylov subspace iterative solution methods (CG, CGS, BiCGStab, QMR, GMRES(m), DefGMRES(m), FGMRES(m), CGNE (normalised equations), CGNR (normalised residuals)) and preconditioners (diagonal, block Jacobi, polynomial (Neumann and least squares), sparse parallel approximate inverse (SPAI), composed (combines polynomial with block Jacobi or SPAI)) as well as both uniprocessor and multi-processor matrix and vector classes. It is designed to facilitate integration of components from various othet sparse libraries

Systems:

Contact: Robert L. Clay, Kyran Mish and Alan B. Williams
Distributed Computing Research
Sandia National Labs, Livermore, CA 94550, USA

Email: `rlclay@ca.sandia.gov`

URL/FTP: `http://ziggurat.ca.sandia.gov/isis`

Comments: Source code down-loadable after submitting an automated e-mail request from the Web page. Latest version 1.1 (March 1999)

References:

3.5 KSP

Name: KSP: Krylov Space methods Package

Description: Package of iterative methods for the solution of linear systems of equations. Methods provided include conjugate gradients, GMRES, BiCGSTAB, transpose-free QMR, and others. New methods can easily be added to the package.

Systems: can run on single workstations, or in parallel using MPI on UNIX and Windows NT and 95

Contact: William Gropp,
Mathematics and Computer Science Division,
Argonne National Laboratory, USA.

Email: `gropp@mcs.anl.gov`

URL/FTP: `http://www.mcs.anl.gov/petsc`,
`ftp://info.mcs.anl.gov/pub/petsc`

Comments: The methods are designed to be "data-structure-neutral" – they are based on a number of main operations which the package user provides for reverse calling (for example matrix-vector multiply or vector product), thus the user is not restricted to any particular data representation or storage scheme. Some of the more common storage schemes are provided with the package. Part of the PETSc software toolkit for scientific computing KSP is usually called from SLES (Simplified Linear Equation Solvers), the higher level front-end package of PETSc

References: [18, 19] See section 2.5 for more information

3.6 ParPre

Name:	ParPre: Parallel Preconditioners for Iterative Methods
Description:	ParPre is a library of parallel preconditioners for iterative solution methods for linear systems of equations. It is an add-on package to PETSc
Systems:	
Contact:	Victor Eijkhout or Tony Chan Department of Computer Science, 6363 Mathematical Sciences Bldg University of Tennessee at Knoxville UCLA Dept of Mathematics, Los Angeles, CA 90095-1555,USA
Email:	`eijkhout@cs.utk.edu` or `chan@math.ucla.edu`
URL/FTP:	`http://www.cs.utk.edu/~eijkhout/parpre.html`
Comments:	part of the ScaLAPACK project. Also available from Netlib in directory "scalapack". It uses the PETSc library, see Section 2.5
References:	[15]

3.7 PCG

Name:	PCG: Parallel Conjugate Gradient methods
Description:	A range of parallel iterative solvers including CG, BCG, GMRES, QMR. Some preconditioners are provided but alternatively a preconditioner and matrix-vector product routine can be provided by the user through reverse communication.
Systems:	Intel iPSC/860, Intel Paragon, CM series, nCUBE 2, f77/MPI, f77/PVM, Cray T3D
Contact:	W. Joubert and G.F. Carey University of Texas at Austin
Email:	`carey@cfdlab.ae.utexas.edu`
URL/FTP:	`http://www.cfdlab.ae.utexas.edu/pcg/index.html`, `ftp://ftp.c3.lanl.gov/pub/pcg`
Comments:	Joint project between Los Alamos National Laboratory and University of Austin in Texas. FTP site last updated in 1996!
References:	[26, 27]

3.8 PIM

Name:	PIM: Parallel Iterative Methods

Description: FORTRAN77 package containing a number of iterative methods for the solution of systems of sparse linear equations. Methods provided include a number of variants of conjugate gradients (CG, Bi-CG, CGS, Bi-CGSTAB, CGNR), generalised minimum residual (GMRES), generalised conjugate residual (GCR) and transpose-free quasi minimum residual (TFQMR). The user may choose the particular stopping criteria required for the iterative method. The user needs to supply reverse-called external routines for the matrix-vector product, preconditioner application and norms and inner products.

Systems: ports exist for networks of workstations using message-passing systems (PVM-3 and MPI), SGI Challenge, Kendall Square Research KSR1, Cray Y-MP2E/232, Cray C9016E, Cray T3D, Intel Paragon XP/S, Intel iPSC/860, IBM 9070 SP/1, TMC CM-5

Contact: Rudnei Dias da Cunha and Tim Hopkins,
Computing Laboratory, University of Kent at Canterbury, Kent CT2 7NF UK

Email: `rdd@ukc.ac.uk` or `trh@ukc.ac.uk`

URL/FTP: `http://www.mat.ufrgs.br/pim-e.html`. Codes and user guide available from `ftp://ftp.mat.ufrgs.br/pub/pim`

Comments: Joint project between University of Kent and Universidade Fedaral do Rio Grande do Sul in Brasil.

References: [14]

3.9 PINEAPL

Name: PINEAPL: Parallel Industrial NumErical Applications and Portable Libraries

Description: Within this general parallel library, there are iterative algorithms for sparse systems, including most of the Krylov-space algorithms, (CG, CGS, BICGSTAB, TFQMR, GMRES) with Jacobi, SOR, SSOR, ILU, overlapping and non-overlapping additive Schwarz preconditioners. Other library material being developed by the PINEAPL partners includes optimisation, a fast Fourier transform and a fast Poisson routine.

Systems: Based on PVM and MPI. Should work on most systems including vector systems.

Contact: Sven Hammarling or Anne Trefethan
The Numerical Algorithms Group Ltd.
Wilkinson House, Jordan Hill Road, Oxford OX2 8DR UK

Email: `sven@nag.co.uk`

URL/FTP: `http://www.nag.co.uk/Projects/Pineapl`

Comments:

References: [29]

3.10 PSPARSLIB

Name:	PSPARSLIB: A Portable Library of Parallel Sparse Iterative Solvers
Description:	A library of parallel iterative algorithms. The library consists of the four major parts, accelerators; preprocessing tools; preconditioning routines; and message-passing tools. Accelerators include CG, GMRES, FGMRES, DQGMRES, BICGSTAB, QMR and TFQMR. Preconditioners includes additive and multiplicative Schwartz, local ILUT, local block ILU.
Systems:	Tested on the CM5, Cray T-series, Convex Exemplar, IBM SP2, IBM and SGI workstation clusters. Uses MPI and BLAS-1.
Contact:	Authors: Yousef Saad, Andrei V. Malevsky, G. C. Lo, Sergey Kuznetsov, Masha Sosonkina, Irene Moulitsa Contact: Yousef Saad Department of Computer Science and Engineering University of Minnesota 200 Union Street S.E. Minneapolis, MN 55455
Email:	`saad@cs.umn.edu`
URL/FTP:	`http://www.cs.umn.edu/Research/arpa/p_sparslib/psp-abs.html`
Comments:	Latest version 3.0 (Feb 1999) can be downloaded as source code.
References:	[36]

4 Direct Linear Solvers for Sparse Matrices

4.1 CAPSS

Name:	CAPSS: Cartesian Parallel Sparse Solver
Description:	CAPSS is a parallel C package which solves a sparse linear system, where the matrix is symmetric positive definite, using Cholesky factorisation.
Systems:	Intel iPSC/860 machines. The code uses message passing calls in PICL, a Portable Instrumented Communications Library from Oak Ridge National Laboratory, USA, and a few native iPSC/860 functions.
Contact:	Padma Raghavan, National Centre for Supercomputing Applications, University of Illinois, USA.
Email:	`padma@ncsa.uiuc.edu`
URL/FTP:	`http://www.ncsa.uiuc.edu/Apps/MCS/CompSci/CAPSS/CAPSS.html`. Also available from Netlib in directory "scalapack"
Comments:	
References:	[35]

4.2 MUMPS

Name:	MUMPS: MUltifrontal Massively Parallel Solver
Description:	MUMPS solves sparse systems based on the multifrontal method. The principal feature of this approach is that the matrix factorisation can be represented by a tree where each edge represents the communication of data and each node some elimination operations on dense submatrices
Systems:	Written in Fortran 90 and MPI. Performance available for tests on IBM SP and SGI Origin 2000.
Contact:	Iain Duff CLRC Rutherford Appleton Laboratory Chilton, Didcot, Oxfordshire OX11 0QX, UK
Email:	`I.Duff@rl.ac.uk`
URL/FTP:	`http://www.genias.de/parasol`
Comments:	Collaboration between CLRC and CERFACS, France. Current version is 2.1.3. Part of the PARASOL project.
References:	[3]

4.3 PSPASES

Name:	PSPASES: Parallel SPArse Symmetric dirEct Solver)
Description:	An MPI-based library for solving linear systems of equations involving sparse symmetric positive definite matrices
Systems:	Any systems with MPI and BLAS libraries, and Fortran 90 and C language compilers. Tested on SGI Origin 2000, SGI PowerChallenge, Cray T3E, IBM SP, and networks of IBM RS/6000 workstations
Contact:	Anshul Gupta, Mahesh Joshi, George Karypis, Vipin Kumar and Fred Gustavson Department of Computer Science and Engineering University of Minnesota, Minneapolis, MN55455, USA
Email:	`mjoshi@cs.umn.edu`
URL/FTP:	`http://www-users.cs.umn.edu/~mjoshi/pspases`
Comments:	PSPASES uses ParMETIS and METIS as its default ordering libraries. Latest version PSPASES 1.0.2 (Sept. 1998)
References:	[21]

4.4 SPARSPAK

This is now superceded by WSSMP for parallel systems.

4.5 SuperLU

Name:	SuperLU: Sparse Gaussian Elimination on High Performance Computers
Description:	A C-based software package. SuperLU_MT is for Shared Memory Parallel Processors (SMPs). SuperLU_Dist, aimed at distributed memory processors, is to be released in early 1999.
Systems:	
Contact:	Xiaoye S. Li or NERSC, MS 50F Lawrence Berkeley National Laboratory 1 Cyclotron Rd, Berkeley, CA 94720 James W. Demmel Comuter Science Division University of California Berkeley, CA 94720
Email:	xiaoye@nersc.gov or demmel@cs.berkley.edu
URL/FTP:	http://www.cs.berkeley.edu/~demmel/SuperLU.html
Comments:	
References:	[32]

4.6 WSSMP

Name:	WSSMP: Watson Symmetric Sparse Matrix Package
Description:	Watson Symmetric Sparse Matrix Package, WSSMP, is a software package for solving large sparse linear systems. It uses a modified multifrontal algorithm and scalable parallel algorithms for sparse symmetric factorisation and triangular solves. It is organised in a two-tier structure with the message-passing parallel interface PWSSMP able to call the serial WSSMP or multi-threaded TWSSMP (which uses Pthreads).
Systems:	IBM platforms (serial, shared memory or distributed memory)
Contact:	Anshul Gupta IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598.
Email:	anshul@watson.ibm.com
URL/FTP:	http://www.research.ibm.com/mathsci/ams/ams_WSSMP.htm
Comments:	Written by some of the same authors as PSPASES, but is mainly tuned and intended for IBM platforms.
References:	[22]

5 Direct Linear Solvers for Dense Matrices and Eigen-solvers

A separate report has been prepared which gives example results for a number of eigen-solvers [1]. This is available from the Web site http://www.cse.clrc.ac.uk/Activity/HPCI or from r.j.allan@dl.ac.uk.

5.1 ARPACK

Name:	ARPACK: Arnoldi's method Package
Description:	ARPACK is a FORTRAN77 package for solving large scale nonsymmetric, symmetric and generalised eigenvalue problems. The package is based on Arnoldi's method and can compute a few eigenvalues and eigenvectors of a large, possibly sparse, matrix. It requires a user-supplied matrix-vector multiply to do this. It uses the implicit restart method of Sorensen et al. A parallel version (P_ARPACK) and a C++ version (ARPACK++) are now available
Systems:	Parallel version based on BLACS and MPI
Contact:	Rich Lehoucq, Kristi Maschhoff, Danny Sorensen and Chao Yang Department of Computational and Applied Mathematics, Rice University, USA.
Email:	`sorensen@rice.edu` or `lehoucq@rice.edu`
URL/FTP:	`http://www.caam.rice.edu/software/ARPACK` or `ftp://ftp.caam.rice.edu/pub/software/ARPACK` Available from netlib in directory "scalapack"
Comments:	
References:	[30] An evaluation of eigen-solvers can be found in [1]

5.2 PeIGS

Name:	PeIGS: Parallel Eigensolver for General Symmetric Systems
Description:	PeIGS [16] (pronounced "pigs") is a collection of commonly used linear algebra subroutines for computing the eigensystem of the real standard problem $\mathbf{Ax} = \lambda\mathbf{x}$ and the general eigensystem $\mathbf{Ax} = \lambda\mathbf{Bx}$, with $\mathbf{A}$ a dense real symmetric matrices and $\mathbf{B}$ positive definate using Cholesky decomposition.
Systems:	Current v3.0 is running on Cray T3D, IBM SP2 and many other systems. Uses MPI or TCGMSG message passing and BLAS and LAPACK for serial speed
Contact:	It was developed by George I. Fann, Richard J. Littlefield (PNNL) and Robert van der Geijn (U. Texas, Austin). Daresbury Laboratory has a research collaboration with PNNL.
Email:	`rj_littlefield@pnl.gov` or `g_fann@pnl.gov`
URL/FTP:	`ftp://ftp.pnl.gov`
Comments:	
References:	It is documented [16] and there are also papers benchmarking several methods tested at PNL [33, 17]. An evaluation of eigen-solvers can be found in [1]

5.3 ScaLAPACK

Name:	ScaLAPACK: Scalable Linear Algebra Package
Description:	ScaLAPACK is a distributed memory version of LAPACK (Linear Algebra Package), written in FORTRAN77. It includes routines for the solution of dense, banded, and tridiagonal linear systems of equations, condition estimation and iterative refinement, for LU and Cholesky factorisation, matrix inversion, full-rank linear least squares problems, orthogonal and generalised orthogonal factorisations, orthogonal transformation routines, reductions to upper Hessenberg, bidiagonal and tridiagonal form, reduction of a symmetric-definite/Hermitian-definite generalised eigenproblem to standard form, the symmetric/Hermitian, generalised symmetric/Hermitian, the nonsymmetric eigenproblem, and the singular value decomposition.
Systems:	The software has been written to be portable across a wide range of distributed-memory environments such as the Cray T-series, IBM SP, Intel series, SGI Power Challenge Array and Origin 2000, clusters of workstations, and any system for which PVM or MPI is available.
Contact:	Jack J. Dongarra, Department of Computer Science, University of Tennessee at Knoxville, USA.
Email:	`scalapack@cs.utk.edu`
URL/FTP:	`http://www.netlib.org/scalapack/index.html`
Comments:	The ScaLAPACK package sits on top of BLAS, PBLAS and BLACS. Current version 1.6 (Nov. 1997)
References:	[12, 11]

5.4 SYISDA

Name:	SYISDA: Symmetric Invariant Subspace Decomposition Algorithm
Description:	SYISDA is part of the PRISM research project aimed at producing portable parallel eigensolvers and also lower-level kernels for use in building these solvers. The project makes use of algorithms based on invariant subspace decomposition approaches, which have a higher sequential complexity than other more commonly used algorithms but are significantly more scalable on a parallel machine.
Systems:	Using MPI, it should work on most platforms.
Contact:	Steve Lederman, Supercomputing Research Center, USA
Email:	
URL/FTP:	`http://www-unix.mcs.anl.gov/prism`
Comments:	
References:	[8, 5] An evaluation of eigen-solvers can be found in [1]

6 PDEs and ODEs

6.1 ParSODES

Name:	ParSODES
Description:	ParSODES is a parallel, stiff, initial value, ODE integrator which is based on an "across the method" parallelisation of multi-implicit Runge-Kutta methods.
Systems:	The code is written in Fortran 90, and the parallelism has been obtained through MPI, so should work on most systems.
Contact:	Claus Bendtsen The Danish Computer Centre for Research and Education DK-2800 Lyngby Denmark
Email:	`Claus.Bendtsen@uni-c.dk`
URL/FTP:	`http://www.netlib.org/ode/parsodes.tar.gz` or `http://unidhp.uni-c.dk/~nicbe`
Comments:	Latest version 1.1 (1996)
References:	

6.2 //ELLPACK

Name:	//ELLPACK: Parallel Elliptic Equation Package
Description:	designed as an object-oriented interface for describing and solving systems of elliptic and parabolic pdes.
Systems:	binary only for SUN4 architecture
Contact:	S. Weerawarana, E.N. Houstis, J.R. Rice and A.C. Catlin Department of Computer Science Purdue University West Lafayette, Indiana, 47907-1398, USA.
Email:	`pellpack-beta@cs.purdue.edu`
URL/FTP:	`http://www.cs.purdue.edu/research/cse/pellpack/pellpack.html`
Comments:	Available as a beta release by special agreement.
References:	[37, 38]

7 Nonlinear Equations and Optimisation

7.1 GALOPPS

Name:	GALOPPS: Genetic ALgorithm Optimised for Portability and Parallelism System
Description:	a genetic algorithm tool in C that provides an enormous range of options for genetic algorithm experiments.
Systems:	It is available for both PC and Unix systems. The other versions are GALOPPS3.2 (two forms, for PC and generic Unix), and PVM GALOPPS (Unix only). A threaded version of GALOPPS (Unix only) is available by special request.
Contact:	Erik Goodman Michigan State University East Lansing, MI 48824-1226
Email:	`goodman@egr.msu.edu`
URL/FTP:	`http://GARAGe.cps.msu.edu/software/galopps`
Comments:	
References:	

7.2 PDS

Name:	PDS: Parallel Direct Search algorithm
Description:	PDS is a collection of Fortran subroutines for solving unconstrained nonlinear optimisation problems using direct search methods.
Systems:	Intel iPSC/2, iPSC/860 or Touchstone Delta, Sun workstation. The software is written so that execution on sequential machines is straightforward while execution on Intel distributed memory machines can be accomplished simply by including a few well-defined routines containing calls to Intel-specific Fortran libraries.
Contact:	J.E. Dennis, Department of Computational and Applied Mathematics Rice University, Houston, Texas, 77005, USA.
Email:	`dennis@caam.rice.edu`
URL/FTP:	`http://softlib.rice.edu/softlib/catalog/pds.html`
Comments:	This coordinate search algorithm does not require derivatives, thus is particularlly useful when optimising based on black-box code.
References:	[28]

7.3 PGAPack

Name:	PGAPack: Parallel Genetic Algorithm Library
Description:	PGAPack is a general-purpose, data-structure-neutral, parallel genetic algorithm library. It is intended to provide most capabilities desired in a genetic algorithm library, in an integrated, seamless, and portable manner.
Systems:	it runs on uniprocessors and, using MPI, on parallel computers and workstation networks.
Contact:	David Levine Mathematics and Computer Science Division Argonne National Laboratory
Email:	`levine@mcs.anl.gov` or `pgapack@mcs.anl.gov`
URL/FTP:	`http://www-unix.mcs.anl.gov/~levine/PGAPACK/index.html`, `ftp://ftp.mcs.anl.gov/pub/pgapack`
Comments:	Written in C and MPI, latest version 1.0 (1996)
References:	[31]

7.4 SNES

Name:	SNES: Simplified Nonlinear Equation Solvers
Description:	SNES provides Newton-like iterative methods for the solution of nonlinear systems of equations and unconstrained optimisation. The package allows the user a great deal of flexibility in the choice of data structures and solution methods used.
Systems:	can run on single workstations, or in parallel using MPI on UNIX and Windows NT and 95
Contact:	William Gropp, Mathematics and Computer Science Division, Argonne National Laboratory, USA.
Email:	`gropp@mcs.anl.gov`
URL/FTP:	`http://www.mcs.anl.gov/petsc`, `ftp://info.mcs.anl.gov/pub/petsc`
Comments:	Uses the SLES package (which in term calls KSP, see separate entry) for intermediate linear solves, although this can be replaced by the user if required. Part of the PETSc software toolkit for scientific computing Latest version 2.0.22 (April 1998).
References:	See section 2.5 for more information.

8 FFTs

A separate report has been prepared on serial and parallel FFT packages [2]. This is available from the Web site `http://www.clrc.cse.ac.uk/Activity/HPCI` or by email from `r.j.allan@dl.ac.uk`.

9 Other Sources of Information

9.1 Netlib

A number of the packages described in this document are available from Netlib. This is a large software repository which contains numerical software and tools, including a large amount of parallel software. Software on Netlib can be accessed in a number of different ways:

- by anonymous ftp from `ftp://netlib2.cs.utk.edu`;
- by Web URL `http://www.netlib.org`;
- by email with a message of the form "send index from pvm3" sent to `netlib@ornl.gov`. The general form is "send *file* from *library*". To get a list of all the libraries on netlib use "send index".
- using the Xnetlib package which allows interactive browsing of the Netlib directories. This can be obtained from Netlib via anonymous ftp in directory xnetlib, or via email with the message "send xnetlib.shar from xnetlib" to `netlib@ornl.gov`.

In the UK Hensa contains a mirror of Netlib.

9.2 Hensa

The HENSA (Higher Education National Software Archives) is a UK national service which benefits the higher education and research community in the UK. It is funded by JISC, the Joint Information Systems Committee of the Higher Education Funding Councils.

It maintains copies of electronic archives from all over the world, providing access to a wide range of up-to-date software and other material, including:

- achieves of numerical and statistical tools and libraries;
- copies of the MPI and HPF standards.;
- parallel research papers;
- details of conferences.

The site can be accessed by anonymous ftp to `ftp://unix.hensa.ac.uk`. It can also be accessed via the WWW with URL `http://www.hensa.ac.uk`.

The entire contents of Netlib are mirrored by Hensa at `ftp://unix.hensa.ac.uk/netlib`, this may be more convenient to use from the UK.

Hensa also contains a mirror of NHSE (below) at `http://www.hensa.ac.uk/parallel/nhse`.

9.3 National HPCC Software Exchange

The NHSE is a distributed collection of software, documents, data and information for use by the high-performance computing community. Development of the NHSE is being carried out by the Center for Research on Parallel Computation (CRPC). Access via WWW at URLs `http://www.nhse.org`.

Existing NHSE repositories include HPC-Netlib, PTlib, and CSIR. HPC-Netlib is the high performance branch of the Netlib mathematical software repository. PTlib is the Parallel Tools software repository and CSIR is Chemistry Software and Information Resources.

9.4 Templates

A useful reference to the underlying methodology of iterative solvers is Templates [7]. This is available via the Web from `http://www.netlib.org/templates/Templates.html`. It is intended to enable people to build their own solvers.

Methods covered are: Jacobi, Gauss-Seidel, successive over-relaxation (SOR); conjugate gradient (CG); minimal residual (MINRES) and symmetric LQ (SYMMLQ); conjugate gradients on the normal equations (CGNE and CGNR); generalised minimal residual (GMRES); biconjugate gradient (BiCG), conjugate gradient squared (CGS), biconjugate gradient stabilised (Bi-CGSTAB) Chebyshev iteration.

9.5 Other Public-domain Sources

Some other public-domain software repositories are listed below.

ManMohan S. Sodhi's survey on management and operations research
`http://www.iems.nwu.edu/orms.repository`

MathProg
`ftp://ftp.zib-berlin.de/pub/mathprog`

Multigrid resources MGNET
`http://www.mgnet.org`

Ken Stanley's diagonaliser page
`http://www.cs.berkeley.edu/~stanley/symeig/index.html`

Scientific applications on Linux
`http://sal.kachinatech.com`

TOMS-CALGO
`http://gams.nist.gov/toms/CALGO.html`

Jörg Arndt's FFT pages
`http://www.jjj.de/fxt/fxtpage.html`

FFTW
`http://theory.lcs.mit.edu/~fftw`

BenchFFT
`http://theory.lcs.mit.edu/~benchfft`

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