Remap Project (Lyon)

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1. Parallel direct solvers for large sparse linear systems: MUMPS package,
2. Scilab //
   - **Idea**: provide access to metacomputing resources (ex: sparse solvers) from the workstation using scilab,
   - **Goal**: efficiency, transparency and interactivity.
3. Use of sparse solvers in scilab

Direct solvers

collaboration with
Patrick Amestoy (ENSEEIHT-IRIT, Toulouse),
Iain Duff (CERFACS-RAL),
Jacko Koster (PARALLAB, Bergen),
and Miroslav Tuma (ICS, Prague)

- MUMPS = MUltifrontal Massively Parallel Solvers

  parallel package for the direct solution of large-scale sparse linear systems,

- partially funded by the PARASOL project

Direct solvers: MUMPS 4.1

- distributed memory code (message passing),
- solves $\mathbf{Ax} = \mathbf{b}$ or $\mathbf{A}^T\mathbf{x} = \mathbf{b}$ using Gaussian elimination ($\mathbf{LU}$ or $\mathbf{LDL}^T$)
  - $\mathbf{A}$ unsymmetric (partial pivoting with threshold),
  - $\mathbf{A}$ general symmetric (with pivoting),
  - $\mathbf{A}$ symmetric positive definite (no pivoting),
  - $\mathbf{A}$ deficient (with null space basis),
- accepts matrices
  - assembled or in elemental form,
  - centralized or distributed.

Direct Solvers: MUMPS 4.1

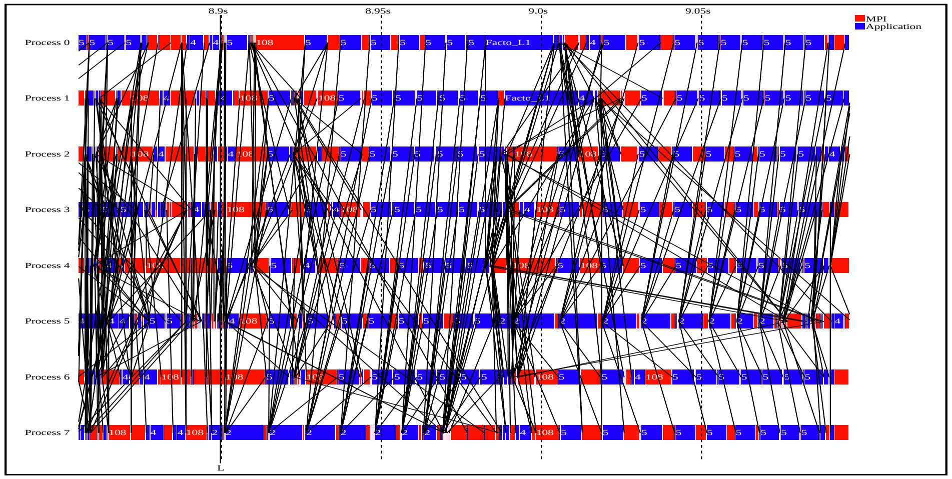
- several pre- & postprocessing facilities
  - accepts ordering of unknowns provided by user,
  - permutes large entries to diagonal (MC64, Duff/Koster) + matrix scaling,
  - return a Schur complement $\mathbf{A}_{22} - \mathbf{A}_{21}{\mathbf{A}_{11}}^{-1}\mathbf{A}_{12}$
  - return rank and null space basis for deficient $\mathbf{A}$
  - (backward) error analysis
  - iterative refinement
- public domain (non commercial use)
  `http://www.enseeiht.fr/apo/MUMPS`

  $\approx$ a couple of hundred users
- competitive performance

1- Direct solvers: MUMPS approach

- Multifrontal method (*Duff, Reid, 1984*),

  tree parallelism + node parallelism (1D or 2D),
- relies on MPI, BLAS, BLACS, ScaLAPACK,
- Asynchronous approach with dynamic data structures to allow for pivoting,

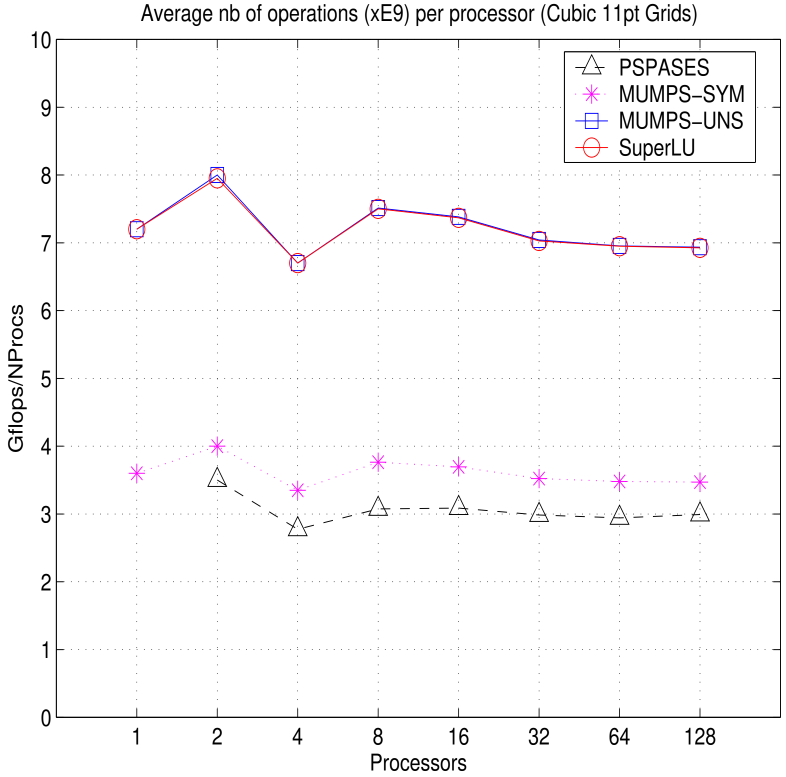


- Dynamic scheduling with decentralized decisions: assign tasks to less loaded procs,

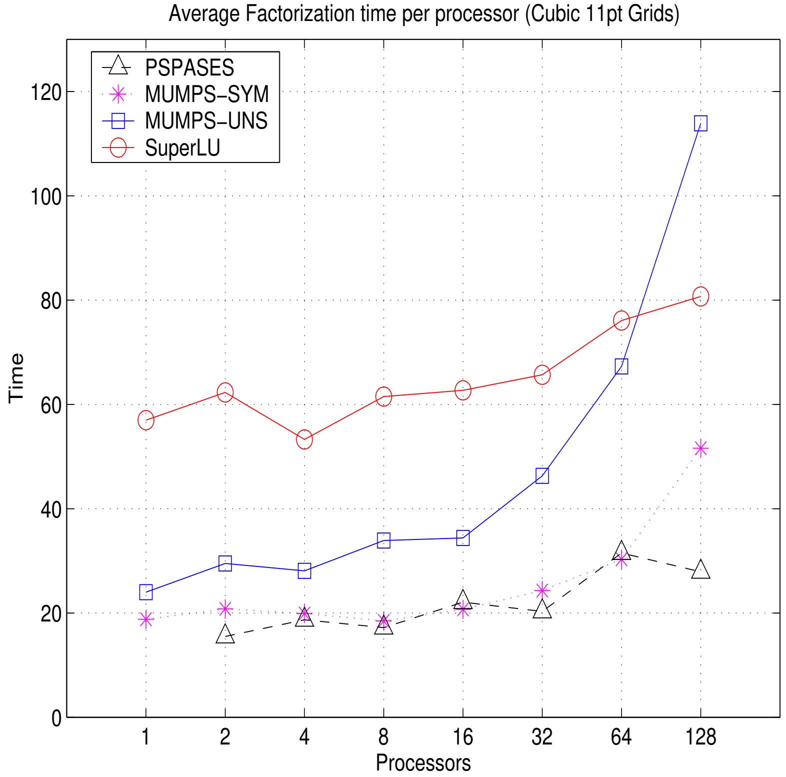
Direct Solvers: Performance on 3-D grids

- Regular cubic grids such that $\frac{flops}{processors} = Cste$,
- PSPASES v1.0.2: static LL^T *(Gupta et.al, Univ. Minnesota)*,
- SuperLU$_{dist}$: static LU *(Demmel, Li, Berkeley)*.

Flops/processor ($\times 10^9$)



Factorization Time



Direct Solvers: On-going work

- improve scalability on large numbers of processors: inject static info (candidate processors),
- complex version,
- tighter integration of ordering packages:
  - AMF *(ENSEEIHT)*
  - MeTiS *(University of Minnesota)*
  - PORD *(University of Paderborn)*
  - SCOTCH *(LaBRI)*
- experimentation/tuning on various platforms.
- New features (longer term): Out-of-core, sparsification of frontal matrices, 2 by 2 pivots in LDL^T, rank-revealing, incomplete LU, QR factorization, …

SCILAB to SCILAB//

The OURAGAN Project

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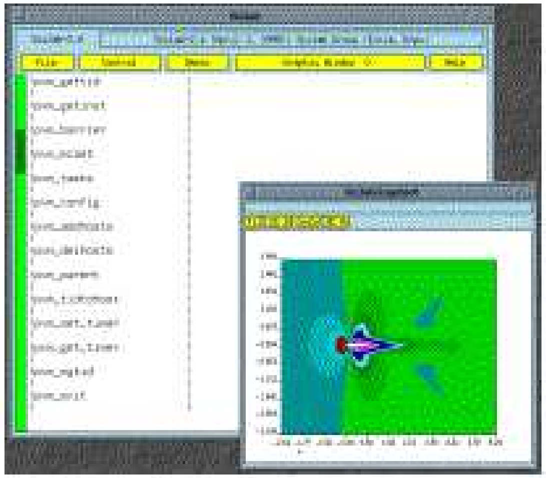
Scilab // features

Message passing between Scilab tasks (PVM, MPI),



Mixed parallelism management (task/data-parallelism)

Parallel libraries interfaces, (ScaLAPACK),

Mixed compilation/run-time support

Out-of-core parallelism (ScaLAPACK extension)

CORBA approach (management of servers)

Multithreaded Scilab scheduling & migration

Netsolve Interface (Univ. of Tennessee),

Computational servers (SLIM, FAST)

Sparse matrix solvers in heterogeneous environments

3- Use of sparse solvers in scilab:

- MUMPS:

  parallel, uses MPI, F90, BLACS, ScaLAPACK,

  $\rightarrow$ tight software integration not straightforward,

- metacomputing approach:

  $\rightarrow$ access to high performance servers/sparse direct methods from scilab console

  $\rightarrow$ interface MUMPS with Netsolve and DIET,

  $\rightarrow$ interface with other sparse solvers (ex: PETSc),

- Proposition (with F. Desprez): centralize informations about sparse developments in scilab

Related projects/collaborations

- France-Berkeley project: Analysis and tuning of two Sparse Direct Solvers (Amestoy, Duff, Li, L'Excellent, 1999-2000),
- MA41, MA49 (HSL, Amestoy, Duff, Puglisi): shared memory codes for resp. LU and QR factorization,
- Parallab (Univ. of Bergen, Norway): use MUMPS for domain decomposition,
- NSF-INRIA with IRISA, Minnesota, Berkeley, . . . : couple direct + iterative, metacomputing interface,
- NSF-INRIA with Univ. Tennessee (submitted) : improve netsolve + grid aware library (netlib)
- ACI Grid "Grid ASP" and RNTL GASP
  $\rightarrow$ DIET: Distributed Interactive Engineering Toolbox,
  $\rightarrow$ large computational applications from scilab.