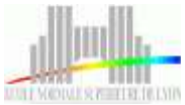
GEOREP, november 2005

Direct methods for the solution of large-scale systems of sparse linear equations






Aurélia FEVRE

Ingénieur associé

équipe GRAAL, INRIA

Outline of the presentation

- Introduction
- Sparse direct solvers
- Work in progress
- GEOREP

Introduction

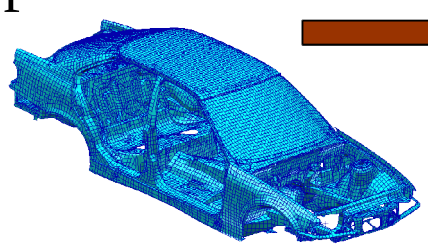
- Goal : overview of the MUMPS package
- Understand the needs of GEOREP in term of solving linear systems

Sparse direct solvers

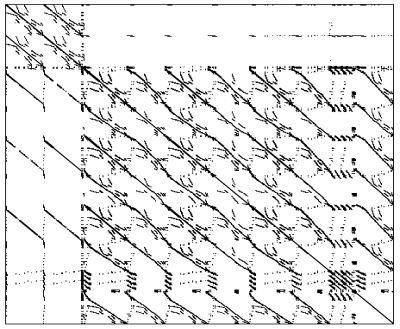
1. Introduction
2. Iterative vs Direct solvers
3. MUMPS Package

Introduction

Simulation of a physical problem



Solution of a sparse system A x = b



- Solving systems of linear equations of the form Ax=b
- Three steps approach :
  - Analysis : ordering, symbolic factorization
  - Factorization : **A=LU** or **A=LDLt**
  - Solve : **L**y=b, then **U**x=y

Direct vs Iterative solvers

DIRECT

- Very general technique
  - High numerical accuracy
  - Sparse matrices with irregular patterns
- Factorization of A
  - May be costly in terms of memory for factors
  - Facto can be reused for multiple Right Hand Sides

ITERATIVE

- Efficiency depends on the type of the problem
  - Convergence – preconditionning
  - Numerical properties/structure of A
- Requires the product of A by a vector
  - Less costly in terms of memory and possibly flops
  - Solutions with multiple Right Hand Sides can be prohibitive

The MUMPS Package

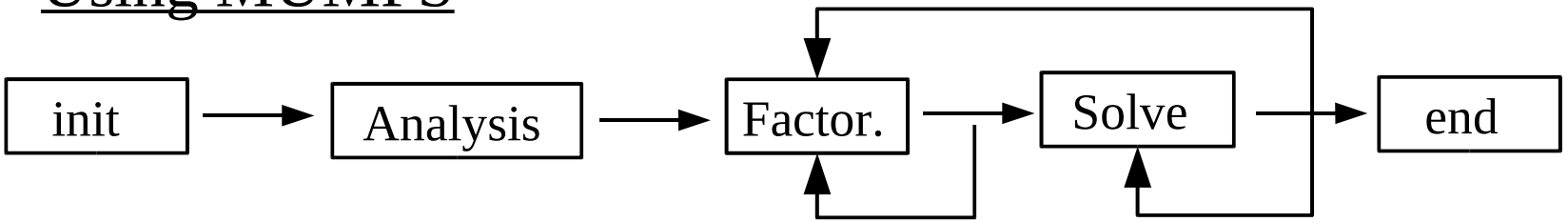
- Multifrontal Massively Parallel Solver
- http://graal.ens-lyon.fr/MUMPS
  http://www.enseeiht.fr/apo/MUMPS
- Background :
  - LTR (long term research) european project (1996-1999)
  - Supporting institutions : CERFACS, ENSEEIHT-IRIT, INRIA Rhône-Alpes
- MUMPS
  - Provided to approx. 1000 users (industrial or academic, for example : EADS, CEA, Boeing, DASSAULT, several USA labs)
  - ≈ 200 000 lines of code
  - Available free of charge (latest release 4.5.5)

The MUMPS Package

- Very general, competitive, many functionalities:
  - types of matrices : symmetric/unsymmetric
  - Input format : assembled or element-entry, distributed matrix entry
  - Arithmetic : real or complex
  - Numerical pivoting, scalings, backward errror analysis, iterative refinement
  - can be called from C or Fortran
- Parallel version : MPI, BLAS, BLACS, ScaLAPACK,

The MUMPS Package

Using MUMPS



The 3 steps can be called separately. For example :

- Several “solve” with successive Right Hand Sides (it uses the same factorized matrix)
- Redo “Factor” with the same analysis if only numerical values of the matrix changed
- several matrices can be handled

The MUMPS Package

Some typical numbers

- Statistic for typical test problems (old version of MUMPS)

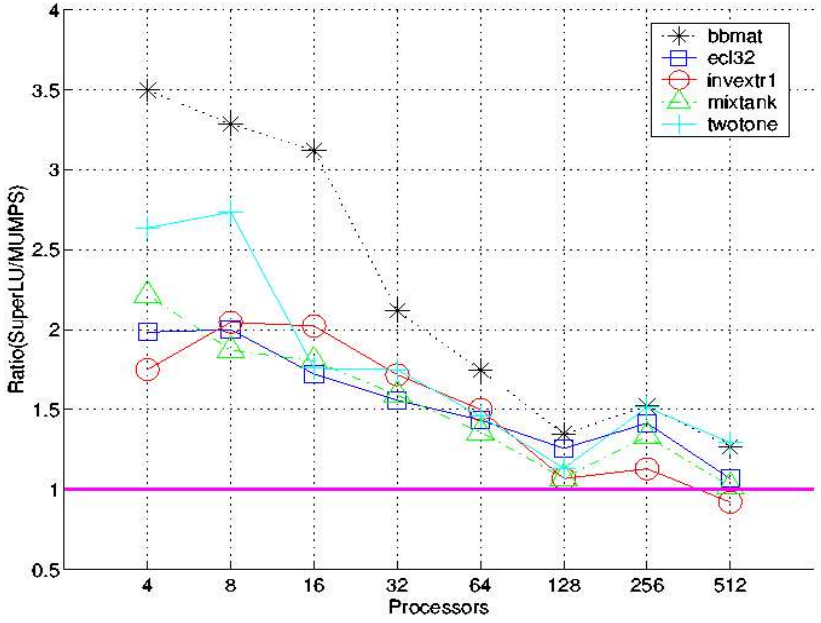
Matrix	N	NZ	Factors	flops	Application area
WANG3	26064	177168	71 MB	5.3 Giga	3d electron continuity
ULTRASOUND3	185193	11390625	1.8 GB	470 Giga	3d wave propagation
CONV3D64	836550	12548250	21.5 GB	23.9 Tera	provided by CEA/CESTA

- Time for factorization (in seconds)
  - Laptop (pentium III, 700 MHz)
    - WANG3: 13.5 s (1 proc)
  - P2CHPD cluster (AMD Athlon 1.6 GHz)
    - WANG3 4.3 s (1 proc)
    - ULTRASOUND3 175 s (2 procs) 105 s (4 procs)
  - IDRIS (Power4):
    - ULTRASOUND3 143 s (1 proc) 87 s (2 procs) 46.5 s (4 procs)
    - CONV3D64 228 s (64 procs) 150 s (128 procs)

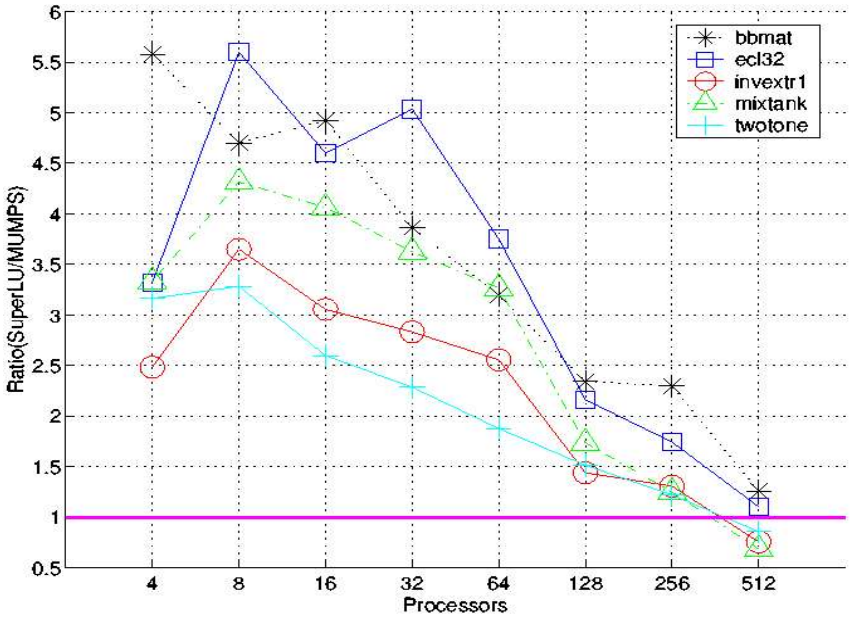
The MUMPS Package

Parallel performance : Comparison of SuperLu and Mumps (old version) [ACM TOMS '01]

factorization time ratio



solve time ratio



Work in Progress

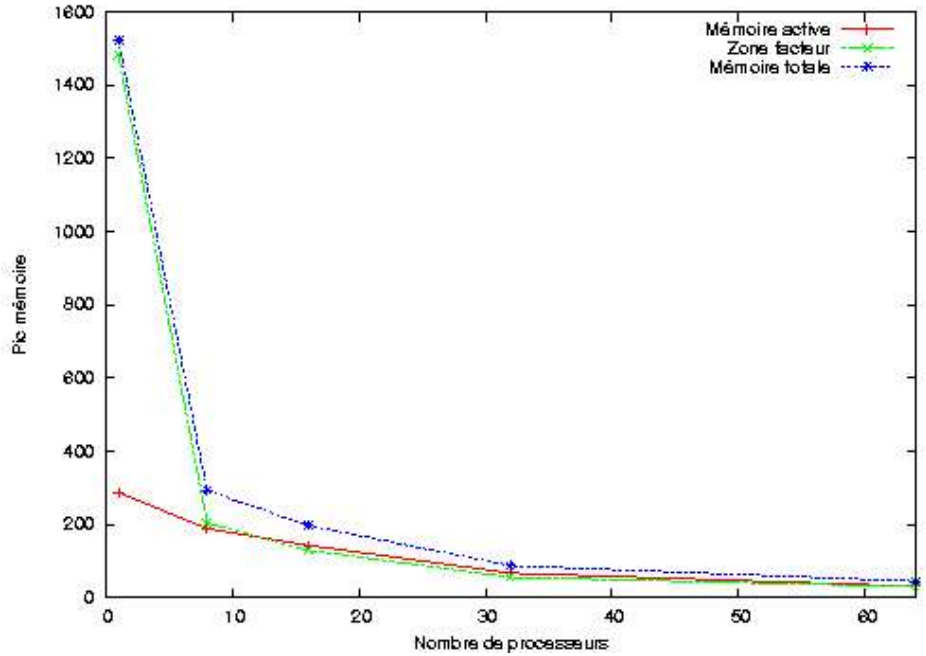
1. Interfaces to MUMPS
2. Out of Core (OOC)
3. Other works

Interfaces to MUMPS

- 2 interfaces : Scilab and Matlab
- Purpose : access to a performant solver (and its functionalities) in Scilab or Matlab
- Available within the next release of MUMPS

Out of Core

- solve larger linear systems
- uses the disk when the physical memory is too small : currently write factors on disk during the factorization, and read them during the solve



Typical memory behaviour (Audikw_1 matrix) on a various number of processors

ordre : 943695

nnz : 39297771

Other work

- Grid TLSE : expertise web site for sparse linear algebra (coordinator: ENSEEIHT-IRIT)
- Provide functionalities for iterative solvers

GEOREP

THE NEEDS ??

GEOREP

- GRAAL in GEOREP :
  - Provide support for MUMPS intallation, usage
  - New application area and types of matrices for our research
  - Get feedback
- questions :
  - Matrices : size, type, structure, …?
  - Parallel version : MPI ?