On the direct solution of very large sparse linear systems using out-of-core techniques

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Joint work with John Reid

Sparse systems

We are interested in solving

$$\mathbf{Ax} = \mathbf{b}$$

where $\mathbf{A}$ is

LARGE

s p a r s e

- Problem sizes of order $> 10^7$ not uncommon and growing larger
- Direct methods (eg $A = PLUQ$) are popular because they are robust
- But their storage requirements generally grow more rapidly than problem size

Options for large problems

Possibilities:

- Iterative method ... but preconditioner?
- Combine iterative and direct methods? Important new area.
- Buy a bigger machine and use exisiting direct solver ... but **expensive** and **inflexible**
- Parallel direct solver?
- Use an out-of-core direct solver

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- Use an out-of-core direct solver

An **out-of-core solver** holds the matrix factors in **files** and may also hold the matrix data and some work arrays in files.

Note: out-of-core working becoming even more important because of more limited local memories on distributed memory machines

Out-of-core solvers

- Idea of out-of-core solvers **not** new: band and frontal solvers developed in 1970s and 1980s held matrix data and factors out-of-core.
- For example, `MA32` in HSL (superseded in 1990s by `MA42`).
- 30 years ago John Reid at Harwell developed a Cholesky out-of-core multifrontal code `TREESOLV` for element applications.

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More recent codes include:

- `BCSEXT-LIB` (Boeing)
- `Oblio` (Dobrian and Pothen)
- `TAUCS` (Toledo and students)
- `MUMPS` currently developing out-of-core version
- Also work by Rothberg and Schreiber

HSL_MA77

Our new out-of-core solver is HSL_MA77

- HSL_MA77 is designed to solve **LARGE** sparse symmetric systems
- HSL_MA77 implements a **multifrontal algorithm**
- First release for **positive definite** problems (Cholesky $\mathbf{A} = \mathbf{L}\mathbf{L}^\mathbf{T}$); coming VERY soon is version for **symmetric indefinite problems** ($\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^\mathbf{T}$)
- Matrix data, matrix factor, and the main work space (multifrontal stack) held in **files**

Aim today: to provide brief introduction to HSL_MA77 and to present some numerical results .... hope you will go away wanting to try the code

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- Separate calls for each phase
  - Entering of integer and real matrix data
  - Analyse phase (set up data structures using user-supplied pivot order)
  - Factorization (compute and store factor plus optional solve)
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- Separate code (HSL_MA54) written to perform the (partial) factorizations of the dense frontal matrices

Input/Output in HSL_MA77

For HSL_MA77 to perform well, the I/O **must** be efficient. I/O involves:

- writing the original real and integer data
- analyse phase (integer data only)
  - reading data for input matrix
  - writing data at each node of the assembly tree
  - reading data at each node
  - writing reordered data ready for factorization
- factorization phase
  - reading integer data at each node of the tree
  - reading real data for each leaf node
  - writing columns of L as they are computed
  - writing Schur complements to stack
  - reading matrix from stack
- solve phase
  - reading integer/ real factor data once for forward sub. and once for back sub.

Input/Output in Fortran

In Fortran 77/90/95 - standard I/O is entirely **record based**

- Fine if every read/write is of the same amount of data
- **But** we need to read/write different numbers of reals and integers at each stage of the computation
- Also, we do not want to be restricted to only accessing the data in the same order as it was written

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We have got around these limitations while adhering to the strict Fortran standard by writing our own **virtual memory management system**

Virtual memory management

We have a separate Fortran 95 package `HSL_OF01` that handles all i/o

- `HSL_OF01` provides read/write facilities for one or more direct access files through a single **in-core buffer** (work array)
- Version for real data and another for integer data. Each has its own buffer.
- The buffer is divided into fixed length pages ... a page is the same length as a record in the file
- Careful handling of the buffer within `HSL_OF01` avoids actual input-output operations whenever possible

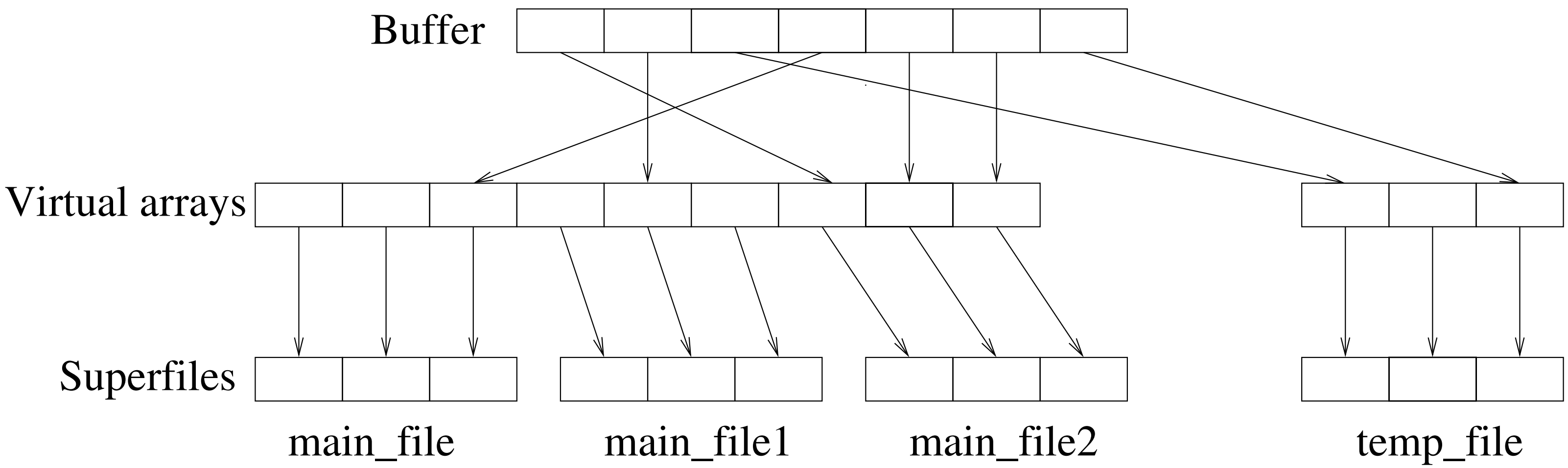
Virtual memory management

Each set of data (such as the reals in the matrix and its factor) is accessed as a **virtual array** i.e. as if it were a very long array

- Long integers (64-bit) are used for addresses in the virtual array
- Any contiguous section of the virtual array may be read or written
- Each virtual array is associated with a **primary file**
- For very large problems, the virtual array may be too large for a single file so **secondary files** are used

The primary and secondary files are **direct access files**.

Virtual memory management



- In this example, two superfiles associated with the in-core buffer
- First superfile has two secondaries, the second has none
- **Important:** user shielded from this but can control where the files are stored (primary and secondary files may be on different devices).
- Actual i/o is **not** needed if user has supplied long buffer

Use of HSL_OF01 within HSL_MA77

- HSL_MA77 has one **integer** buffer and one **real** buffer
- The integer buffer is associated with a file that holds the integer data for the matrix A and the matrix factor
- The real buffer is associated with two files:
  - one holds the real data for the matrix A and the matrix factor
  - the other is used for the multifrontal stack (work space)
- The indefinite case also uses a further real file to hold data associated with delayed pivots
- The user supplies pathnames together with names for the primary files

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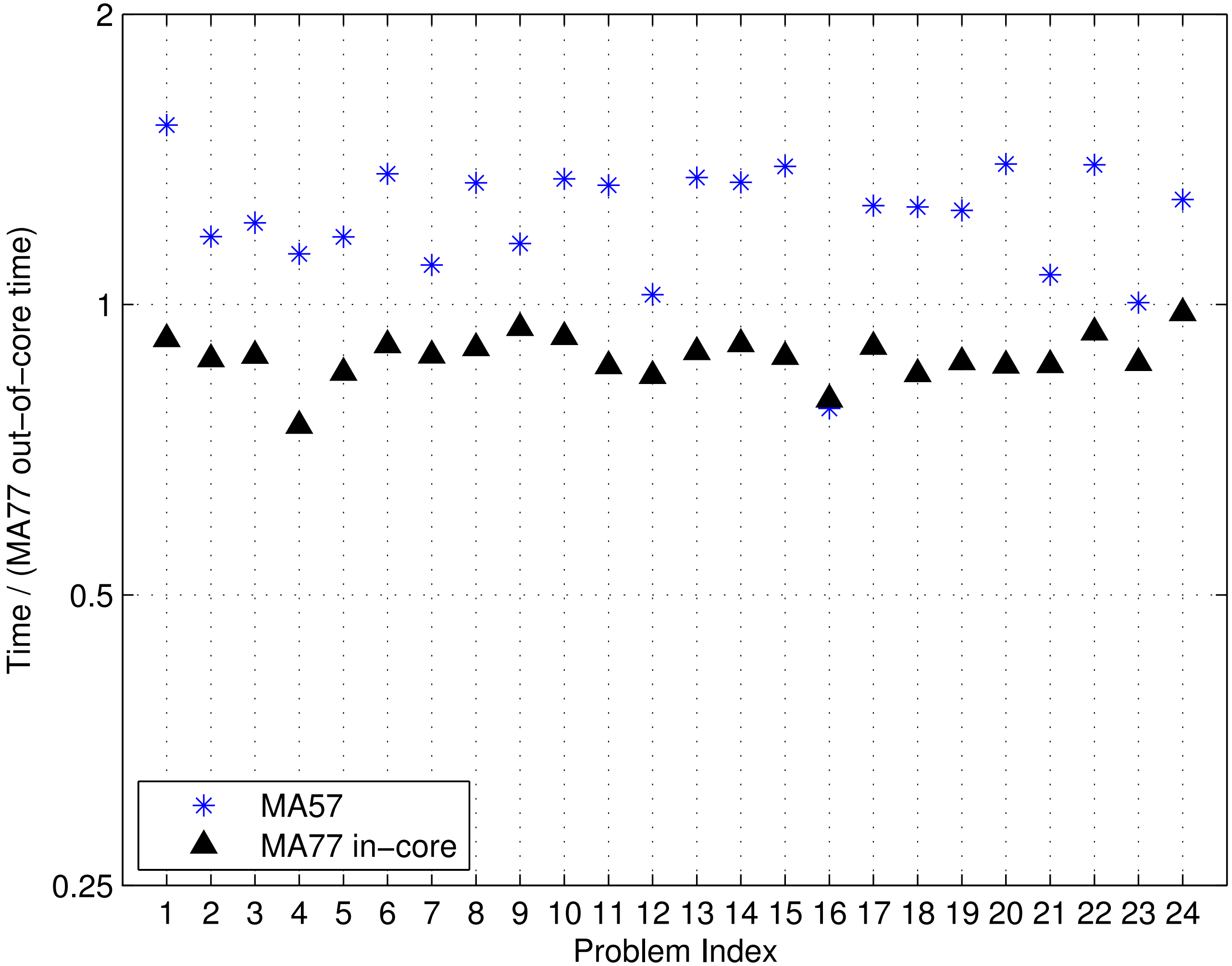
NOTE: HSL_MA77 includes option for the files to be replaced by **in-core arrays** (faster for problems for which user has enough memory) . A combination of files and arrays may be used.

Comparisons with MA57

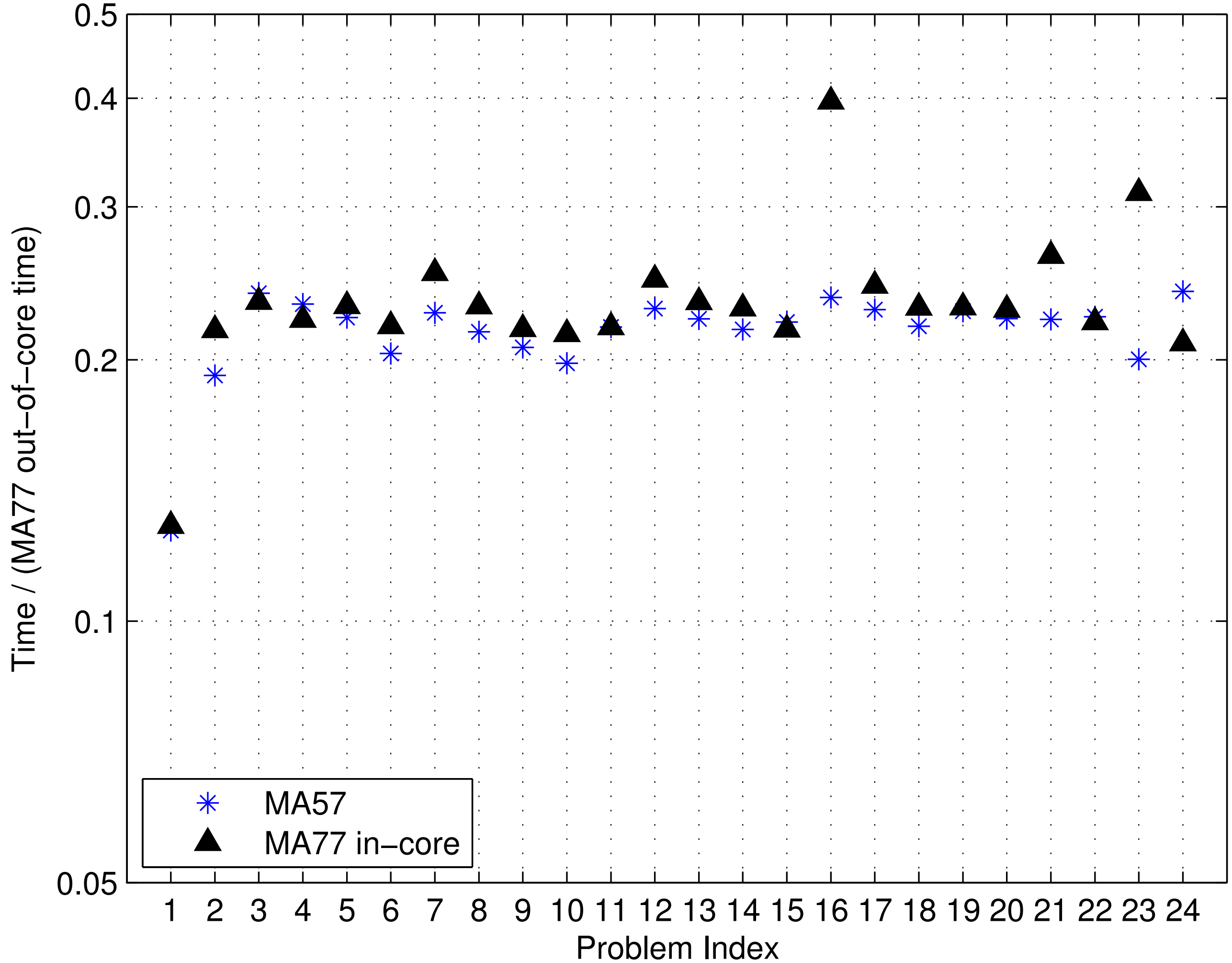
Want to compare the performance of HSL_MA77 with existing solvers.

- Test set of 24 problems of order up to $1.5 * 10^6$ from a range of applications
- All available in University of Florida Sparse Matrix Collection
- Tests used double precision (64-bit) reals on a single 3.6 GHz Intel Xeon processor of a Dell Precision 670 with 4 Gbytes of RAM
- f95 compiler with the -O3 option and ATLAS BLAS and LAPACK
- Comparisons with flagship HSL solver MA57 (Duff)
  - Multifrontal solver (replaced earlier package MA27)
  - Primarily designed for indefinite problems (we use the option to switch off numerical pivoting)

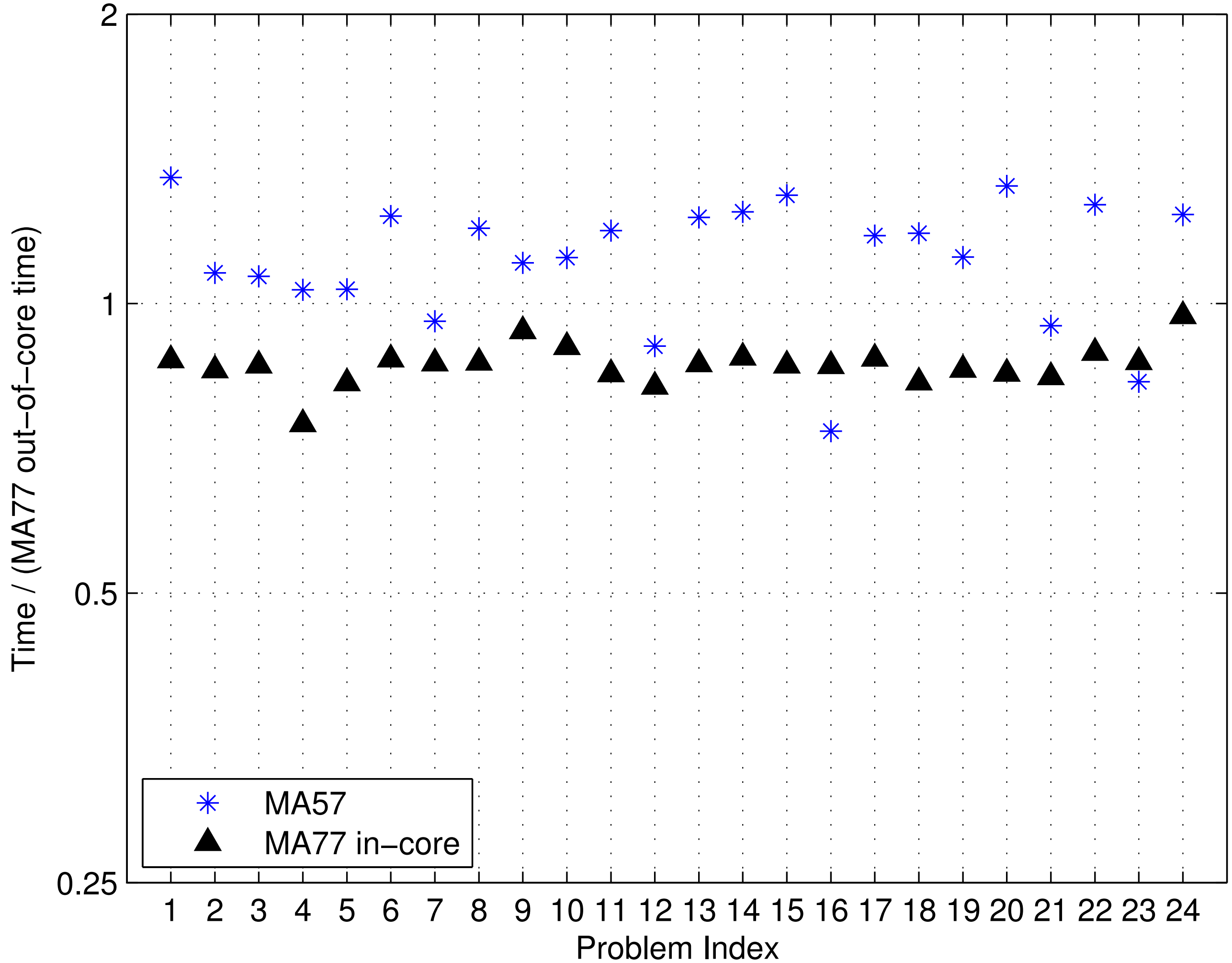
HSL_MA77 factor time compared with MA57



HSL_MA77 solve time compared with MA57



HSL_MA77 total time compared with MA57



Times (in seconds) for large problems

Phase	inline_1 ($n = 503,712$)	bones10 ($n = 914,898$)	nd24k ($n = 72,000$)	bone010 ($n = 986,703$)
Input	4.87	6.25	2.86	8.00
Ordering	14.2	22.8	16.4	34.7
MA77_analyse	4.20	6.70	22.1	26.7
MA77_factor	90.6	174.6	1284	1491
MA77_solve(1)	5.30	36.0	10.4	311
MA77_solve(8)	10.6	41.3	20.7	331
MA77_solve(64)	60.5	141.0	90.2	499

MA57 not able to solve these on our test computer (insufficient memory).

Unsymmetric element problems

- Recently developed out-of-core multifrontal code for unsymmetric element problems. Code is called HSL_MA78
- Based on the design of HSL_MA77
- Again uses HSL_OF01 to handle out-of-core
- Separate package HSL_MA74 written to compute the partial factorization of the dense unsymmetric frontal matrices
  - Implements a block factorization ... employs level 3 BLAS
  - Incorporates threshold pivoting (options for partial, diagonal or rook pivoting)
  - Also option for static pivoting (prevents delayed pivots but may produce inaccurate factorization)
- HSL_MA78 solves $AX = B$ or $A^T X = B$

Comparison with frontal solver

HSL_MA42_ELEMENT is an unsymmetric out-of-core (uni-)frontal code

	n	Time (secs)		Factors ($*10^6$)	
		MA42_ELEMENT	MA78	MA42_ELEMENT	MA78
crplat2	18010	1.85	1.84	4.35	2.94
ship_001	34920	10.5	13.4	15.5	15.6
m_t1	97578	552	101	135.5	56.2
shipsec8	114919	950	101	196.0	55.6
troll	213453	3042	74	672.0	63.7

These results illustrate the benefits of the multifrontal algorithm.

Appeal: We need large test problems in element form from real applications.

Concluding remarks

- Writing these solvers has been (and still is) a major project
- Positive definite code and unsymmetric element code performing well
- Out-of-core working adds an overhead but appears not to be prohibitive (exception is solve phase)
- Indefinite code written, currently testing the indefinite kernel
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Out-of-core solvers and virtual memory management package will be in HSL 2007

For details of HSL see `www.cse.scitech.ac.uk/nag/hsl`