Lecture 25
Linear Algebra Software

MIT 18.335J / 6.337J

Introduction to Numerical Methods

Per-Olof Persson

December 12, 2006

BLAS

- *Basic Linear Algebra Subroutines* (BLAS)
  - Standardized interface for simple vector and matrix operations
  - Manufacturers provide optimized implementations for their machines
- History:
  - BLAS1 (1970s) – Vector operations: $\alpha = x^T y$, $y = \alpha x + y$
  - BLAS2 (mid 1980s) – Matrix-vector operations: $y = Ax + y$
  - BLAS3 (late 1980s) – Matrix-matrix operations: $C = AB + C$
- Efficient cache-aware implementations give almost peak performance for BLAS3 operations
- High level algorithms (Gaussian elimination, etc) use BLAS but no other machine dependent code
  - Performance and portability

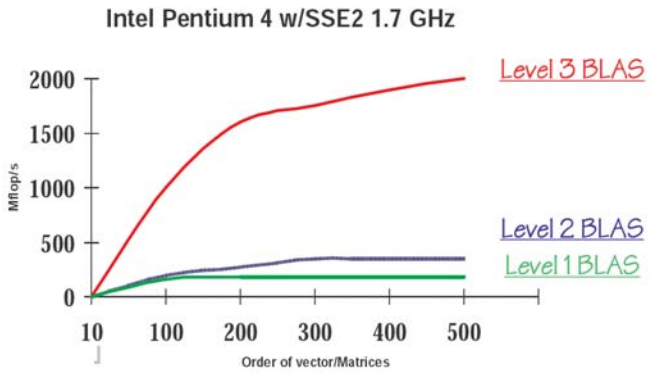
Memory Hierarchy and High Level BLAS

- Modern computers use a *memory hierarchy*
- From fast/expensive to cheap/slow: Registers, L1 cache, L2 cache, local memory, remote memory, secondary memory
- Fast algorithms perform many operations on each memory block to minimize memory access (*cache reuse*)
- Only BLAS3 has potential for very high performance

BLAS	Memory Refs	Flops	Flops / Memory Ref
Level 1 ($y = \alpha x + y$)	$3n$	$2n$	$2/3$
Level 2 ($y = Ax + y$)	n^2	$2n^2$	2
Level 3 ($C = AB + C$)	$4n^2$	$2n^3$	$n/2$

BLAS Performance

- For high performance write algorithms in terms of BLAS3 operations



BLAS Implementations

- Vendor provided:
  - Intel Math Kernel Library (MKL), AMD Core Math Library (ACML)
  - Sun Performance Library
  - SGI Scientific Computing Software Library
- Automatically Tuned Linear Algebra Software (ATLAS)
  - Analyzes hardware to produce BLAS libraries for any platform
  - Used in MATLAB, precompiled libraries freely available
  - Sometimes outperforms vendor libraries
- GOTO BLAS (mainly for Intel processors)
  - Manually optimized assemly code, currently the fastest implementation

Calling BLAS from C

- BLAS standard based on Fortran 77:
  - All memory must be preallocated
  - All variables are passed by reference
- Example: Double precision matrix-matrix multiply ($C = \alpha AB + \beta C$):

```
dgemm_(&transa,&transb,&m,&n,&k,&alpha,A,&lda,
       B,&ldb,&beta,C,&ldc);
```

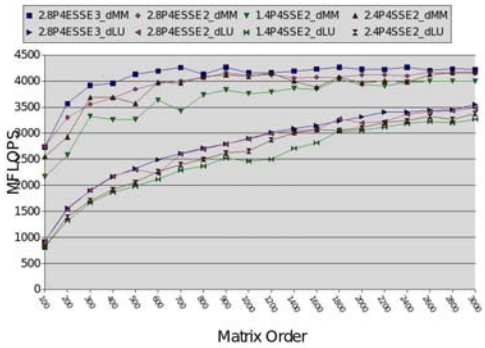
  - `transa`, etc: Matrix transpose (`'T'`) or not (`'N'`)
  - `lda`, etc: Leading dimensions of matrices
  - Some platforms/compilers do not require the trailing underscore
  - In C++, declare functions with `extern "C"`
- See also C BLAS interface in ATLAS

LAPACK

- Standard library for dense/banded linear algebra
  - Linear systems: $Ax = b$
  - Least squares problems: $\min_x \|Ax - b\|_2$
  - Eigenvalue problems: $Ax = \lambda x$, $Ax = \lambda Bx$
  - Singular value decomposition (SVD): $A = U\Sigma V^T$
- Algorithms use BLAS3 as much as possible
- Used by MATLAB (since version 6)
- *LAPACK Search Engine* useful for finding routines

LAPACK Performance

- Matrix-matrix multiply and LU factorization as function of matrix size
- About 80% of peak performance for LU factorization of large matrices



Sparse Solver Packages

- UMFpack (Unsymmetric MultiFrontal method)
  - Used in MATLAB (since version 7.1), no parallel version
- PARADISO
  - Serial and shared memory, used in Intel MKL
- SuperLU
  - Versions for serial and parallel computers (shared/distributed)
  - “Static pivoting” for distributed machines (increase small pivots, iterative refinement for accuracy)
- MUMPS (MUltifrontal Massively Parallel sparse direct Solver)
  - Versions for serial and parallel computers (distributed)