Scientific Computing (PHYS 2109/Ast 3100 H)
II. Numerical Tools for Physical Scientists

SciNet HPC Consortium
University of Toronto

Winter 2014

Lecture 13: Numerical Linear Algebra

Part I - Theory

- Solving $Ax = b$
- System Properties
- Direct Solvers
- Iterative Solvers
- Dense vs. Sparse matrices

Lecture 13: Numerical Linear Algebra

Part I - Theory

- Solving $Ax = b$
- System Properties
- Direct Solvers
- Iterative Solvers
- Dense vs. Sparse matrices

Part II - Application

- Using packages for Linear Algebra
- BLAS
- LAPACK
- etc...

SciNet compute • calcul CANADA

How to write numerical linear algebra

As much as possible, rely on existing, mature software libraries for performing numerical linear algebra computations. By doing so...

- Focus on your code details
- Reduce the amout of code to produce/debug
- Libraries are tuned and optimized, ie. your code will run faster
- More options to switch methods if necessary

Software

Packages

- Netlib (http://www.netlib.org)
  - Maintained by UT and ORNL
  - Most of the code is public domain or freely licensed
  - Mostly written in FORTRAN 77 !
  - BLAS & LAPACK

Software

Packages

- Netlib (http://www.netlib.org)
  - Maintained by UT and ORNL
  - Most of the code is public domain or freely licensed
  - Mostly written in FORTRAN 77 !
  - BLAS & LAPACK
- PETSc (http://www.mcs.anl.gov/petsc/)
  - Argonne National Labs
  - Open Source
  - C++
  - PDE & Iterative Linear Solvers

Software

Packages

- Netlib (http://www.netlib.org)
  - Maintained by UT and ORNL
  - Most of the code is public domain or freely licensed
  - Mostly written in FORTRAN 77 !
  - BLAS & LAPACK
- PETSc (http://www.mcs.anl.gov/petsc/)
  - Argonne National Labs
  - Open Source
  - C++
  - PDE & Iterative Linear Solvers
- Trilinos (http://trilinos.sandia.gov/)
  - Sandia National Labs
  - Collection of 50+ packages
  - Linear Solvers, Preconditioners, etc.

Software

Packages

- Netlib (http://www.netlib.org)
  - Maintained by UT and ORNL
  - Most of the code is public domain or freely licensed
  - Mostly written in FORTRAN 77 !
  - BLAS & LAPACK
- PETSc (http://www.mcs.anl.gov/petsc/)
  - Argonne National Labs
  - Open Source
  - C++
  - PDE & Iterative Linear Solvers
- Trilinos (http://trilinos.sandia.gov/)
  - Sandia National Labs
  - Collection of 50+ packages
  - Linear Solvers, Preconditioners, etc.
- Others
  - http://www.netlib.org/utk/people/JackDongarra/la-sw.html

BLAS

Basic Linear Algebra Subroutines

- A well defined standard interface for these routines
- Many highly-tuned implementations exist for various platforms. (Atlas, Flame, Goto, PLASMA, cuBLAS...)
- (Interface vs. Implementation! Trick is designing a sufficiently general interface.)
- Higher-order operations (matrix factorizations, like as we'll see, gaussian elimiation) defined in LAPACK, on top of BLAS.

SciNet compute • calcul CANADA

Typical BLAS routines

- Level 1: sdot (dot product, single), zaxpy (a**x** + **y**, dbl complex)
- Level 2: dgemv (dbl matrix*vec), dsymv (dbl symmetric matrix*vec)
- Level 3: sgemm (general matrix-matrix), ctrmm (triangular matrix-matrix)
- Incredibly cryptic names, interfaces.

Prefixes:

S: Single C: Complex
D: Double Z: Double Complex

Matrix Types:

GE: General
GB: General Banded
HY: Hermetian
TR: Triangular
TP: Triangular Packed
SY: Symmetric
SB: Symmetric Banded
HB: Hermetian Banded
TB: Triangular Banded

SciNet compute • calcul CANADA

Why bother?

- Finding, downloading library
- Figuring out how to link
- C/Fortran issues
- Just write it - it's not rocket science.

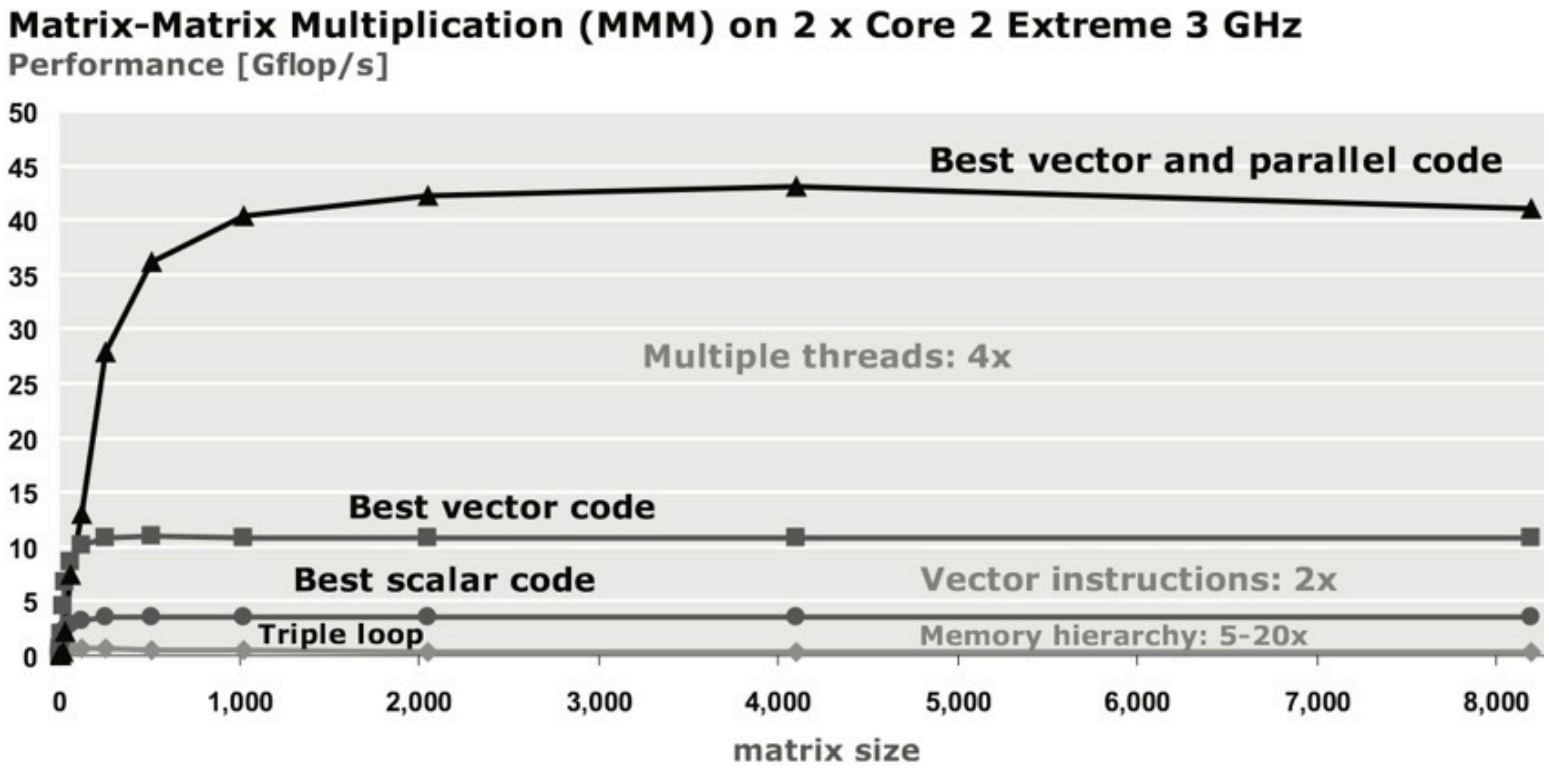
$$C = AB$$

$$c_{i,j} = \sum_k a_{i,k} b_{k,j}$$

```
for (i=0; i<N; i++)
    for (j=0; j<N; j++)
        for (k=0; k<N; k++)
            c[i][j] = a[i][k]*b[k][j];
```

SciNet compute • calcul CANADA

Never, ever, write your own



"How to Write Fast Numerical Code: A Small Introduction", Chellappa *et al*
www.ece.cmu.edu/~franzf/papers/gttse07.pdf

SciNet compute • calcul CANADA

Using BLAS

BLAS & LAPACK

- netlib provides “reference” implementation
- Most vendors provide optimized versions
- Commercial: Intel (MKL), AMD (ACML), IBM (ESSL)
- Open Source: ATLAS, GotoBLAS, OpenBLAS
- Fortran functions
- C interface using CBLAS and LAPACKE

Using BLAS

Install OpenBLAS (http://www.openblas.net/)

```
$git clone git://github.com/xianyi/OpenBLAS.git
$cd OpenBLAS
$make FC=gfortran
$make install PREFIX=$HOME/OpenBLAS/
```

Put

the following in .bashrc

```
export BLAS_INC=${HOME}/OpenBLAS/include/
export BLAS_LIB=${HOME}/OpenBLAS/lib/
export LD_LIBRARY_PATH=${LD_LIBRARY_PATH}:${HOME}/OpenBLAS/lib/
```

BLAS Example: DSCAL ($\mathbf{x} \leftarrow \alpha\mathbf{x}$)

```
#include <iostream>
#include <cblas.h>
int main(int argc, char **argv) {
  double x[] = { 1.0, 2.0, 3.0 };
  double coeff = 4.323;
  int one = 1;
  int n = 3;
  //Direct Fortran call
  dscal_(&n, &coeff, &x[0], &one);
  for (int i = 0; i < n; i++)
  std::cout<<" "<<x[i];
  return 0;
}
```

BLAS Example: DSCAL ($\mathbf{x} \leftarrow \alpha\mathbf{x}$)

```
#include <iostream>
#include <cblas.h>
int main(int argc, char **argv) {
  double x[] = { 1.0, 2.0, 3.0 };
  double coeff = 4.323;
  int one = 1;
  int n = 3;
  //Using CBLAS interface
  cblas_dscal(n,coeff,x,one);
  for (int i = 0; i < n; i++)
  std::cout<<" "<<x[i];
  return 0;
}
```

BLAS Example: DSCAL ($\mathbf{x} \leftarrow \alpha\mathbf{x}$)

```
$g++ dscal.cc -o dscal -I${BLAS_INC} -L${BLAS_LIB} -lopenblas
$./dscal
$4.323 8.646 12.96
```

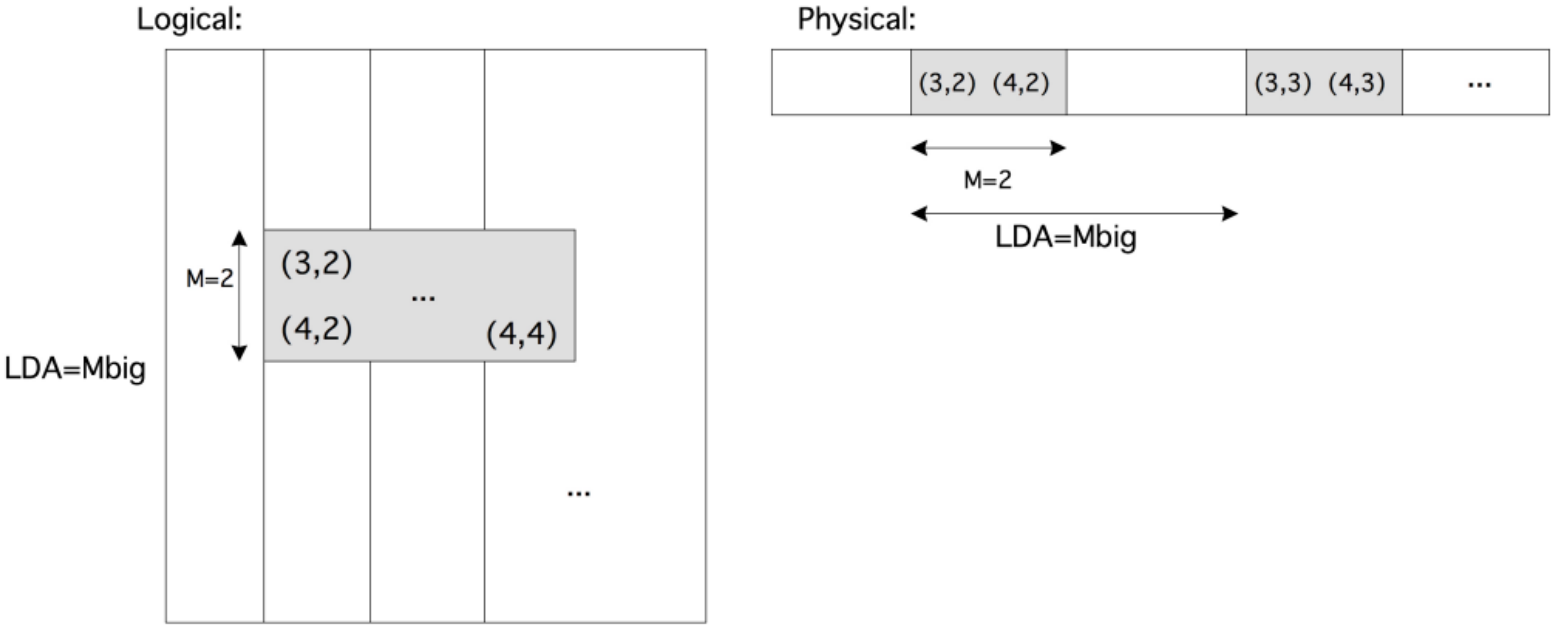
BLAS Example: DGEMM ($\mathbf{C} \leftarrow \alpha\mathbf{AB} + \beta\mathbf{C}$)

Documentation

- http://www.netlib.org/blas/blast-forum/
- **$ man dgemm**

```
NAME
       DGEMM - performs one of the matrix-matrix operations   C := alpha*op( A )*op( B ) + beta*C,

SYNOPSIS
       SUBROUTINE DGEMM(TRANSA,TRANSB,M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)

           DOUBLE                                                    PRECISION ALPHA,BETA
           INTEGER                                                   K,LDA,LDB,LDC,M,N
           CHARACTER                                                 TRANSA,TRANSB
           DOUBLE                                                    PRECISION
                                                                     A(LDA,*),B(LDB,*),C(LDC,*)

PURPOSE
       DGEMM  performs one of the matrix-matrix operations

       where  op( X ) is one of

          op( X ) = X   or   op( X ) = X',

       alpha and beta are scalars, and A, B and C are matrices, with op( A ) an m by k matrix,
       op( B ) a  k by n matrix and C an m by n matrix.
```

BLAS



Misc. Details

- LDA - Leading Dimension of "A" used to access subblocks of
- CBLAS additions **`CblasRowMajor`**, **`CblasColMajor`**

BLAS Example: DGEMM ($\mathbf{C} \leftarrow \alpha\mathbf{AB} + \beta\mathbf{C}$)

```
#include <iostream>
#include <cblas.h>
int main(int argc, char **argv) {
  int m = 5, k = 5, n = 5;
  double alpha = 1.0, beta = 0.0;
  double *A = new double[m*k];
  double *B = new double[k*n];
  double *C = new double[m*n];
  for (int i=0; i<(m*k); i++) A[i] = (double)(i+1);
  for (int i=0; i<(k*n); i++) B[i] = (double)(-i-1);
  for (int i=0; i<(m*n); i++) C[i] = 0.0;
  cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
  m, n, k, alpha, A, k, B, n, beta, C, n);
  ...
}
```

BLAS Example: DGEMM ($\mathbf{C} \leftarrow \alpha\mathbf{AB} + \beta\mathbf{C}$)

```
Matrix A : 5 by 5
1 2 3 4 5
6 7 8 9 10
11 12 13 14 15
16 17 18 19 20
21 22 23 24 25

Matrix B: 5 by 5
-1 -2 -3 -4 -5
-6 -7 -8 -9 -10
-11 -12 -13 -14 -15
-16 -17 -18 -19 -20
-21 -22 -23 -24 -25

Matrix C: 5 by 5
-215 -230 -245 -260 -275
-490 -530 -570 -610 -650
-765 -830 -895 -960 -1025
-1040 -1130 -1220 -1310 -1400
-1315 -1430 -1545 -1660 -1775
```

LAPACK

The Linear Algebra PACKage (LAPACK)

LAPACK contains a variety of subroutines for solving linear systems, matrix decompositions, and factorizations.

- Intermally uses BLAS calls
- Supports the same data types (single/double precision, real/complex and matrix structure types (symmetric, banded, etc.) as BLAS
- Three categories: auxiliary routines, computational routines, and driver routines
- C interface with prefix **LAPACKE_**
  - http://www.netlib.org/lapack/lapacke.html

The Linear Algebra PACKage (LAPACK)

Computational routines are designed to perform single, specific computational tasks:

- factorizations: LU , LL^T /LL^H , LDL^T /LDL^H , QR, LQ, QRZ generalized QR and RQ
- symmetric/Hermitian and nonsymmetric eigenvalue decompositions
- singular value decompositions
- generalized eigenvalue and singular value decompositions

LAPACK Example: DGESV (Solve $\mathbf{Ax} = \mathbf{b}$)

```
NAME
       DGESV - computes the solution to a real system of linear equations  A * X = B,

SYNOPSIS
       SUBROUTINE DGESV( N, NRHS, A, LDA, IPIV, B, LDB, INFO )

           INTEGER        INFO, LDA, LDB, N, NRHS

           INTEGER        IPIV( * )

           DOUBLE         PRECISION A( LDA, * ), B( LDB, * )

PURPOSE
       DGESV computes the solution to a real system of linear equations
          A  *  X = B, where A is an N-by-N matrix and X and B are N-by-NRHS matrices.
       The LU decomposition with partial pivoting and row interchanges is used to factor A as
          A = P * L * U,
       where P is a permutation matrix, L is unit lower triangular, and U is upper triangular.
       The factored form of A is then used to solve the system of equations A * X = B.
```

LAPACK Example: DGESV (Solve $\mathbf{Ax} = \mathbf{b}$)

```
#include <iostream>
#include <lapacke.h>
const int N=3, NRHS=2, LDA=N, LDB=N;
int main(int argc, char **argv) {
  int ipiv[N], info;
  double a[LDA*N] = {
    6.80, -2.11, 5.66,
    -6.05, -3.30, 5.36,
    -0.45, 2.58, -2.70
  };
  double b[LDB*NRHS] = {
    4.02, 6.19, -8.22,
    -1.56, 4.00, -8.67
  };
  info = LAPACKE_dgesv( LAPACK_COL_MAJOR, N, NRHS,
  a, LDA, ipiv, b, LDB );
  ...
}
```

LAPACK Example: DGESV (Solve $\mathbf{Ax} = \mathbf{b}$)

```
$g++ dgesv.cc -o dgesv -I${BLAS_INC} -L${BLAS_LIB} -lopenblas
$./dgesv
```

```
Solution ‘‘x’’
-0.0517981 -0.892398
 -0.819976 -0.736171
 1.30806   -0.121056

Details of LU factorization
6.8         -6.05      -0.45
0.832353    10.3957    -2.32544
-0.310294   -0.49802   1.28225

Pivot indices
1 3 3
```

What about non-dense martices?

$$\begin{pmatrix} -2 & 1 & & & & & \\ 1 & -2 & 4 & & & & \\ & 4 & -2 & 4 & & & \\ & & 4 & -2 & 4 & & \\ & & & 4 & -2 & 4 & \\ & & & & & \ddots & \\ & & & & 4 & -2 & 1 \\ & & & & & 1 & -2 \end{pmatrix}$$

Types

- Banded: **DGBSV**
- Tri-Diagonal: **DGTSV**
- Symmetric Positivve Def. **DPOSV**

SciNet compute • calcul CANADA

LAPACK Example: DGTSV (Solve $\mathbf{Ax} = \mathbf{b}$)

```
#include <iostream>
#include <lapacke.h>
const int N=5, NRHS=2;
int main(int argc, char **argv) {
  int ldb=N, info;
  double dl[N-1] = { 1, 4, 4, 1 };
  double d[N] = { -2, -2, -2, -2, -2 };
  double du[N-1] = {1, 4, 4, 1 };
  double b[N*NRHS] = {
    3, 5, 5, 5, 3,
    -1.56, 4.00, -8.67, 1.75, 2.86,
    9.81, -4.09, -4.57, -8.61, 8.99
  };
  info = LAPACKE_dgtsv(LAPACK_COL_MAJOR, N, NRHS,
  dl, d, du, b, ldb );
  ...
}
```

LAPACK Example: DGTSV (Solve $\mathbf{Ax} = \mathbf{b}$)

```
$g++ dgesv.cc -o dgtsv -I${BLAS_INC} -L${BLAS_LIB} -lopenblas
$./dgtsv
```

```
Solutions ‘‘x’’
 -0.93   0.29  -6.10
  1.14  -0.99  -2.39
  2.05   0.43  -0.69
  1.14  -0.96   0.90
 -0.93  -1.91  -4.05
```

Sparse Matrices

Sparse BLAS ?

Unfortunately there is not a mature, de facto standard sparse matrix BLAS library. Three potential options:

- Official Sparse BLAS: a reference implementation is not yet available http://www.netlib.org/blas/blast-forum
- NIST Sparse BLAS: An alternative BLAS system; a reference implementation is available http://math.nist.gov/spblas
- The Matrix Template Library : The C++ library mentioned above also provides support for sparse matrices http://www.osl.iu.edu/research/mtl/intro.php3

Conclusions

Conclusions

- Linear algebra pops up everywhere
- Statistics, data fitting, graph problems, PDE/coupled ODE solves, signal processing...
- Exploit structure in your matrices
- Chose best method based on system properties (condition number, sparsity, etc..)
- Many very highly tuned packages for any sort of problem that can be cast into matrices
- LAPACK, BLAS, etc..

Assignment

Assignment #7

The implicit Euler time discretization applied to the 1d heat/diffusion equation with 2nd order finite difference spatial discretization has the form:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - D\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} = 0$$

Assignment #7

When rearranged to solve for $\mathbf{u}^{n+1}$ and ignoring BC's it has the form:

$$\mathbf{u}^{n+1} - \frac{D\Delta t}{(\Delta x)^2} \begin{pmatrix} -2 & 1 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & 1 & -2 & 1 & & \\ & & & 1 & -2 & 1 & \\ & & & & \ddots & & \\ & & & & 1 & -2 & 1 \\ & & & & & 1 & -2 \end{pmatrix} \mathbf{u}^{n+1} = \mathbf{u}^n$$

Assignment #7

- Ignoring the constants, use the D__EV Lapack routines and 100 points to determine the eigenvalues for this problem. What might we expect to get amplified/damped? How does this affect our choice of time-step.
- For a 1d grid of size 100 (eg, a 100x100 matrix A), use the most appropriate D__SV Lapack routine(s) to evolve this PDE.
- Start with initial conditions with $u = 1$ at the first point, and zero everywhere else (hot plate turns on in a cold domain).
- Use D=1, Δx=1/N, and Dirchlet BC's $u(0) = 1$ and $u(N-1) = 0$.
- Using a small enough timestep, timestep the temperature evolution, plot the final solution, and explain the results.
- Submit code, makefile, git-log, plot and text file with comments.