HPC Linear Algebra

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Logistics

Assignments

- A1 grading in progress, look for results in the next day
- A2 will go up by Thu and feature MPI Coding

MSI Accounts

- MSI has set up class accounts for students in 5451
- Should allow you to `ssh X500@mesabi.msi.umn.edu`
- UMN User/Password/Duo Authenication to get on mesabi
- Off campus requires UMN VPN enabled

Today

- Complete Discussion of MPI Collective Communication
- Overview of some Linear Algebra Libraries

Hand-Coded Matrix Algebra

- Very common for students to learn how to code up some basic linear algebra routines
- In reality, prototype and production code benefits from use of mature libraries for these
- Existing libraries for Linear Algebra already exist, are reliable and fast, both important in HPC / Parallel Computing

```
void matmult(
   int arows, int bcols, int midim,
   double A[][], // arows * midim
   double B[][], // midim * bcols
   double C[][]) // arows * bcols
{
  for (int i=0 ; i < arows ; ++i ){
    for (int j=0 ; j < bcols ; ++j ){
      C[i][j] = 0.0;
      for (int k=0 ; k < midim ; ++k ){
        C[i][j] += A[i][k] * B[k][j];
      }
    }
  }
}
// try dgemm() instead
```

BLAS: Basic Linear Algebra Subroutines

- Started in the 1970's and now WIDELY deployed
- Defines a set of numerical operations in 3 Levels
  1. Vector/Scalar operations (add constant onto all vector elements) and Vector/Vector operations (dot product)
  2. Matrix/Vector operations (mat-vec multiply)
  3. Matrix/Matrix operations (mat-mat multiply)
- Interestingly these are all mostly $O(N), O(N^2), O(N^3)$ operations respectively
- The names for the function suck and take significant study to understand and use effectively

  `axpy()`? `ddot()`? `sgemm()`? Are these rappers, hacker handles, or did someone just punch the keyboard repeatedly to name all the functions?
  According to legend, all the function names are 5 letters or less as this was the limit imposed by the Fortran compiler which originally compiled them.

BLAS Introductory Example

`dgemm()` : Multiply 2 double precision, general format matrices

```
dgemm(opa, opb,                 // transpose A,B or not
      arows, bcols, midim,      // matrix dimensions
      alpha,                    // scaling factor for product
      A, lda, B, ldb,           // A and B matrix + cols
      beta, C, ldc)             // answer scaling + storage + dim

C := alpha * opa( A )* opb( B ) + beta*C
```

Super transparent, excellent software engineering...

- Targets Fortran77: different calling conventions than C
- Complex due to flexibility: 4 variants based on `opa,opb`

$$C \leftarrow \alpha AB + \beta C \qquad C \leftarrow \alpha A^T B + \beta C$$
$$C \leftarrow \alpha AB^T + \beta C \qquad C \leftarrow \alpha A^T B^T + \beta C$$

- Allows for scaling with `alpha,beta` but both often are 1
- Naming Convention: `d ge mm ()`
  - `d`: double precision real
  - `ge`: general matrix, not symmetric or banded
  - `mm`: matrix multiply

C BLAS Example

- cblas are C language bindings to BLAS routines
- Slightly easier to understand, uses symbolic names for some (extra) arguments
- Accounts for C being Row-Major vs Fortran being Column-Major

```
// dgemm_example.c
// A : arows * midim matrix
// B : midim * bcols matrix
// B : arows * bcols matrix
// C <- A*B
cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
            arows, bcols, midim,
            alpha,
            A, midim, B, bcols,
            beta, C, bcols);
```

LAPACK: Linear Algebra Package

- Basic Operations like Matrix Multiply are covered in BLAS
- Many Linear Algebra problems come up in HPC
  - Solve a Linear System: $Ax = b$, find x give A, b
  - Determine eigenvectors / eigenvalues for matrix A
  - Calculate Singular Value Decomposition on A
- LAPACK builds on BLAS to provide algorithms for all of these
- Has many of the same properties as BLAS
  - Netlib version Written in Fortran77
  - Has bindings for C in LAPACKE
  - Naming conventions are difficult: `dgesv()`

    `d`: double precision real

    `ge`: general format matrix

    `sv`: "solve" linear system via a LUP decomposition
- LAPACK / BLAS often packaged together in single libraries

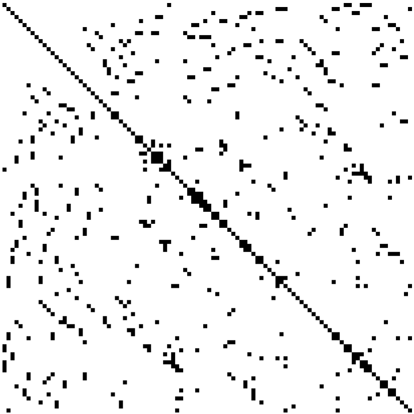
Implementations of BLAS+LAPACK

Package	Notes
Netlib	The official LAPACK. (BSD/Open Source)
ATLAS	Automatically Tuned Linear Algebra Software (BSD/Open Source)
GSL	GNU Scientific Library (GNU / Open Source)
Intel MKL	Intel's Math routines for their x86 CPUs. (Freeware/Closed Source)
ARM PL	ARM Processor Performance Libraries (Freeware/Closed Source)
NVBLAS	NVIDIA BLAS, optimized for CUDA / GPU execution
cuSOLVER	NVIDIA LAPACK, optimized for CUDA / GPU execution
...	

- Note vendor implementations for specific processors / architectures: target efficient operation on these chips
- ATLAS is notable as on install, runs a series of benchmarks to set parameters in BLAS that give the best performance (Automatically Tuned)

Sparse Matrices

- Various scientific problems in HPC involve matrices with **many** Zero elements
- Referred to as **sparse matrices** especially when stored in data structures that reduce their size
- Contrast with **dense matrices** which we have assumed so far
- Example: `LINKS` matrix in Page Rank could benefit a lot from sparse storage
- BLAS / LAPACK deal with dense matrices, Sparse Matrices are their own beast



Example of a sparsity pattern in a large matrix: **black** indicates non-zero element, white is zero

Data Structures to Store Sparse Matrices

- Dense Matrices
  - Use $NROW \times NCOL$ space
  - Provide $O(1)$ lookup for element `(i,j)`
  - Easily provides $O(N)$ iteration through matrix elements
- Sparse Matrix formats
  - Use $O(NNZ)$ storage: NNZ is the **Number of NonZeros**
  - Provide worse than $O(1)$ lookup for element `(i,j)`
  - Store only elements that are nonzero, assume if an index is not present that it is zero
  - Try to provide $O(NNZ)$ iteration through matrix elements
- Storage savings for sparse formats can be significant when matrix is mostly zeros ($NNZ \ll NROW \times NCOL$)

Octave Example of Sparse Matrix Storage

- Octave is an open-source scientific computing environment, mostly compatible with Matlab
- Has built-in support for sparse matrices
- Uses the Compressed Sparse Column format (CSC) internally
- Makes it easy to show space savings

```
octave:2> A=[
 [10   20    0    0    0    0]
 [ 0   30    0   40    0    0]
 [ 0    0   50   60   70    0]
 [ 0    0    0    0    0   80]];

octave:3> As = sparse(A);

octave:4> B = [ A zeros(4,94);
                zeros(96, 100)];

octave:5> Bs=sparse(B);

octave:6> whos
Variables visible from the current scope:

variables in scope: top scope

   Attr Name        Size        Bytes  Class
   ==== ====        ====        =====  =====
        A           4x6           192  double
        As          4x6           184  double
        B         100x100       80000  double
        Bs        100x100         936  double
        ans         1x1             8  double

Total is 20049 elements using 81320 bytes
```

Coordinate Format (COO)

- Store `(row,col,val)` for all non-zero elements
- Values/Indices stored in separate arrays
- Justify operational complexities:
  1. Space requirement is `3*NNZ`
  2. Finding element `(i,j)` is $O(\log(NNZ))$
  3. Transpose is $O(NNZ)$

```
     0    1    2    3    4    5
0  [10   20    0    0    0    0]   SAMPLE DENSE MATRIX
1  [ 0   30    0   40    0    0]
2  [ 0    0   50   60   70    0]
3  [ 0    0    0    0    0   80]

NNZ = 8, NROW=4, NCOL=6
               0  1  2  3  4  5  6  7
VALUES    = [ 10 20 30 40 50 60 70 80 ]  COO DATA ARRAYS
ROW_INDEX = [  0  0  1  1  2  2  2  3 ]
COL_INDEX = [  0  1  1  3  2  3  4  5 ]
```

Compressed Sparse Row Format (CSR)

- Save space by "compressing" rows : store only row start positions
- Length of Row `I` is `ROW_START[I+1]-ROW_START[I]`
- Justify operational complexities:
  1. Space requirement is `2*NNZ + NROW+1`
  2. Finding element `(i,j)` is close to $O(1)$
  3. Transpose is $O(NNZ)$

```
      0     1     2     3     4     5
0   [10    20     0     0     0     0]     SAMPLE DENSE MATRIX
1   [ 0    30     0    40     0     0]
2   [ 0     0    50    60    70     0]
3   [ 0     0     0     0     0    80]

NNZ = 8, NROW=4, NCOL=6
                 0   1   2   3   4   5   6   7
VALUES    = [ 10  20  30  40  50  60  70  80 ]  CSR DATA ARRAYS
COL_INDEX = [  0   1   1   3   2   3   4   5 ]
ROW_START = [  0   2   4   7   8 ]
                               ^ Extra element = NNZ
```

Algorithms for Sparse Matrices

- BLAS / LAPACK do NOT work for sparse matrices
- Must utilize different algorithms
- Less standardization around sparse matrices but libraries / vectors exist
- Sparse BLAS spec exists but fewer implementations
- Factorization like in LAPACK require significant algorithm changes to work for sparse matrices
- Prof. Yousef Saad is our local expert in this area and is worth chatting up if you want to learn more

Related Materials

Stephen Boyd's EE364 Linear Algebra Oveview

https://stanford.edu/class/ee364b/lectures/num-lin-alg-software.pdf

- Discusses many of the same items we talked about here
- Focus is on optimization problems like linear programming
- Very similar considerations

CSCI 5304 - Computational Aspects of Matrix Theory

- Great course on doing linear algebra for scientific problems
- Some coverage of BLAS/LAPACK and sparse matrices
- Often taught by Prof Saad who is a resident expert on all things Matrix/Sparse