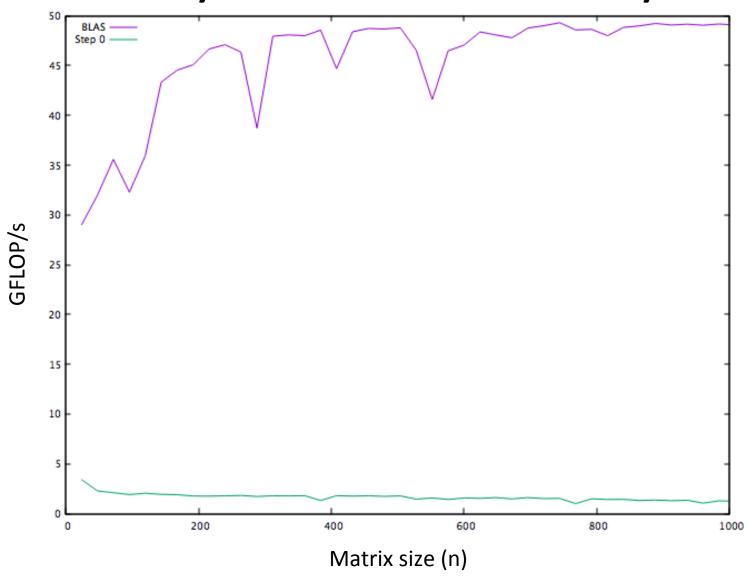
Devin A. Matthews
UT Austin

MolSSI Software Summer School 2017

- Dense Linear Algebra (DLA) is the field of operations on vectors and matrices.
- The "dense" part refers to the fact that all of the vector and matrix elements may be non-zero.
   There are also extensions of BLAS and LAPACK for sparse matrices.
- The BLAS includes basic operations like matrix multiplication, while LAPACK builds on the BLAS to calculate eigenvalues and –vectors, solutions of linear systems, matrix factorizations, etc.

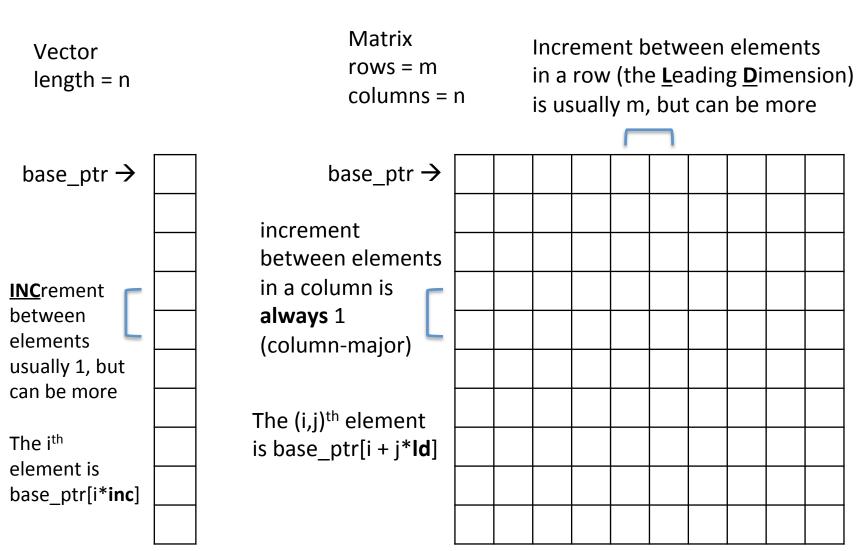
## Why do I need a library?



- The traditional BLAS and LAPACK implementations are in Fortran.
- Modern implementations are in C or C++, but still export a Fortran interface.
- This means that:
  - All parameters are pointers.
  - The name is mangled (usually a \_ gets added).
  - Fortran INTEGER != C/C++ int.

- (Almost) all BLAS and LAPACK routines support four data types:
  - Single precision (float, real\*4)
  - Double precision (double, real\*8)
  - Single complex (std::complex<float>, complex\*8)
  - Double complex (std::complex<double>, complex\*16)
- The data type for an operation is denoted by a prefix: s (single), d (double), c (single complex), or z (double complex).
  - Ex: zdotc = double complex dot product with conjugation

### The anatomy of vectors and matrices



#### **BLAS**

- BLAS includes three levels:
  - Level 1: vector-vector operations such as:
    - Dot product
    - Vector scaling
    - Scale and accumulate (AXPY)
  - Level 2: matrix-vector operations such as:
    - Matrix-vector product
    - Outer product (rank-1 update)
  - Level 3: matrix-matrix operations such as:
    - Matrix-matrix product
    - Triangular solve
    - Symmetric rank-k update

## BLAS level 1 examples

$$y_i = y_i + \alpha * x_i$$

result = 
$$\Sigma_i x_i^* \overline{y}_i$$

## BLAS level 2 examples

$$A_{ij} = \alpha^* x_i^* y_j + A_{ij}$$

$$y_i = \Sigma_j \alpha^* op(A_{ij})^* x_j + \beta^* y_i$$

## BLAS level 3 example

$$C_{ij} = \Sigma_p \alpha^* op_A(A_{ip})^* op_B(B_{pj}) + \beta^* C_{ij}$$

## LAWrap

- This is a header library I wrote to make using BLAS/LAPACK in C and C++ a little easier.
  - Give arguments by values instead of by reference (pointer).
  - Const-correct interface.
  - Function overloading (e.g. "gemm").
  - Automatically allocate workspace in LAPACK.
- CBLAS and LAPACKe are also good low-level interfaces.

# LAPACK

#### **Symmetric (Hermitian) Eigenvalue Problems**

$$\langle \phi_i | \hat{H} | \phi_j \rangle \langle \phi_j | \Psi \rangle = E \langle \phi_i | \Psi \rangle$$

#### Generalized Eigenvalue Problems

$$\mathbf{\tilde{F}}\mathbf{\tilde{C}} = \mathbf{\tilde{C}}\mathbf{E}$$

$$FC = SCE$$

#### **Non-symmetric Eigenvalue Problems**

$$\left(\hat{H}e^{\hat{T}}\right)_c \hat{R}_i |0\rangle = E_i R_i |0\rangle$$

#### **Matrix Factorizations and Linear Equations**

$$\langle K|\tilde{B}|\mu\nu\rangle = \langle K|V|L\rangle^{-\frac{1}{2}}\langle L|B|\mu\nu\rangle$$

(This is Cholesky + triangular solve, not inverse square root!)

## LAPACK example

(FOR EXAMPLE ONLY, also may have bugs/missed steps)

```
int norb = 1000;
int nocc = 100;
std::vector<double> C(norb*norb), S(norb*norb), F(norb*norb), D(norb*norb);
std::vector<double> e(norb);
C = F:
int info = LAWrap::hegv(LAWrap::AXBX, 'V', 'U',
                      norb, C.data(), norb, S.data(), norb, e.data());
std::cout << "Current SCF Eigenvalues:\n";
std::cout << std::setprecision(12) << std::fixed;</pre>
for (int i = 0;i < nocc;i++)</pre>
   std::cout << i << " " << e[i] << '\n';
for (int i = nocc;i < norb;i++)</pre>
   std::cout << i << " " << e[i] << '\n';
LAWrap::gemm('N', 'T', norb, norb, nocc,
            1.0, C.data(), norb, C.data(), norb, 0.0, D.data(), norb);
```

#### **BLAS** and LAPACK libraries

- Netlib (<u>http://www.netlib.org/blas</u>) (OSS)
  - Reference implementation; really slow.
- Intel Math Kernel Library (MKL) (free)
  - Optimized BLAS, LAPACK, FFT, etc.
- AMD Compute Library (ACL) (OSS)
  - AMD vendor BLAS/LAPACK
- IBM Engineering and Scientific Subroutine Library (ESSL)
  - IBM vendor BLAS/LAPACK (e.g. BlueGene/Q, POWER)
- OpenBLAS (OSS)
  - Optimized BLAS and Netlib LAPACK
- BLIS (OSS)
  - Optimized BLAS
- libflame (OSS)
  - Some LAPACK operations optimized
- Apple Accelerate
  - Default BLAS and LAPACK on OSX/macOS

### Wrapper libraries

- Wrapper libraries offer convenient interfaces in higher-level languages. Here is a non-exhaustive list for C++:
  - Eigen
  - Boost::uBLAS
  - Armadillo
  - CPPLapack
    - The "CPPBlas" project is unrelated.
- Distributed-memory BLAS and LAPACK:
  - Elemental
  - ELPA
  - PBLAS, ScaLAPACK

## Questions