





## Using high performance libraries

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#### 7 Motifs in HPC...

Phil Colella (LBL) identified 7 kernels of which most simulation and data analysis program are composed:

- Dense Linear Algebra
  - Ex: solve Ax=B or Ax=lambdax where A is a dense matrix
- Sparse Linear Algebra
  - Ex: solve Ax=B or Ax=lambdax where A is a sparse matrix (mostly zero)
- Operation on structured Grids:
  - Ex: ANEWj()=4\*(A(i,j)-A(i-1,j)-A(i+1,j)-A(i,j-1)-A(i,j+1)
- Operation on unstructured Grids:
  - Ex; similar but list of neighbours varies from entry to entry
- Spectral Methods
  - Ex: Fast Fourier Transform (FFT)
- Particle Methods
  - Ex: Compute electrostatic forces on n-particles
- Monte Carlo
  - Ex: many independent simulation using different inputs

Where should you start optimizing your application?

#### **Optimization Techniques**

- There are basically three different categories:
  - Improve memory performance (the most important)
  - Improve CPU performance



• The easiest and more efficient way..

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#### What are Performance libraries?

- Routines for common (math) functions such as vector and matrix operations, fast Fourier transform etc. written in a specific way to take advantage of capabilities of the CPU.
- Each CPU type normally has its own version of the library specifically written or compiled to maximally exploit that architecture

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#### Why use performance libraries?

- Compilers can optimize code only to a certain point. Effective programming needs deep knowledge of the platform
- Performance libraries are designed to use the CPU in the most efficient way, which is not necessarily the most straightforward way.
- It is normally best to use the libraries supplied by or recommended by the CPU vendor
- On modern hardware they are hugely important, as they most efficiently exploit caches, special instructions and parallelism

#### Any other reason apart from optimization?

- Usage of libraries
  - Make coding easier. Complicated math operations can be used from existing routines
  - Increase portability of code as standard (and well optimized)
     libraries exist for ALL computing platforms.
- Lego approach: build your own code using already available bricks..

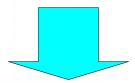
#### What is available?

- Linear Algebra: BLAS/LAPACK/SCALAPACK
- FFT:
  - FFTW
- ODE/PDE
  - PETSC
- Machine Learning:
  - Tensorflow / Caffe etc...

## Should I write my own algorithm for L. A.?

#### 99.99% of time NO

- Tons of libraries out there
- Well tested
- Extremely efficient in 99.99% of the case
- With some "de facto" standard implemented



PORTABILITY IS COMING (almost) FOR FREE

#### Why Linear algebra?

- 3 Basic Linear Algebra Problems in
  - Linear Equations: Solve Ax=b for x
  - 2. Least Squares: Find x that minimizes  $||r||_2 = \sqrt{\Sigma} r_i^2$  where r=Ax-b
    - Statistics: Fitting data with simple functions
  - 3a. Eigenvalues: Find  $\lambda$  and x where  $Ax = \lambda x$ 
    - Vibration analysis, e.g., earthquakes, circuits
  - 3b. Singular Value Decomposition:  $A^TAx = \sigma^2x$ 
    - Data fitting, Information retrieval

Lots of variations depending on structure of A

A symmetric, positive definite, banded, ...

## Why dense Linear Algebra?

- Many large matrices are sparse, but ...
  - Dense algorithms easier to understand
  - Some applications yields large dense matrices
  - LINPACK Benchmark (www.top500.org)
    - "How fast is your computer?" =
      "How fast can you solve dense Ax=b?"
  - Large sparse matrix algorithms often yield smaller (but still large) dense problems

**BLAS: Basic Linear Algebra Subprograms** 

## BLAS history (1/3)

- In the beginning it was libraries like EISPACK (for eigenvalue problems)
- Then the BLAS-1 were invented (1973-1977)
  - Create a standard library of 15 operations (mostly) on vectors
  - "AXPY" (  $y = \alpha \cdot x + y$  ), dot product, scale ( $x = \alpha \cdot x$  ), etc
  - Up to 4 versions of each (S/D/C/Z), 46 routines, 3300 LOC
  - Language: FORTRAN
- Goals
  - Common "pattern" to ease programming, readability
  - Robustness, via careful coding (avoiding over/underflow) --> Accuracy
  - Portability (common interface)
  - Efficiency via machine specific implementations
  - Maintaibility
- Why BLAS-1? They do O(n) ops on O(n) data
  - Used in libraries like LINPACK (for linear systems)
  - Source of the name "LINPACK Benchmark" (not the code!)

## BLAS history (2/3)

- But the BLAS-1 weren't enough
  - Consider AXPY ( $y = \alpha \cdot x + y$ ): 2n flops on 3n read/writes
  - Computational intensity = (2n)/(3n) = 2/3
  - Too low to run near peak speed (read/write dominates)
- So the BLAS-2 were developed (1984-1986)
  - Standard library of 25 operations (mostly) on matrix/vector pairs
  - "GEMV":  $y = \alpha \cdot A \cdot x + \beta \cdot x$ , "GER":  $A = A + \alpha \cdot x \cdot yT$ ,  $x = T-1 \cdot x$
  - Up to 4 versions of each (S/D/C/Z), 66 routines, 18K LOC
- Why BLAS-2?
  - They do O(n2) ops on O(n2) data
  - So computational intensity still just  $\sim (2n^2)/(n^2) = 2$
  - OK for vector machines, but not for machine with caches

## BLAS history (3/3)

- The next step: BLAS-3 (1987-1988)
  - Standard library of 9 operations (mostly) on matrix/matrix pairs
    - "GEMM":  $C = \alpha \cdot A \cdot B + \beta \cdot C$ ,  $C = \alpha \cdot A \cdot A^T + \beta \cdot C$ ,  $C = T^{-1} \cdot B$
    - Up to 4 versions of each (S/D/C/Z), 30 routines, 10K LOC
  - Why BLAS 3? They do O(n3) ops on O(n2) data
  - So computational intensity (2n³)/(4n²) = n/2 big at last!
    - Good for machines with caches, other mem. hierarchy levels
  - Performing implementations left to others..



#### Where are BLAS?

#### http://www.netlib.org/blas

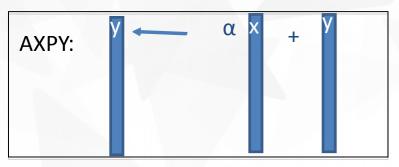
- Source: 142 routines, 31K LOC,
- Testing: 28K LOC
- Reference (unoptimized) implementation only!
  - http://www.netlib.org/blas/#\_reference\_blas\_version\_3\_5\_0
  - Ex: 3 nested loops for GEMM

## **BLAS** list

Seminary	Level 1 BLAS			
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XHEMR ( SIDE, UPLO,   N. N. ALPHA, A. LDA, B. LDB, BETA, C. LDC ) $C \leftarrow \alpha AB + \beta C, C \leftarrow \alpha BA + \beta C, C - m \times n, A = A^H$				
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XSTRICK ( UPLD, TRANS, N. K. ALPHA, A. LDA, B. LDB, BETA, C. LDC ) $C \leftarrow \alpha AB^T + \alpha BA^T + \beta C, C \leftarrow \alpha A^TB + \alpha B^TA + \beta C, C - n \times n$ S. D. C. Z XHENZK ( UPLD, TRANS, N. K. ALPHA, A. LDA, B. LDB, BETA, C. LDC ) $C \leftarrow \alpha AB^H + \beta BA^H + \beta C, C \leftarrow \alpha A^HB + \alpha B^HA + \beta C, C - n \times n$ C. Z XTRUM ( SIDE, UPLD, TRANSA, DIAG, N. N. ALPHA, A. LDA, B. LDB ) $B \leftarrow \alpha Bop(A)B, B \leftarrow \alpha Bop(A), op(A) = A, A^T, A^H, B - m \times n$ S. D. C. Z				
XHERZX( UPLO, TRANS, N. K. ALPHA, A. LDA, B. LDB, BETA, C. LDC ) $C \leftarrow \alpha AB^H + \beta BA^H + \beta C, C \leftarrow \alpha A^H B + \delta B^H A + \beta C, C - n \times n$ C, Z XTRMM ( SIDE, UPLO, TRANSA, DIAG, N. N. ALPHA, A. LDA, B. LDB ) $B \leftarrow \alpha \alpha \beta (A)B, B \leftarrow \alpha B \alpha \beta (A), \alpha \beta (A) = A, A^T, A^H, B - m \times n$ S, D, C, Z TRANSA ( SIDE, UPLO, TRANSA, DIAG, N. N. ALPHA, A. LDA, B. LDB ) $B \leftarrow \alpha \beta (A)B, B \leftarrow \alpha B \alpha \beta (A) = A, A^T, A^H, B - m \times n$ S, D, C, Z				
XTRMM ( SIDE, UPLO, TRANSA, DIAG, M, N, ALPHA, A, LDA, B, LDB ) $B \leftarrow osp(A)B, B \leftarrow osp(A), op(A) = A, A^T, A^H, B - m \times n$ S, D, C, Z	xSYR2X( UPLO, TRANS, N, K, ALPHA, A, LDA	, B, LDB, BETA, C, LDC )		S, D, C, Z
AMONG A CORP HOLD STATE AND A STATE OF THE S	xHER2K( UPLO, TRANS, N, K, ALPHA, A, LDA	, B, LDB, BETA, C, LDC )		1 (a) M. 100
where I every more entreet that we will the every time of the property of the				
and the transfer that the transfer to the tran	xTRSM ( SIDE, UPLO, TRANSA, DIAG, M. N. ALPHA, A. LDA	, 8, LDB )	$B \leftarrow oop(A^{-1})B$ , $B \leftarrow \alpha Bop(A^{-1})$ , $op(A) = A$ , $A^T$ , $A^H$ , $B - m \times n$	S. D. C. Z

#### Level 1, 2 and 3 BLAS

#### Level 1 BLAS Vector-Vector operations

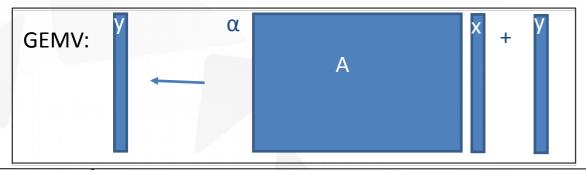




2n FLOP
2n memory reference

RATIO: 1

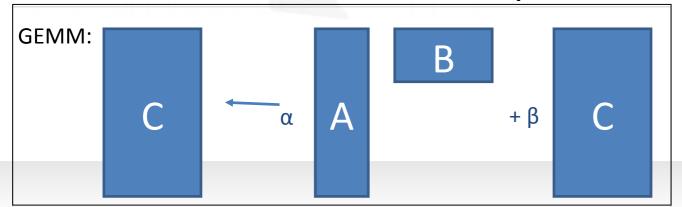
#### Level 2 BLAS Matrix-Vector operations



2n<sup>2</sup> FLOP n<sup>2</sup> memory references

RATIO: 2

#### Level 3 BLAS Matrix-Matrix operations



2n³ FLOP 4n² memory references

RATIO: 2 n

#### Why BLAS so important?

- Because the BLAS are efficient, portable, parallel, and widely available, they are commonly used in the development of high quality linear algebra software.
- Performance of lot of applications depends a lot on the performance of the underlying BLAS

## Standardization (BLAS example)

- Each BLAS Subroutines have a standardized layout
- BLAS is documented in the source code
- Man pages exist
- Vendor supplied docs
- Different BLAS implementations have the same calling sequence

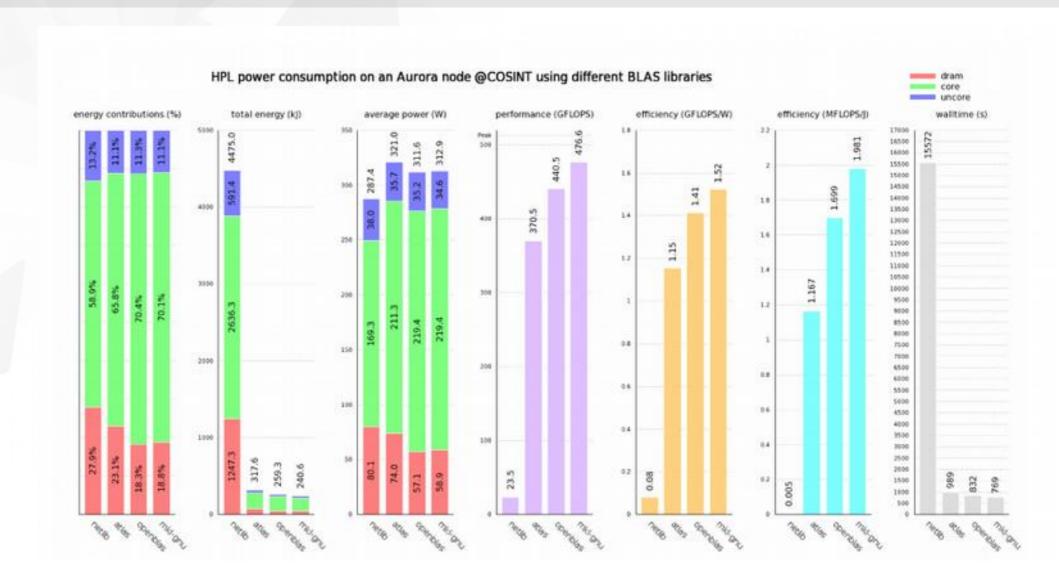
```
SCALAR ARGUMENTS ..
                     TRANSA, TRANSB
                     M. N. K. LDA, LDB, LDC
                    A( LDA, * ), B( LDB, * ), C( LDC, * )
FURPOSE
DGEMM PERFORMS ONE OF THE MATRIX-MATRIX OPERATIONS
  C := ALPHA*OP( A )*OP( B ) + BETA*C.
WHERE OP(X) IS ONE OF
  OP(X) = X OR OP(X) = 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.
PARAMETERS
.....
TRANSA - CHARACTER*1.
        ON ENTRY, TRANSA SPECIFIES THE FORM OF OP( A ) TO BE USED IN
        THE MATRIX MULTIPLICATION AS FOLLOWS:
           TRANSA = 'N' OR 'N', OP(A) = A.
           TRANSA = 'T' OR 'T', OP(A) = A',
           TRANSA = 'C' OR 'C', OP( A ) = A'.
        UNCHANGED ON EXIT.
TRANSB - CHARACTER*1.
        ON ENTRY, TRANSB SPECIFIES THE FORM OF OP( B ) TO BE USED IN
        THE MATRIX MULTIPLICATION AS FOLLOWS:
           TRANSB = 'N' OR 'N'. OP( B ) = B.
           TRANSB = 'T' OR 'T', OP(B) = B'.
```

#### **Vendor/Optimized BLAS libraries**

- ACML
  - The AMD Core Math Library, supporting the AMD processors
- ATLAS
  - Automatically Tuned Linear Algebra
     Software, an open source implementation of BLAS APIs for C and Fortran 77
- Intel MKL
  - The Intel Math Kernel Library, supporting x86 32-bits and 64-bits. Includes optimizations for Intel Pentium, Core and Intel Xeon CPUs and Intel Xeon Phi; support for Linux, Windows and Mac OS X
- cuBLAS
  - Optimized BLAS for NVIDIA based GPU cards
- clBLAS
  - An OpenCL implementation of BLAS

- ESSL
  - IBM's Engineering and Scientific
     Subroutine Library, supporting the
     PowerPC architecture under AIX and Linux
- GotoBLAS
  - Kazushige Goto's BSD-licensed implementation of BLAS, tuned in particular for Intel Nehalem/Atom, VIA Nanoprocessor, AMD Opteron
- BLIS
  - BLAS-like Library Instantiation Software framework for rapid instantiation
- OpenBLAS
  - Optimized BLAS based on Goto BLAS hosted at GitHub, supporting Intel platform and other

## Blas efficiency: (from Moreno B. MHPC's thesis)



## What about my C++/C program ??

- BLAS routines are Fortran-style, when calling them from Clanguage programs, follow the Fortran-style calling conventions:
  - Pass variables by address, not by value.
  - Store your data in Fortran style, that is, column-major rather than row-major order.
- be aware that because the Fortran language is case-insensitive, the routine names can be both upper-case or lower-case, with or without the trailing underscore. For example, the following names are equivalent:

dgemm, DGEMM, dgemm\_, and DGEMM\_

#### **Use CBLAS**

- C-style interface to the BLAS routines ( http://www.netlib.org/blas/blast-forum/cblas.tgz)
- You can call CBLAS routines using regular C-style calls.
- The header file specifies enumerated values and prototypes of all the functions.
- For details and examples:

https://software.intel.com/en-us/mkl-tutorial-c-multiplying-matrices-using-dgemm

# Efficiency: q parameter (aka computational efficiency)

Table 2: Basic Linear Algebra Subroutines (BLAS)

Operation	Definition	Floating	Memory	q
		point	references	
		operations		
вахру	$y_i \!=\! \alpha x_i \!+\! y_i,  i \!=\! 1,,n$	2n	3n + 1	2/3
Matrix-vector mult	$y_i = \sum_{j=1}^n A_{ij}x_j + y_i$	$2n^2$	$n^2 + 3n$	2
Matrix-matrix mult	$C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj} + C_{ij}$	$2n^3$	$4n^2$	n/2

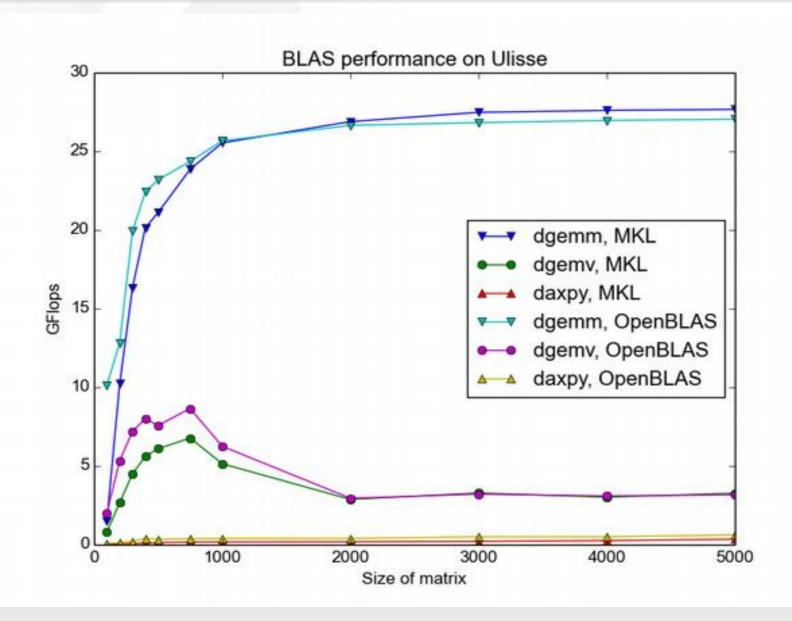
The parameter q is the ratio of flops to memory references. Generally:

- 1.Larger values of q maximize useful work to time spent moving data.
- 2. The higher the level of the BLAS, the larger q.

#### It follows...

- BLAS1 are memory bounded! (for each computation a memory transfer is required)
- BLAS2 are not so memory bounded (can have good performance on super-scalar architecture)
- BLAS3 can be very efficient on super-scalar computers because not memory bounded

#### **Blas Performance on ULISSE**



#### **Proposed Exercise**

- Create the previous graph for the HW/software we are using:
  - Using MKL
  - Using OpenBLAS
  - On a Ulisse old/new nodes
- Steps:
  - Install, if missing needed libraries in your directory
  - Write a small program to call the three routines
  - Write a script to collect all sizes of interest
  - Make nice plots

#### comment on BLAS

## **Basic Linear Algebra Subroutines**

Name	Description	Examples
Level-1 BLAS	Vector Operations	$C = \sum X_i Y_i$
Level-2 BLAS	Matrix-Vector Operations	$\boldsymbol{B}_i = \sum_k \boldsymbol{A}_{ik} \boldsymbol{X}_k$
Level-3 BLAS	Matrix-Matrix Operations	$C_{ij} = \sum_{k} A_{ik} B_{kj}$

#### How to link optimized libraries?

- Reference implementation: order matters!
  - LAPACK uses BLAS
  - => -L/usr/local/lib -llapack -lblas
- OpenBLAS:
  - Automatically includes lapack reference implementation so no need to specify anything else. Please check!
- ATLAS is written C with f77 wrappers:
  - -L/opt/atlas/lib -lf77blas -latlas
- MKL:
  - Generally complex and highly dependent on version and/or HW/SW implementation

https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

## Exercise 2: Running HPL on our clusters

Check the README on github account

#### A few notes:

- Standard input file should be present
- Beware of threads
  - How to control them?



#### What about N?

- N should be large enough to take ~75% of RAM..
  - N = sqrt ( 0.75 \* Number of Nodes \* Minimum memory of any node / 8 )
- You can compute it via:
  - http://www.advancedclustering.com/act-kb/tune-hpl-dat-file/

#### HPL benchmark input file HPL.dat

```
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
HPL.out
             output file name (if any)
             device out (6=stdout,7=stderr,file)
6
             # of problems sizes (N)
50000 Ns
              # of NBs
768
           NBs
             PMAP process mapping (0=Row-,1=Column-major)
             # of process grids (P x Q)
4 1 2 1
               Ps
4 2 2 4
               0s
16.0
             threshold
             # of panel fact
0 1 2
             PFACTs (0=left, 1=Crout, 2=Right)
             # of recursive stopping criterium
2 8
             NBMINs (>= 1)
1
             # of panels in recursion
2
             NDIVs
             # of recursive panel fact.
0 1 2
             RFACTs (0=left, 1=Crout, 2=Right)
             # of broadcast
0 2
             BCASTs (0=1rq, 1=1rM, 2=2rq, 3=2rM, 4=Lnq, 5=LnM)
             # of lookahead depth
1 0
             DEPTHs (>=0)
             SWAP (0=bin-exch,1=long,2=mix)
1
192
             swapping threshold
1
             L1 in (0=transposed,1=no-transposed) form
             U in (0=transposed,1=no-transposed) form
1
             Equilibration (0=no,1=yes)
             memory alignment in double (> 0)
```

## Parameters for HPL.dat input file

N	Problem size	Pmap	Process mapping
NB	Blocking factor	threshold	for matrix validity test
Р	Rows in process grid	Ndiv	Panels in recursion
Q	Columns in process grid	Nbmin	Recursion stopping criteria
Depth	Lookahead depth	Swap	Swap algorithm
Bcasts	Panel broadcasting method	L1, U	to store triangle of panel
Pfacts	Panel factorization method	Align	Memory alignment
Rfacts	Recursive factorization method	Equilibration	

## Tips to get performance..

- Figure out a good block size (NB) for the matrix multiply routine. The best method is to try a few out. If you happen to know the block size used by the matrix-matrix multiply routine, a small multiple of that block size will do fine. This particular topic is discussed in the FAQs section.
- The process mapping should not matter if the nodes of your platform are single processor computers. If these nodes are multi-processors, a row-major mapping is recommended.
- HPL likes "square" or slightly flat process grids. Unless you are using a very small process grid, stay away from the 1-by-Q and P-by-1 process grids.

## What are you supposed to do?

• Let us read together the readme file.





Thank you ...



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