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Advanced School in High Performance and GRID Computing

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Mathematical Libraries.
Part I

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Mathematical Libraries (Part 1)

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Overview

- Opportunities to improve application performance on modern CPUs
- Why use performance libraries?
- Using / linking libraries
- Example:
  Using DGEMM in BLAS

"There are better ways to log off."

Using Cache Efficiently

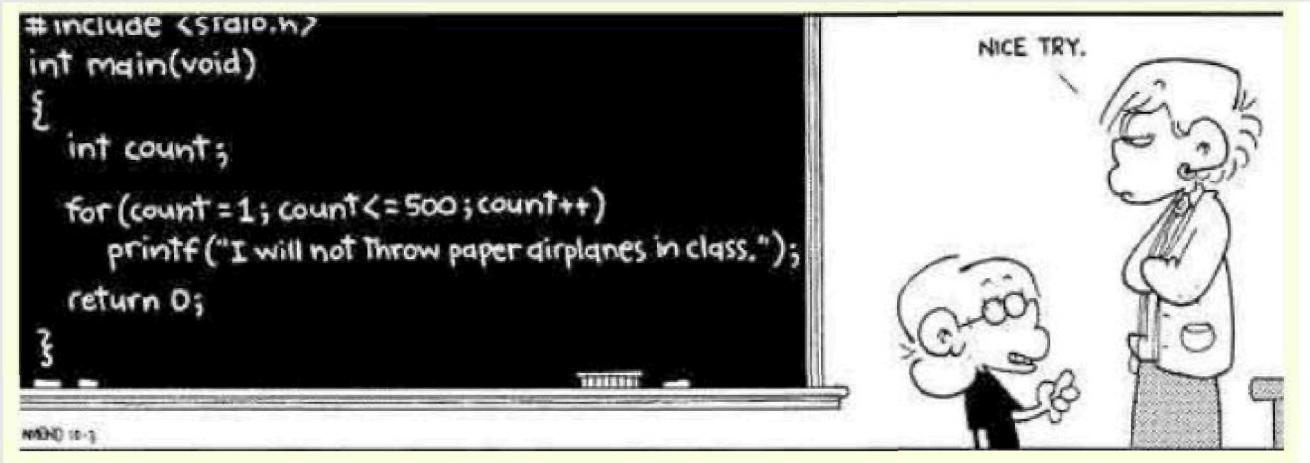
- Cache is a fast but small memory area
- Located on the CPU or close to it
- Compensate for discrepancy between CPU speed (fast) and Memory speed (slow)
- Typically transparently, and kept coherent in multi-core, multi-CPU environment.
- The key for good performance is to write code that maximized the effect of cache memory
- The optimal code structure (blocking) depend on CPU speed, model, and architecture

Using Special Instructions

- Modern CPUs contain many special purpose instructions: MMX,SSE,3d-now,Altivec
- Many allow to operate on multiple data elements in parallel: SIMD, vector instructions
- Programming in assembly required to use them efficiently
- In general not portable between different CPU architectures and models
- Significant speedups for Linear Algebra operations, signal processing.

Using Multi-core / Multi-CPU

- Modern CPUs contain multiple CPU cores
- Need parallel program (MPI, OpenMP, ...) to exploit the additional capability
- Parallelism in code need rewrites/restructuring (MPI), or instrumentation (OpenMP)



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
- 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.

Why use performance libraries?

- Compilers can optimize code only to a certain point (they are dumb). 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

Standardization

- 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

```
      SUBROUTINE DGEMM ( TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB,
     $                   BETA, C, LDC )
*     .. SCALAR ARGUMENTS ..
      CHARACTER*1        TRANSA, TRANSB
      INTEGER            M, N, K, LDA, LDB, LDC
      DOUBLE PRECISION   ALPHA, BETA
*     .. ARRAY ARGUMENTS ..
      DOUBLE PRECISION   A( LDA, * ), B( LDB, * ), C( LDC, * )
*     ..
*
*  PURPOSE
*  =======
*
*  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'.
*
```

How to use libraries in code

```
[rroussea@samson qmc_code]$ more alldet.f90
        subroutine alldet(iopt,indt,nelorb,nelup,neldo,ainv,winv
     1,ainvupb,derl)
        implicit none
        integer iopt,nelorb,nelup,neldo,nelt,i,j,nelorb5
     1,indt
        real*8 ainv(nelup,*),ainvupb(nelup,*)
     1  ,derl(nelorb,*),winv(nelorb,0:indt+4,*)

         nelorb5=(indt+5)*nelorb



        call dgemm('N','T',nelup,nelorb,nelup,1.d0,ainv,nelup
     1,winv(1,0,1),nelorb5,0.d0,ainvupb,nelup)

        call dgemm('N','N',nelorb,nelorb,neldo,1.d0,winv(1,0,nelup+1)
     1,nelorb5,ainvupb,nelup,0.d0,derl,nelorb)
```

Within your code you simply need to call the BLAS/LAPACK routines
As if they are subroutines you would normally write.
Note check the BLAS/LAPACK manuals to know the name of routine
And what variables need to be passed to them and in what order.
NB DGEMM double generic matrix-matrix multiplication

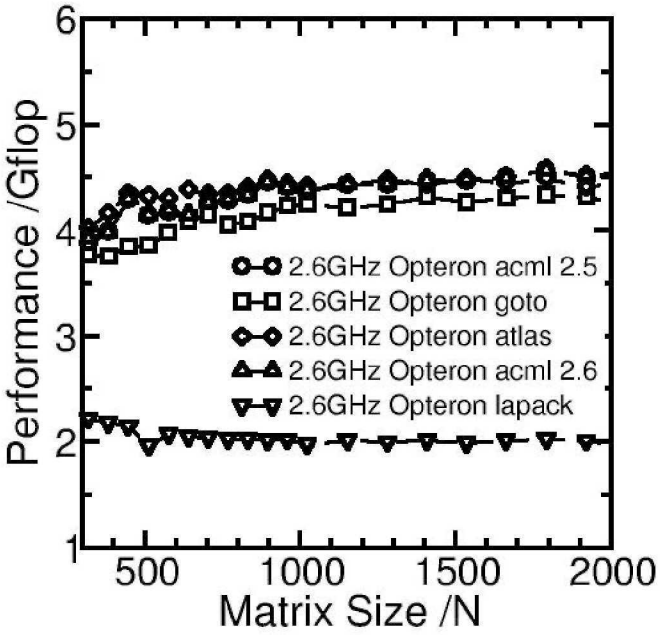
BLAS/LAPACK Implementations

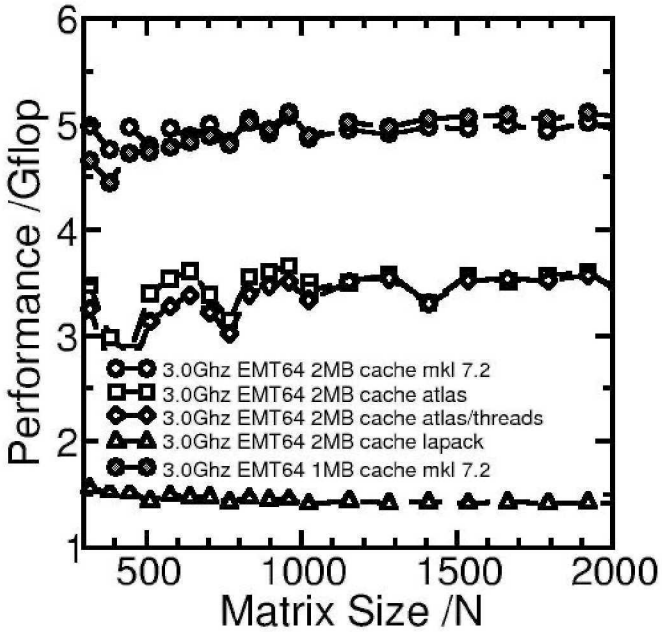
- BLAS and LAPACK reference (portable Fortran77)
- Intel Math Kernel Library (MKL): BLAS/LAPACK (+FFT) routines modified for best performance on IA32/x86, x86_64/AMD64/EM64t, and IA64 based machines.
- AMD Math Core Library (ACML): BLAS LAPACK (+FFT) routines modified for best performance on AMD x86 and x86_64 based machines
- Automatically Tuned Linear Algebra Software (ATLAS): BLAS and LAPACK routines that use empirical tests to tune machine specific parameters.
- GOTO BLAS, a BLAS implementation with special optimization for modern (x86/x86_64) CPU architectures

Linking Your Code to Libraries

- Linker flags: -L/some/other/dir -lm
  -> search for libm.so/libm.a also in /some/dir
- Order matters. Ex.: LAPACK uses BLAS
  => -L/usr/local/lib -llapack -lblas
- ATLAS is written C with f77 wrappers:
  => -L/opt/atlas/lib -lf77blas -latlas
- MKL uses “collections”.
  Using -lmkl links: libmkl_intel_lp64.so,
  libmkl_intel_thread.so libmkl_core.so
  => check with “ldd”
- Check LD_LIBRARY_PATH with shared libs

Library Performance Example





- The absolute and relative performance of a library is very platform dependent
- Vendor optimized libraries are most of the time faster.

Comments on LAPACK and BLAS

- BLAS Levels: 1) vector, 2) vector/matrix, 3) matrix
- BLAS Level 1, has N memory operations for N CPU operations. Whereas Level 3 has $2N^2$ memory/N^4 CPU => more efficient. Thus combining operations over vectors into matrix-matrix operations is useful
- Reference LAPACK/BLAS are better than “coding by hand”, BUT are less efficient than the vendor supplied versions of the same library or ATLAS.
- LAPACK relies heavily on BLAS so the key to good performance is a fast BLAS.

Beware! Multi-threaded Libraries

- FFTW: Thread parallelization through additional library, needs special management
- ATLAS: fixed number of threads compiled in
- MKL: Threading with OpenMP
  - Uses by default **all** available cores
    => conflicts with MPI, NUMA-SMP workstations
  - Modular, can be tuned to compiler, linker, threads
  - Default linking sequence for ifort with Intel threads
    => add -openmp to linker/compiler command
  - Serial: -lmkl_intel_lp64 -lmkl_sequential -lmkl_core
  - GNU: -lmkl_gf_lp64 -lmkl_gnu_thread -lmkl_core
  - See documentation for details (always RTFM!).