Cornell University
Center for Advanced Computing

Per-Core Performance Optimization

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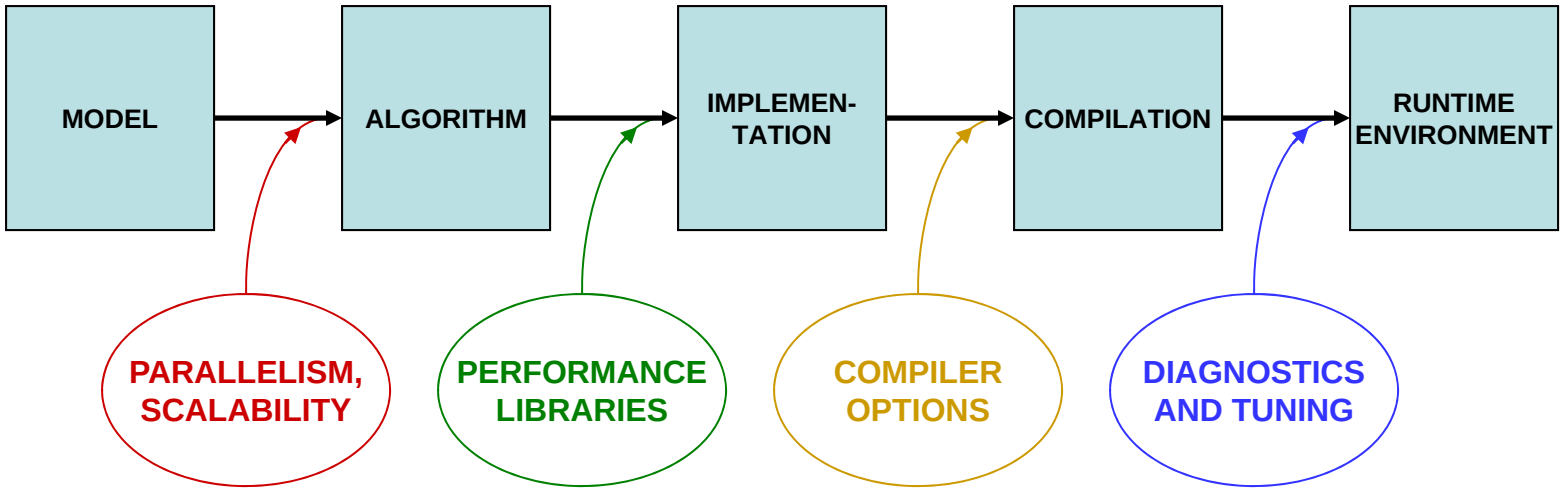
Putting Performance into Design and Development



Designing for parallelism and scalability is a topic in itself…

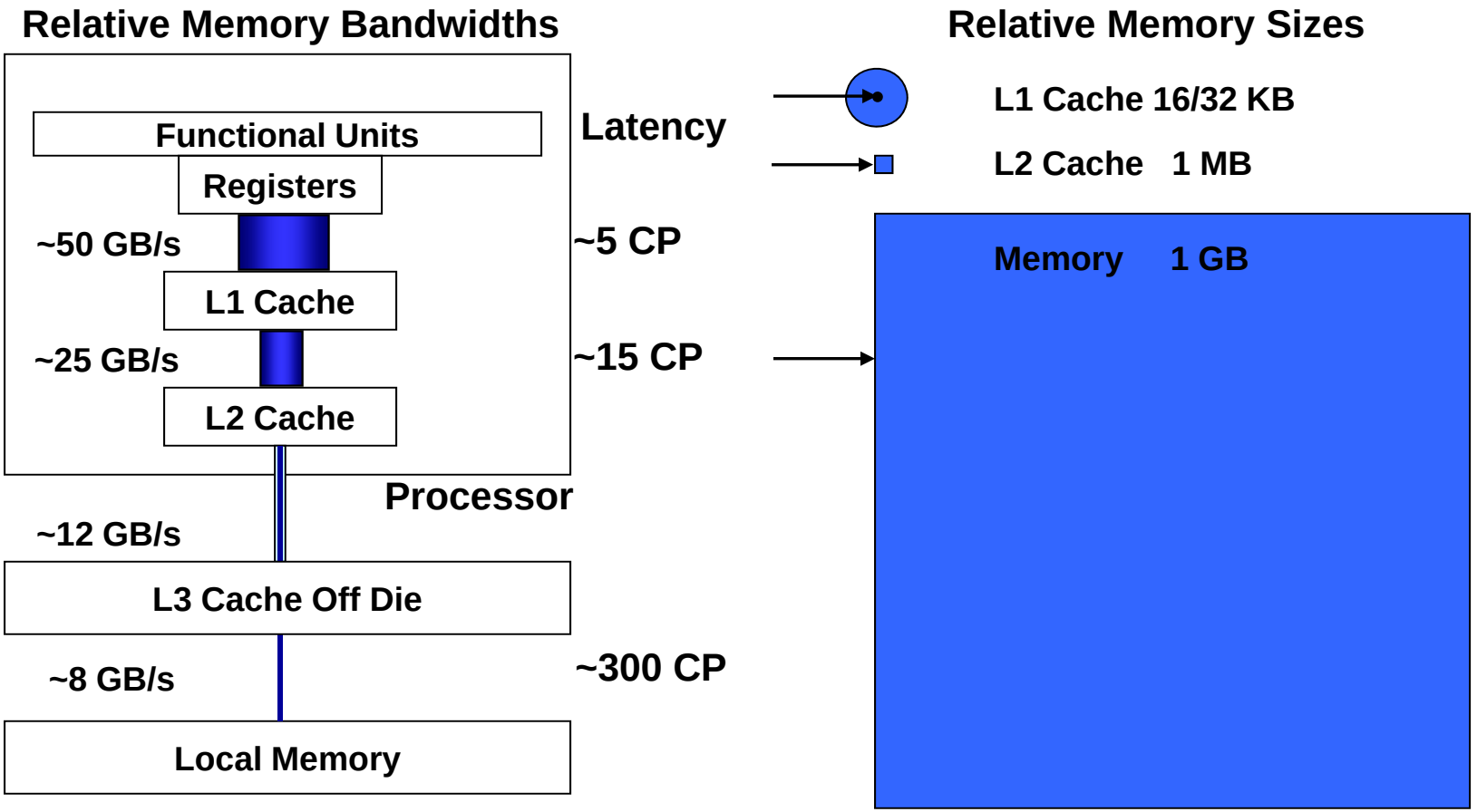
…this talk is about principles and practices during the later stages of development that lead to better performance on a per-core basis

What Matters Most in Per-Core Performance

Good memory locality!

- Code accesses contiguous memory addresses
  - Reason: Data arrives in cache lines, including neighbors
  - Reason: Loops can be vectorized for SSE (explained in a moment)
- Multiple operations involving the same data item are collected together
  - Reason: Access to cache is much faster than to RAM
- Data are aligned on doubleword boundaries
  - Reason: More efficient to have data items not straddling cache lines
- Goal: to have the data stay longer in cache, so that deeper levels of the memory hierarchy are accessed as infrequently as possible

Understanding The Memory Hierarchy



What's the Target Architecture?

- AMD initiated the x86-64 or x64 instruction set
  - Extends Intel's 32-bit x86 instruction set to handle 64-bit addressing
  - Encompasses both AMD64 and EM64T = "Intel 64"
  - Differs from IA-64 (now called "Intel Itanium Architecture")

- Additional SSE instructions access special registers & operations
  - 128-bit registers can hold 4 floats/ints or 2 doubles simultaneously
  - Within an SSE register, "vector" operations can be applied
  - Operations are also pipelined (e.g., load > multiply > add > store)
  - Therefore, multiple results can be produced every clock cycle

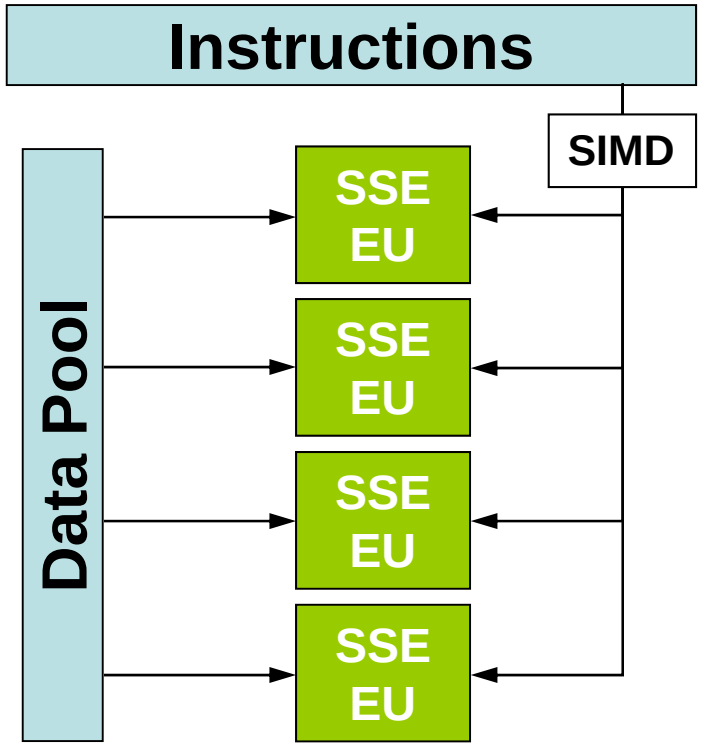
Understanding SSE, SIMD, and Micro-Parallelism

- For “vectorizable” loops with independent iterations, SSE instructions can be employed…

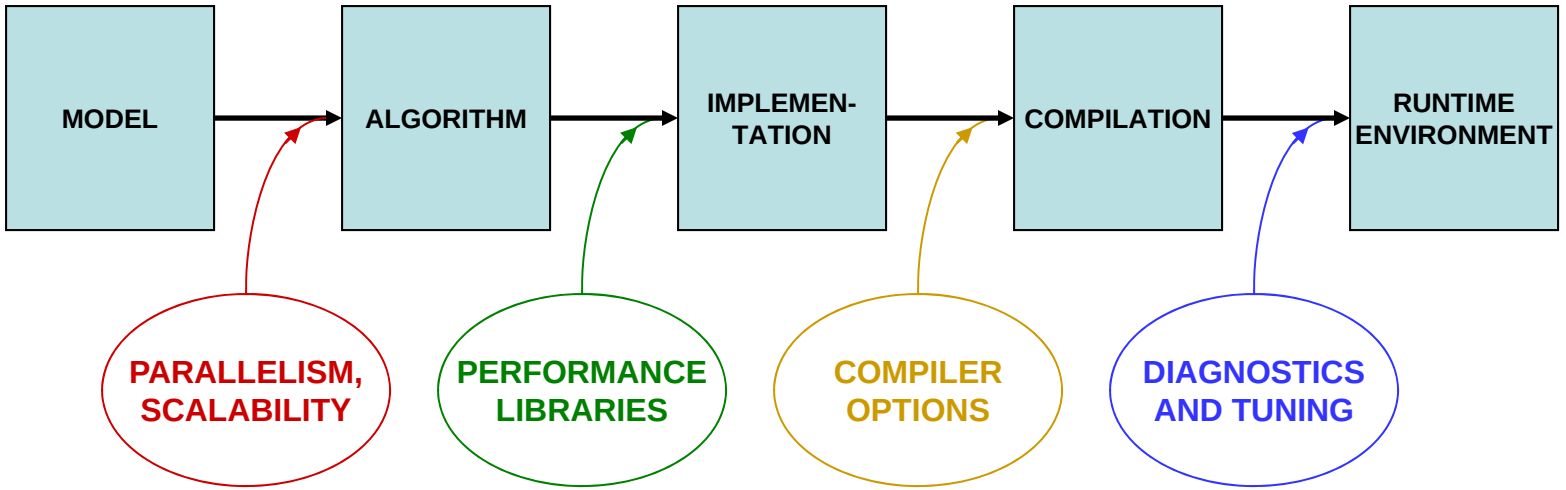
SSE = *Streaming SIMD Extensions*

SIMD = *Single Instruction, Multiple Data*

Instructions operate on multiple arguments simultaneously, in parallel Execution Units



Putting Performance into Development: Libraries



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Performance Libraries

- Optimized for specific architectures (chip + platform + system)
- Offered by different vendors
  - Intel Math Kernel Library (MKL)
  - AMD Core Math Library (ACML)
  - ESSL/PESSL on IBM systems
  - Cray libsci for Cray systems
  - SCSL for SGI systems
- Usually far superior to hand-coded routines for “hot spots”
  - Writing your own library routines by hand is not like re-inventing the wheel; it’s more like re-inventing the muscle car
  - *Numerical Recipes* books are NOT a source of optimized code: performance libraries can run 100x faster

HPC Software on Ranger, from Apps to Libs

Applications	Parallel Libs	Math Libs	Input/Output	Diagnostics
AMBER	PETSc	MKL	NetCDF	TAU
NAMD		ACML	HDF5	PAPI
GROMACS	PLAPACK	GSL	PHDF5	…
	ScaLAPACK	GotoBLAS	…	
GAMESS	SLEPc	GotoBLAS2		
NWChem				
…	METIS	FFTW(2/3)		
	ParMETIS	…		
	SPRNG			
	…			

Intel MKL 10.0 (Math Kernel Library)

- Is optimized for the IA-32, Intel 64, Intel Itanium architectures
- Supports Fortran and C interfaces
- Includes functions in the following areas:
  - Basic Linear Algebra Subroutines, for BLAS levels 1-3 (e.g., Ax+y)
  - LAPACK, for linear solvers and eigensystems analysis
  - FFT routines
  - Transcendental functions
  - Vector Math Library (VML), for vectorized transcendentals
  - …others

Using Intel MKL on Ranger

- Enable MKL
  - module load mkl
  - module help mkl

- Compile and link for C/C++

```
mpicc -I$TACC_MKL_INC mkl_test.c -L$TACC_MKL_LIB -lmkl_em64t
```

- Compile and link for Fortran

```
mpif90 mkl_test.f90 -L$TACC_MKL_LIB -lmkl_em64t
```

GotoBLAS and FFTW

GotoBLAS

- Hand-optimized BLAS, minimizes TLB misses
- Only testing will tell what kind of advantage your code gets

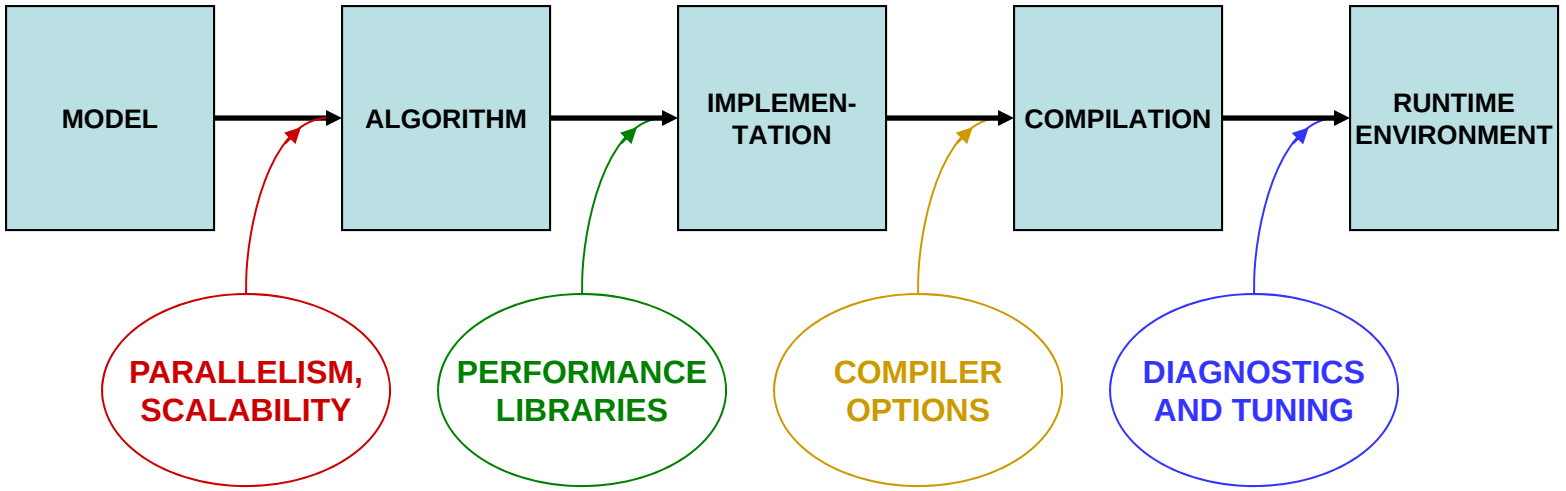
FFTW, the Fastest Fourier Transform in the West

- Cooley-Tukey
- Prime Factor algorithm, most efficient with small prime factors like (2, 3, 5, and 7)
- Automatic performance adaptation

GSL, the Gnu Scientific Library

- Special Functions
- Vectors and Matrices
- Permutations
- Sorting
- Linear Algebra/BLAS Support
- Eigensystems
- Fast Fourier Transforms
- Quadrature
- Random Numbers
- Quasi-Random Sequences
- Random Distributions
- Statistics, Histograms
- N-Tuples
- Monte Carlo Integration
- Simulated Annealing
- Differential Equations
- Interpolation
- Numerical Differentiation
- Chebyshev Approximation
- Root-Finding
- Minimization
- Least-Squares Fitting

Putting Performance into Development: Compilers



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Compiler Options

- There are three important categories:
  - Optimization level
  - Architecture specification
  - Interprocedural optimization

- Generally you'll want to supply one option from each category

Let the Compiler Do the Optimization

- Be aware that compilers can do sophisticated optimization
  - Realize that the compiler will follow your lead
  - Structure the code so it's easy for the compiler to do the right thing (and for other humans to understand it)
  - Favor simpler language constructs (pointers and OO code won't help)

- Use the latest compilers and optimization options
  - Check available compiler options
    `<compiler_command> --help` {lists/explains options}
  - Refer to the User Guides, they usually list "best practice" options
  - Experiment with combinations of options

Basic Optimization Level: -O*n*

- -O0 = no optimization: disable all optimization for fast compilation
- -O1 = compact optimization: optimize for speed, but disable optimizations which increase code size
- -O2 = default optimization
- -O3 = aggressive optimization: rearrange code more freely, e.g., perform scalar replacements, loop transformations, etc.

- Note that specifying -O3 is not always worth it…
  - Can make compilation more time- and memory-intensive
  - Might be only marginally effective
  - Carries a risk of changing code semantics and results
  - Sometimes even breaks codes!

-O2 vs. -O3

- Operations performed at default optimization level, -O2
  - Instruction rescheduling
  - Copy propagation
  - Software pipelining
  - Common subexpression elimination
  - Prefetching
  - Some loop transformations
- Operations performed at higher optimization levels, e.g., -O3
  - Aggressive prefetching
  - More loop transformations

Know Your Chip

- SSE level and other capabilities depend on the exact chip

- Taking an AMD Opteron "Barcelona" from Ranger as an example…
  - Supports AMD64, SSE, SSE2, SSE3, and "SSE4a" (subset of SSE4)
  - Does *not* support AMD's more recent SSE5
  - Does *not* support all of Intel's SSE4, nor its SSSE = Supplemental SSE

- In Linux, a standard file shows features of your system's architecture
  - **`cat /proc/cpuinfo`** {shows cpu information}
  - If you want to see even more, do a Web search on the model number

- This information can be used during compilation

Specifying Architecture in the Compiler Options

With -x<code> {code = W, P, T, O, S… } or a similar option, you tell the compiler to use the most advanced SSE instruction set for the target hardware. Here are a few examples of processor-specific options.

Intel 10.1 compilers:

- -xW = use SSE2 instructions (recommended for Ranger)
- -xO = include SSE3 instructions (also good for Ranger)
- -xT = SSE3 & SSSE3 (no good, SSSE is for Intel chips only)
- In Intel 11.0, these become -msse2, -msse3, and -xssse3

PGI compilers:

- -tp barcelona-64 = use instruction set for Barcelona chip

Interprocedural Optimization (IP)

- Most compilers will handle IP within a single file (option -ip)

- The Intel -ipo compiler option does more
  - It places additional information in each object file
  - During the load phase, IP among ALL objects is performed
  - This may take much more time, as code is recompiled during linking
  - It is **important** to include options in **link** command (-ipo -O3 -xW, etc.)
  - All this works because the special Intel xild loader replaces ld
  - When archiving in a library, you must use xiar, instead of ar

Interprocedural Optimization Options

Intel 10.1 compilers:

- -ip enable single-file interprocedural (IP) optimizations
  - Limits optimizations to within individual files
  - Produces line numbers for debugging
- -ipo enable multi-file IP optimizations (between files)

PGI compilers:

- -Mipa=fast,inline enable interprocedural optimization
  There is a loader problem with this option

Other Intel Compiler Options

- -g — generate debugging information, symbol table
- -vec_report# — {# = 0-5} turn on vector diagnostic reporting
- -C (or -check) — enable extensive runtime error checking
- -CB -CU — check bounds, check uninitialized variables
- -convert *kw* — specify format for binary I/O by keyword {*kw* = big_endian, cray, ibm, little_endian, native, vaxd}
- -openmp — multi-thread the executable based on OpenMP directives
- -openmp_report# — {# = 0-2} turn on OpenMP diagnostic reporting
- -static — load libs statically at runtime – *do not use*
- -fast — same as -O2 -ipo -static; *not allowed on Ranger*

Other PGI Compiler Options

- -fast — use a suite of processor-specific optimizations: -O2 -Munroll=c:1 -Mnoframe -Mlre -Mautoinline -Mvect=sse -Mscalarsse -Mcache_align -Mflushz
- -mp — multithread the executable based on OpenMP directives
- -Minfo=mp,ipa — turn on diagnostic reporting for OpenMP, IP

Best Practices for Compilers

- Normal compiling for Ranger
  - Intel:
    icc/ifort -O3 -ipo -xW prog.c/cc/f90
  - PGI:
    pgcc/pgcpp/pgf95 -fast -tp barcelona-64 -Mipa=fast,inline prog.c/cc/f90
  - GNU:
    gcc -O3 -fast -xipo -mtune=barcelona -march=barcelona prog.c

- -O2 is the default; compile with -O0 if this breaks (very rare)
- Effects of Intel's -xW and -xO options may vary
- Debug options should not be used in a production compilation!
  - Compile like this only for debugging: ifort -O2 -g -CB test.c

Lab: Compiler-Optimized Naïve Code vs. GSL

- Code is from Numerical Recipes to do LU decomposition
- Compare timings with different optimizations
- Compare with implementation in GSL

- Compile with different flags, including “-g”, “-O2”, “-O3”
- Submit a job to see how fast it is
- Recompile with new flags and try again

- Sits in lude.tar.gz

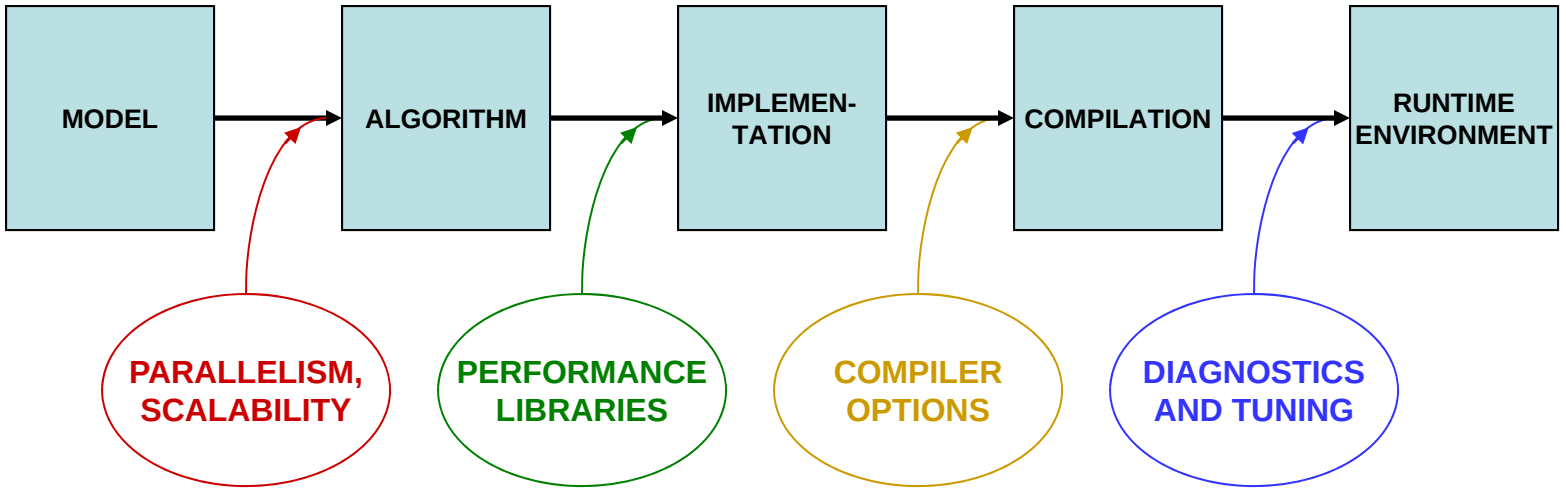
Make/Run Instructions for the Lab

- Edit top of makefile to change compiler and flags
  - COMPILER=pgcc
  - FFLAGS=-O2 -tp barcelona-64
  - VERSION=0
- "VERSION" is tacked onto the end of the executable names
  - nr0 and gsl0 or nr1 and gsl1
- "make" generates executables
- "make list" looks through your directory to find all executables
- ./nr0 -f -o output_file -n 10000
  - -f tells it to tell you how you compiled the executable
  - -o is the name of an optional output file to verify results
  - -n is the size of the nxn matrix

Obtaining Results for the Lab

- Edit makefile to use “FFLAGS=-g” and VERSION=0, then “make”
- Edit makefile to use “FFLAGS=-O2” and VERSION=1, then “make”
- Edit makefile to use “FFLAGS=-O3” and VERSION=2, then “make”
- “make list” to see that they are all there.
  - ./nr0 pgcc -O2 -tp barcelona-64
  - ./gsl0 pgcc -O2 -tp barcelona-64
  - ./nr1 pgcc -O3 -tp barcelona-64
  - ./gsl1 pgcc -O3 -tp barcelona-64
  - ./nr2 pgcc -g -tp barcelona-64
  - ./gsl2 pgcc -g -tp barcelona-64
- “qsub job.sge” or “make submit”
- Find the runtimes in the output to see the speeds

Putting Performance into Development: Tuning



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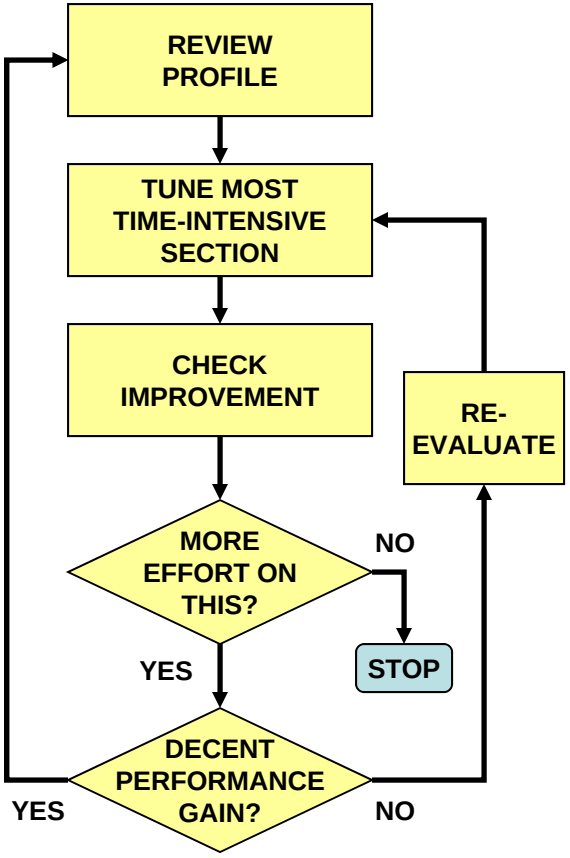
In-Depth vs. Rough Tuning

In-depth tuning is a long, iterative process:

- Profile code
- Work on most time intensive blocks
- Repeat as long as you can tolerate…

For rough tuning during development:

- It helps to know about common microarchitectural features (like SSE)
- It helps to have a sense of how the compiler tries to optimize instructions, given certain features



Rules of Thumb for Writing Optimizable Code

- Minimize stride length
  - Stride length 1 is optimal for vectorizable code
  - It increases cache efficiency
  - It sets up hardware and software prefetching
  - Stride lengths of large powers of two are typically the worst case, leading to cache and TLB misses (due to limited cache associativity)
- Strive for stride-1 vectorizable loops
  - Can be sent to a SIMD unit
  - Can be unrolled and pipelined
  - Can be parallelized through OpenMP directives
  - Can be "automatically" parallelized (be careful…)

G4/5	**Velocity Engine (SIMD)**
Intel/AMD	**MMX, SSE, SSE2, SSE3 (SIMD)**
Cray	**Vector Units**

Best Practices from the Ranger User Guide

- Avoid excessive program modularization (i.e. too many functions/subroutines)
  - Write routines that can be inlined
  - Use macros and parameters whenever possible
- Minimize the use of pointers
- Avoid casts or type conversions, implicit or explicit
  - Conversions involve moving data between different execution units
- Avoid branches, function calls, and I/O inside loops
  - Why pay overhead over and over?
  - Structure loops to eliminate conditionals
  - Move loops into the subroutine, instead of looping around a subroutine call

More Best Practices from the Ranger User Guide

- Additional performance can be obtained with these techniques:
  - Memory Subsystem Tuning: Optimize access to the memory by minimizing the stride length and/or employing “cache blocking” techniques such as loop tiling
  - Floating-Point Tuning: Unroll inner loops to hide FP latencies, and avoid costly operations like division and exponentiation
  - I/O Tuning: Use direct-access binary files to improve the I/O performance
- These techniques are explained in further detail, with examples, in a Memory Subsystem Tuning document found online

Inlining

- What does inlining achieve?
  - It replaces a function call with a full copy of that function's instructions
  - It avoids putting variables on the stack, jumping, etc.

- When is inlining important?
  - When the function is a hot spot
  - When function call overhead is comparable to time spent in the routine
  - When it can benefit from Inter-Procedural Optimization

- As you develop "think inlining"
  - The C "inline" keyword provides inlining within source
  - Use -ip or -ipo to allow the compiler to inline

Example: Procedure Inlining

```
integer :: ndim=2, niter=10000000
real*8  :: x(ndim), x0(ndim), r
integer :: i, j
   ...
   do i=1,niter
      ...
      r=dist(x,x0,ndim)
      ...
   end do
   ...
end program
real*8 function dist(x,x0,n)
real*8  :: x0(n), x(n), r
integer :: j,n
r=0.0
do j=1,n
   r=r+(x(j)-x0(j))**2
end do
dist=r
end function
```

Trivial function *dist* is called *niter* times

```
integer:: ndim=2, niter=10000000
real*8  :: x(ndim), x0(ndim), r
integer :: i, j
   ...
   do i=1,niter
      ...
      r=0.0
      do j=1,ndim
         r=r+(x(j)-x0(j))**2
      end do
      ...
   end do
   ...
end program
```

Low-overhead loop *j* executes *niter* times

function *dist* has been inlined inside the *i* loop

Stride 1 in Fortran and C

- The following snippets of code illustrate the correct way to access contiguous elements of a matrix, i.e., stride 1 in Fortran and C

Fortran Example:

```
real*8 :: a(m,n), b(m,n), c(m,n)
...
do i=1,n
   do j=1,m
      a(j,i)=b(j,i)+c(j,i)
   end do
end do
```

C Example:

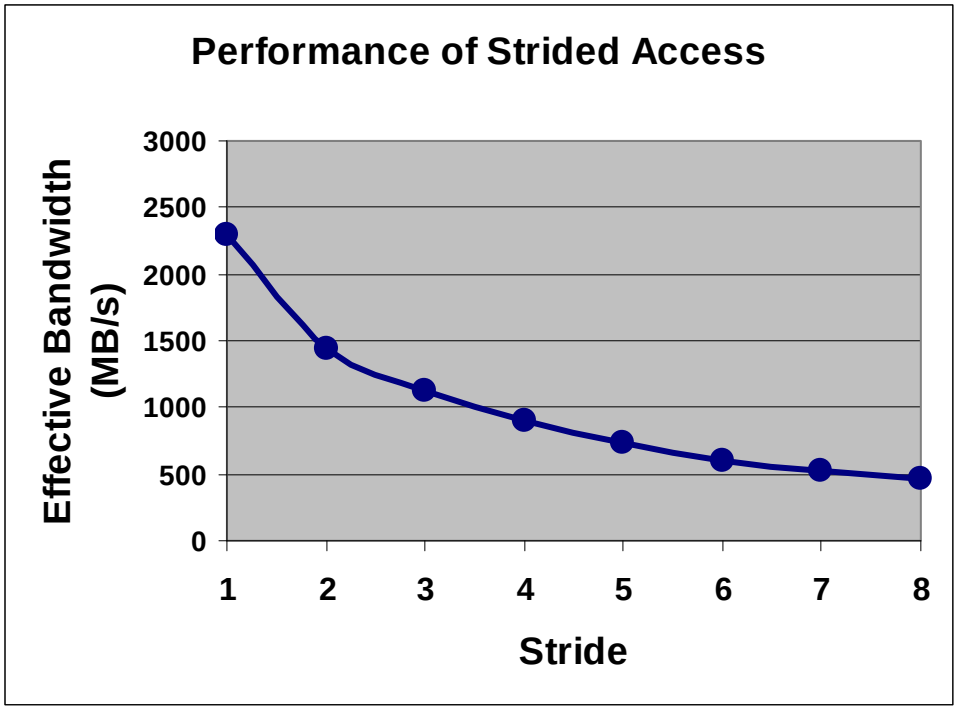
```
double a[m][n], b[m][n], c[m][n];
...
for (i=0;i < m;i++){
   for (j=0;j < n;j++){
      a[i][j]=b[i][j]+c[i][j];
   }
}
```

The Penalty of Stride > 1

- For large and small arrays, always try to arrange data so that structures are arrays with a unit (1) stride.

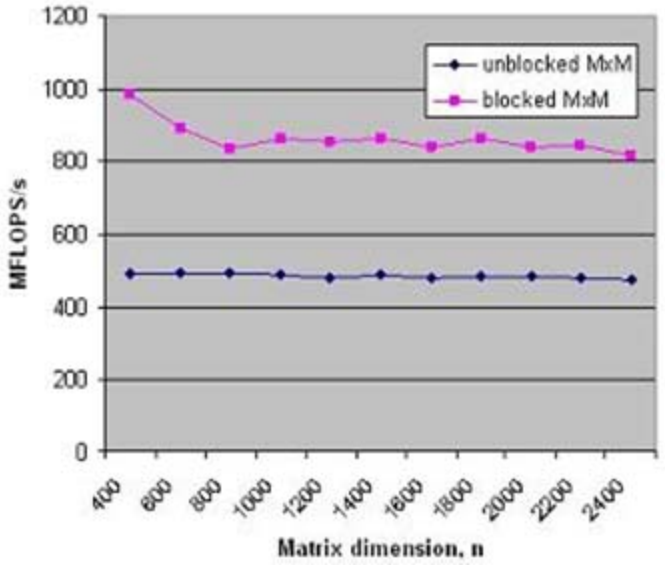
Bandwidth Performance Code:

```
do i = 1,10000000,istride
sum = sum + data( i )
end do
```



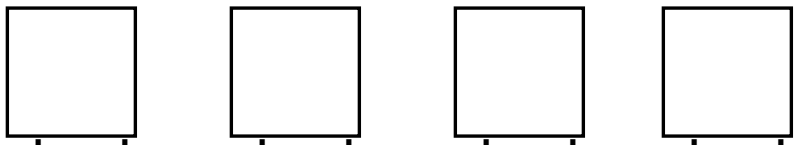
Array Blocking, or Loop Tiling, to Fit Cache

Example: matrix-matrix multiplication




```
real*8 a(n,n), b(n,n), c(n,n)
do ii=1,n,nb
   do jj=1,n,nb
      do kk=1,n,nb
         do i=ii,min(n,ii+nb-1)
            do j=jj,min(n,jj+nb-1)
               do k=kk,min(n,kk+nb-1)

          c(i,j)=c(i,j)+a(i,k)*b(k,j)
```



Takeaway: all the performance libraries do this, so you don't have to