Performance Considerations: Compilers, Optimization, Libraries

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Outline

1. Introduction
2. Compiler Options
3. Performance Libraries
4. Code Optimizations

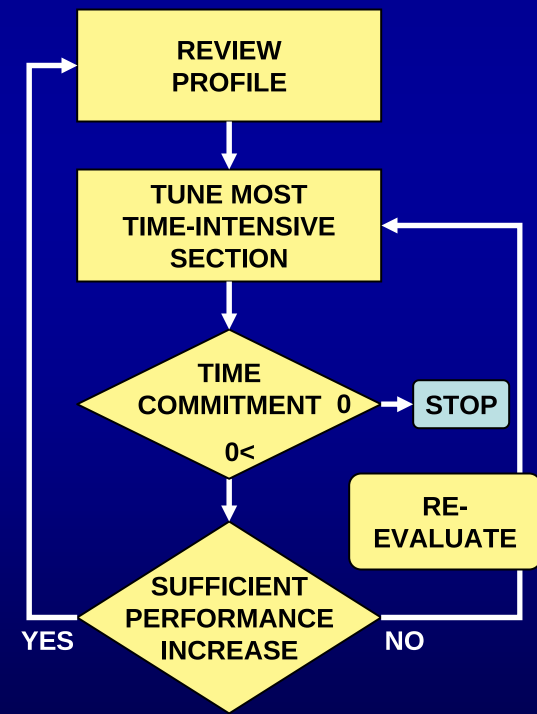
1 General Optimization Procedure

Optimization in code design/development:

- Requires understanding of common architecture features
- Requires sense of how compilers map code to instructions.

Optimization is an iterative process:

- Profile code
- Work on most time intensive blocks
- Repeat



1 Compiler Options

- Three important Categories
  - Optimization Level
  - Architecture Specification
  - Interprocedural Optimization

You should always have at least one option from each category!

2 Compilers and Optimization

- Compilers can perform significant optimization
  - The compiler follows your lead!
  - Structure code to make apparent what the compiler should do (so that the compilers and others can understand it).
  - Use simple language constructs (e.g. don't use pointers, or OO code).
- Use latest compilers.
  - Always check compiler options
    <compiler_command> --help   {lists/explains options}
  - Look for architecture options for your system
    See User Guides – usually lists "best practice" options
    cat /proc/cpuinfo {shows cpu information}
- Experiment with different options.
- May need routine-specific options (use *-ipo*).

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Optimization Level: –O*n*

- -O0 no optimization: Fast compilation, disables optimization
- -O1 optimize for speed, but disables optimizations which increase code size
- -O2 default optimization
- -O3 aggressive optimization: rearrangement of code, i.e. scalar replacement, loop transformation. Compile time/space intensive and/or marginal effectiveness; may change code semantics and *results* (sometimes even breaks codes!)

Optimization Levels

- Operations performed at default optimization level
  - instruction rescheduling
  - copy propagation
  - software pipelining
  - common subexpression elimination
  - prefetching, (some loop transformations)
- Operations performed at aggressive optimization levels
  - Usually enabled by –O3
  - more aggressive prefetching, loop transformations

Architecture Specification

X87 instruction sets are now replaced by SSE "Vector" instruction sets.

(S)SSE = (Supplemental) Streaming SIMD Extension

SSE instructions sets are chip dependent

(SSE instructions pipeline and simultaneously execute independent operations to get multiple results per clock period.)

The –x<codes> { code = W, P, T, O, S} directs the compiler to use most advanced SSE instruction set for the target hardware.

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Architecture Specification

Intel **(SSSE is for Intel chips only!)**

Processor-specific optimization options (all do SSE and SSE2):

-xT	includes SSE3 & SSSE3 instructions for EM64T (Lonestar, v. 10.1)
-xW	**no supplemental** Instructions (Ranger, v. 10.1)
-xO	includes SSE3 Instructions (Ranger, v. 10.1)

PGI

-tp barcelona-64	uses 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 adds additional information to each object file.
  - Then, during loading, the code is recompiled and IP among ALL objects is performed.
  - May take much more time: Code is recompiled during linking
  - It is **Important** to include options in link command (-ipo –O# -xW, etc.) (special Intel xild loader replaces ld)
  - When archiving in a library, you must use xiar, instead of ar.

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Interprocedural Optimization (IP)

Intel

-ip enable single-file interprocedural (IP) optimizations (within files). Line numbers produced for debugging

-ipo enable multi-file IP optimizations (between files)

PGI

-Mipa=fast,inline Interprocedural Optimization

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Other Intel Compiler Options

Other options:

-g debugging information, generates symbol table

-vec_report[#] {#=0-5}, controls vector diagnostic reporting

-C enable extensive runtime error checking (-CA, -CB, -CS, -CU, -CV)

-convert <kwd> specify file format

keyword: big_endian, cray, ibm, little_endian, native, vaxd

-openmp enable the parallelizer to generate multi-threaded code based on the OpenMP directives.

-openmp_report controls level of diagnostic reporting

-static create a static executable for serial applications. MPI applications compiled on Lonestar cannot be built statically.

Other PGI Compiler Options

Processor-specific optimization options:

-fast	-O2 -Munroll=c:1 -Mnoframe -Mlre -Mautoinline -Mvect=sse -Mscalarsse -Mcache_align -Mflushz
-mp	thread generation for OpenMP directives
-Minfo=mp,ipa	OpenMP/Interprocedural Opt. reporting

Compilers - Best Practice

- 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 default opt, compile with –O0 if this breaks (very rare)

- The effects of -xW and -xO options may vary

- Don't include debug options for a production compile!

  ifort –O2 ~~–g~~ ~~–CB~~ test.c

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3 Performance Libraries

- Optimized for specific architectures
- Use library routines instead of hand-coding your own
  In “hot spots”, never write library functions by hand.
- Offered by different vendors (ESSL/PESSL on IBM systems, Intel MKL for x86-64, AMD ACML, Cray libsci for Cray systems, SCSL for SGI)
- Numerical Recipes books DO NOT provide optimized code. (Libraries can be 100x faster).

Linux x86-64 (Lonestar/Ranger) Libraries - 3rd Party Applications

Performance	Math Libs	Method Libs	Applications	I/O
gprof	SPRNG	PETSc	Amber	NetCDF
			NAMD	HDF (4/5)
TAU	Metis/parmetis	PLAPACK	GROMACS	
PAPI		SCALAPACK		Parallel
	FFTW (2/3)	SLEPc	Gamess	I/O
DDT			NWchem	
	MKL			GridFTP
…	GSL	…	…	…
	GotoBLAS			

Intel MKL 10.0 (Math Kernel Library)

- Optimized for the IA32, x86-64, IA64 architectures
- supports both Fortran and C interfaces
- Includes functions in the following areas:
  - BLAS (levels 1-3)
  - LAPACK
  - FFT routines
  - … others
  - Vector Math Library (VML)

Intel MKL 10.0 (Math Kernel Library)

- Enabling MKL
  - module load mkl
  - module help mkl
- Example Compile

```
mpicc -I$TACC_MKL_INC mkl_test.c    -L$TACC_MKL_LIB  -lmkl_<>
mpif90                mkl_test.f90 -L$TACC_MKL_LIB  -lmkl_< >
```

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Code Optimization

- **Always minimize stride length**
  - Stride length 1 is optimal for vectorizable code.
  - This increases cache efficiency, and sets up hardware and software prefetching.
  - Stride lengths of powers of two are typically the worst case scenario leading to cache misses.
- **Strive to write 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…)**

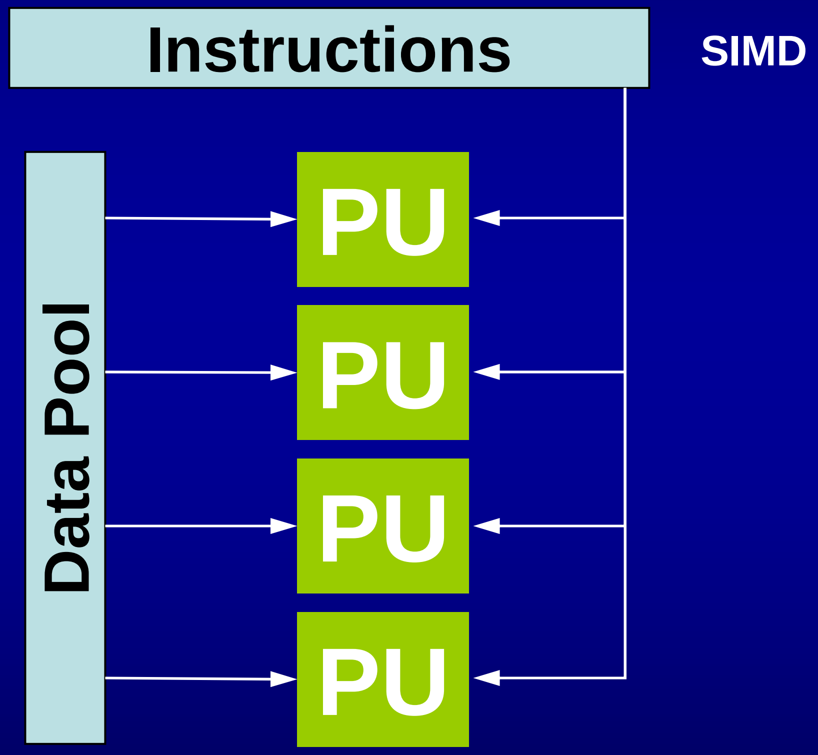
G4/5	**Velocity Engine (SIMD)**
Intel/AMD	**MMX, SSE, SSE2, SSE3 (SIMD)**
Cray	**Vector Units**

4 Code Optimization

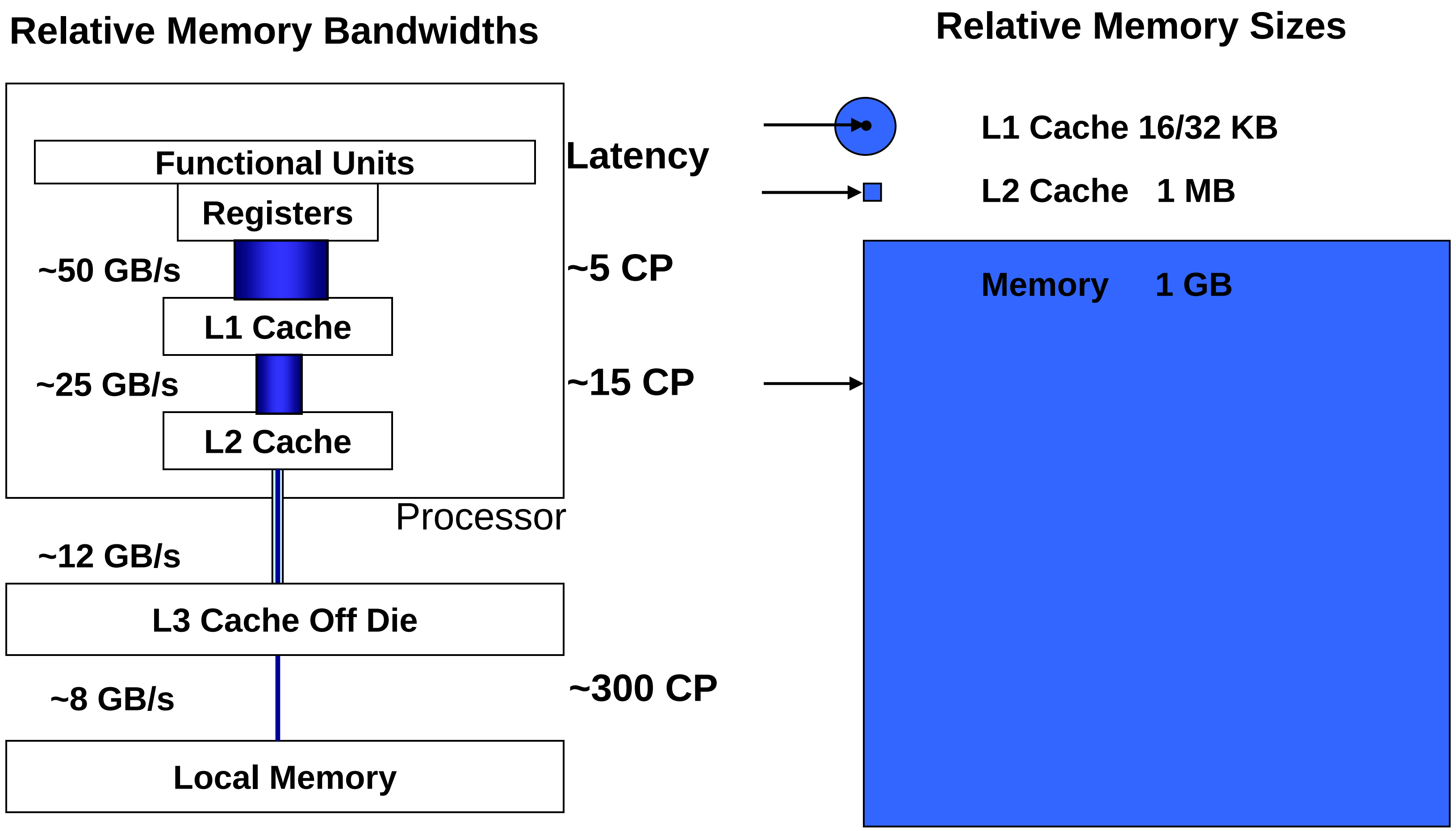
- Write loops with independent iterations, so that SSE instructions can be employed

SIMD (Single Instruction Multiple Data)

SSE (Streaming SIMD Extensions) instructions operate on multiple data arguments simultaneously



Approx. Memory Bandwidths & Sizes



Code Optimization

When is Inlining important?

- When the function is a hot spot
- When the call-overhead to work ratio is high
- When it can benefit from Interprocedural Optimization

The C inline keyword provides inlining within source.
As you develop “think inlining”.
Use –ip or –ipo to allow the compiler to inline.

Code Optimization

Example: procedure inlining

```
program MAIN
integer :: ndim=2, niter=10000000
real*8  :: x(ndim), x0(ndim), r
integer :: i, j
   ...
   do i=1,100000
      ...
      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
```

function dist is called *niter* times

```
program MAIN
integer, parameter :: ndim=2
real*8  :: x(ndim), x0(ndim), r
integer :: i, j
   ...
   do i=1,100000
      ...
      r=0.0
     do j=1,ndim
        r=r+(x(j)-x0(j))**2
     end do
      ...
   end do
   ...
end program
```

function *dist* is expanded inline inside loop

Loop j is called *niter* times

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Code Optimization

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

```
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];
   }
}
```

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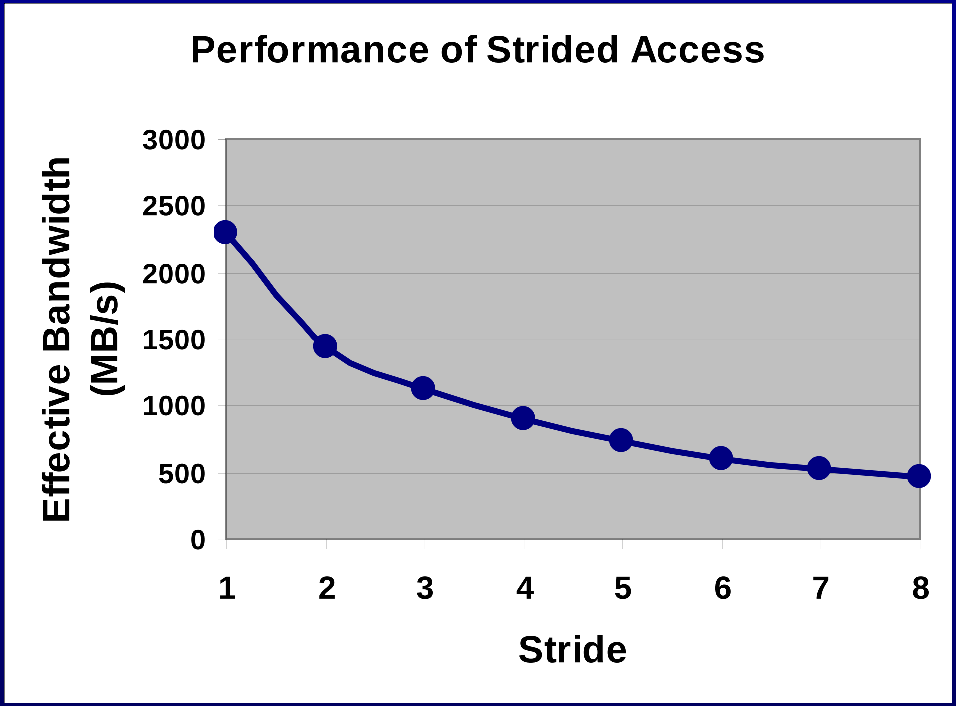
Code Optimization

- Also, 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
```



Code Optimization

Loop interchange can help in the case of a DAXPY loop :

```
integer,parameter::nkb=16,kb=1024,n=nkb*kb/8
real*8           :: x(n), a(n,n), y(n)
...
do i=1,n
   s=0.0
   do j=1,n
      s=s+a(i,j)*x(j)
   end do
   y(i)=s
end do
```

```
integer, parameter :: nkb=16,kb=1024, n=nkb*kb/8
Real*8 :: x(n), a(n,n), y(n)
...
do j=1,n
  do i=1,n
    y(i)=y(i)+a(i,j)*x(j)
  end do
end do
```

Code Optimization

Array Blocking

The objective of array blocking is to work with small array blocks when expressions contain mixed-stride operations. It uses complete cache lines when they are brought in from memory, and hence avoid possible eviction that would otherwise ensue without blocking.

```
do i=1,n
do j=1,n
 A(j,i)=B(i,j)
end do
end do
```

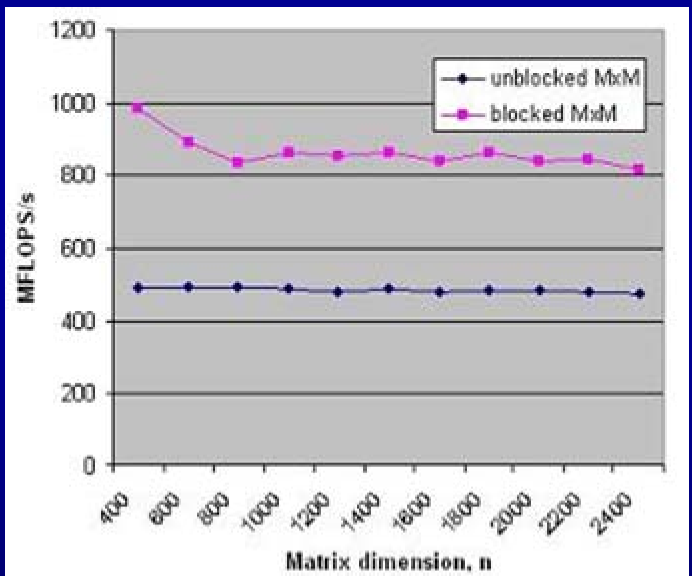
→

```
do i=1,n,2
do j=1,n,2
 A(j  ,i  )=B(i  ,j  )
 A(j+1,i  )=B(i+1,j  )
 A(j  ,i+1)=B(i  ,j+1)
 A(j+1,i+1)=B(i+1,j+1)
end do
end do
```

Code Optimization

Array Blocking

matrix multiplication



results from old system

```
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(j,k)*b(k,i)
```

nb x nb **nb x nb** **nb x nb** **nb x nb**

```
end do; end do; end do; end do; end do; end do
```

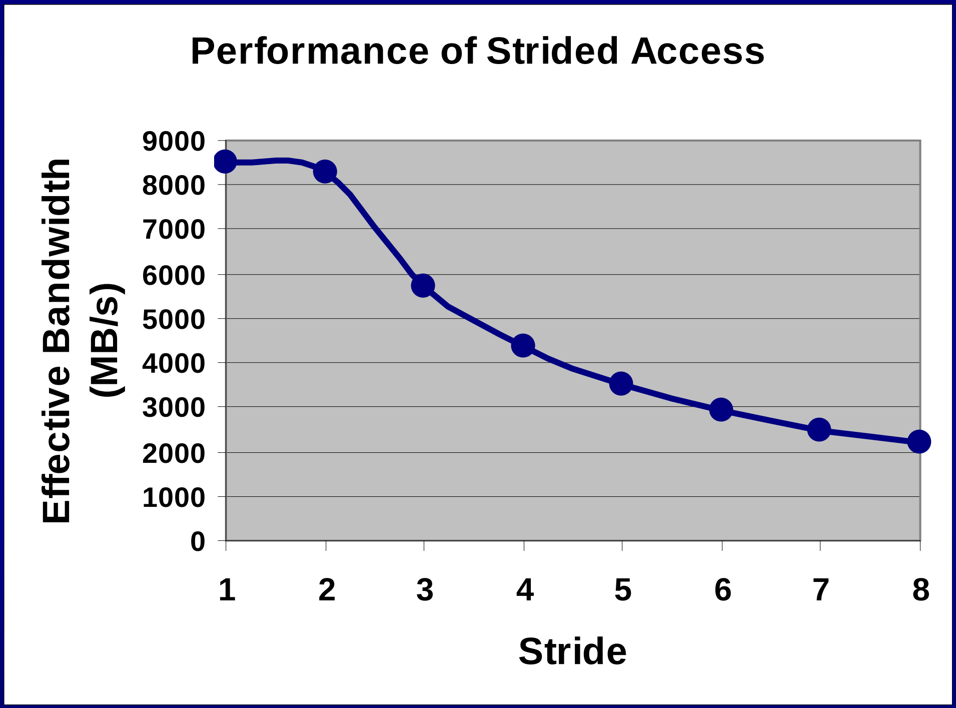
Much more efficient implementations exist, in HPC scientific libraries (ESSL, MKL, ACML,…).

Code Optimization

Even low-stride is effective when accessing data in cache.

```
Bandwidth Performance Code
(assume data is in cache):

do i = 1,50000,istride
sum = sum + data( i )
end do
```



Code Optimization

In some cases, an entire loop can be replaced with a single call to a vector function. For example, the loop below can be written as a call to vdInvSqrt in the Intel VML:

```
for (i=0;i<n;i++) {
   y[i]=1.0/sqrt(x[i]);
}
```
→
```
vdInvSqrt(n,x,y);
```

```
for (i=0;i<n;i++) {
   y[i]=a*sin(x[i]) + b*cos(x[i]);
}
```
→
```
vdSinCos(n,x,s,c);
for (i=0;i<n;i++) {
   y[i]=a*s[i] + b*c[i]);
}
```

But, how do you make something like this portable?
-- "ifdef", in C and F90.

Code Optimization

#IFDEF example

```
program main
integer, Parameter :: n=100, nn=2*n, nap=nn*(nn+1)/2
real(8), Parameter :: xmax=20.0, xmin=-xmax

#ifdef _IBM
                   integer            :: iopt=20
                   integer, parameter :: naux=3*nn
                   real(8):: ap(nap), eval(nn), work(naux)
#elif defined _IA32
                   integer            :: info
                   real(8) ::ap(nap), eval(nn), work(3*nn)
#endif
...
#ifdef _IA32
                   call DSPEV('n','u',nn,ap,eval,evec,nn,work,info)
#elif defined _IBM
                   call DSPEV(iopt,ap,eval,evec,nn,nn,work,naux)
#endif
...
end program
```

Code Optimization

Loop fusion:

Loop fusion combines two or more loops of the same iteration space (loop length) into a single loop:

```
for (i=0;i<n;i++){
   a[i]=x[i]+y[i];
}
for (i=0;i<n;i++){
   b[i]=1.0/x[i]+z[i];
}
```

→

```
for (i=0;i<n;i++){
   a[i]=    x[i]+y[i];
   b[i]=1.0/x[i]+z[i];
}
```

Costly (at least 30 CP)

Only n memory accesses for X array.
Five streams created.
Division many not be pipelined!

Code Optimization

Loop Fission:

The opposite of loop fusion is loop distribution or fission. Fission splits a single loop with independent operations into multiple loops:

```
do i=1,n
  a(i)=b(i)+c(i)*d(i)
  e(i)=f(i)-g(i)*h(i)+p(i)
  q(i)=r(i)+s(i)
end do
```

```
do i=1,n
  a(i)=b(i)+c(i)*d(i)
end do

do i=1,n
  e(i)=f(i)-g(i)*h(i)+p(i)
end do

do i=1,n
  q(i)=r(i)+s(i)
end do
```

References

- Books

  High Performance Computing by Kevin Dowd and Charles Severance (O'Reilly book) -- general study of high performance computing

  Performance Optimization of Numerically Intensive Codes by Stefan Goedecker and Adolfy Hoisie (Siam book, Society for Industrial and Applied Mathematics)

- TACC User Guides

  www.tacc.utexas.edu/services/userguides/ranger/
  www.tacc.utexas.edu/services/userguides/lonestar/

- Compilers

  www.intel.com/cd/software/products/asmo-na/eng/compilers/278607.htm
  www.intel.com/cd/software/products/asmo-na/eng/compilers/279831.htm
  www.pgroup.com/doc/pgiug.pdf

- Optimization

  http://cache-www.intel.com/cd/00/00/21/92/219281_compiler_optimization.pdf

References

- Libraries

  GotoBLAS www.tacc.utexas.edu/resources/software/

  Dense and band matrix software (**ScaLAPACK**)

  www.netlib.org/scalapack

  Large sparse eigenvalue software (**PARPACK** and **ARPACK**)

  www.caam.rice.edu/software/ARPACK/