Performance Optimization of Scientific Applications

Philip J. Mucci

mucci@cs.utk.edu

Innovative Computing Laboratory,

UTK Knoxville, TN

PDC, KTH, Stockholm, Sweden

Outline

- Introduction
- Important Facts about RISC Architecture
- Performance Metrics and Issues
- Compiler Technology
- Serial Code Optimization
- MPI/OpenMP Optimization
- Numerical Libraries
- Performance Analysis Tools

Introduction

Performance

- What is performance?
  - Latency
  - Bandwidth
  - Efficiency
  - Scalability
  - Execution time
- At what cost?

Performance Examples

- Operation Weather Forecasting Model
  - Scalability
- Database search engine
  - Latency
- Image processing system
  - Throughput

What is Optimization?

- Finding **hot spots** *&* **bottlenecks (profiling)**
  - Code in the program that uses a *disproportional* amount of *time*
  - Code in the program that uses system resources *inefficiently*
- Reducing **wall clock** time
- Reducing resource requirements

Types of Optimization

- Hand-tuning
- Preprocessor
- Compiler
- Parallelization

Steps of Optimization

- Integrate libraries
- Optimize compiler switches
- Profile
- Optimize blocks of code that dominate execution time
- Always examine correctness at every stage!

Performance Strategies

- Always use optimal or near optimal algorithms.
  - Be careful of resource requirements and problem sizes.
- Maintain realistic and consistent input data sets/sizes during optimization.
- Know when to stop.

The 80/20 Rule

- Program spends 80 % time in 20 % of its code
- Programmer spends 20 % effort to get 80 % of the total speedup possible in the code.

  "The Law of Diminishing Returns"

How high is up?

- Profiling reveals percentages of time spent in CPU and I/O bound functions.
- Correlation with representative low-level, kernel and application benchmarks.
- Literature search.
- Peak speed of CPU means little in relation to most codes.
- Example: ISIS solver package

Don't Sweat the Small Stuff

- Make the Common Case Fast (Hennessey)

PROCEDURE	TIME
`main()`	13%
`procedure1()`	17%
`procedure2()`	20%
`procedure3()`	50%

- A 20% decrease of `procedure3()` results in 10% increase in performance.
- A 20% decrease of `main()` results in 2.6% increase in performance

Considerations when Optimizing

- Machine configuration, libraries and tools
- Hardware and software overheads
- Alternate algorithms
- CPU/Resource requirements
- Amdahl’s Law
- Communication pattern, load balance and granularity

Important Facts about RISC Architecture

The Pipeline

- Instructions have latencies and bandwidths.
- Important to keep the pipeline full.
  - Avoid step by step dependencies in your code.
    - A -> B
    - B -> C
    - C -> D

The RISC Philosophy

- Reduced Instruction Set Architecture
- We can:
  - Design, place and route more elegantly.
  - Drive a higher clock rate
  - Have a deeper pipeline.
  - Expose opportunities for instruction parallelism to the compiler.
- Guess what? Your Pentium is a RISC.
  - CISC translated to RISC “micro-ops”.

The RISC Philosophy

- Reduced Instruction Set Architecture
- If we:
  - Keep the number of instructions small.
  - Keep the functionality of the instructions orthogonal.
  - Keep the instructions isolated to one piece of hardware on chip.

Cache Architecture

- Small high-speed memories with block access
- Divided into smaller units of transfer called lines
- Address indicates
  - Page number
  - Cache line
  - Byte offset

Caches exploit Locality

Spatial - If location X is being accessed, it is likely that a location *near* X will be accessed *soon.*

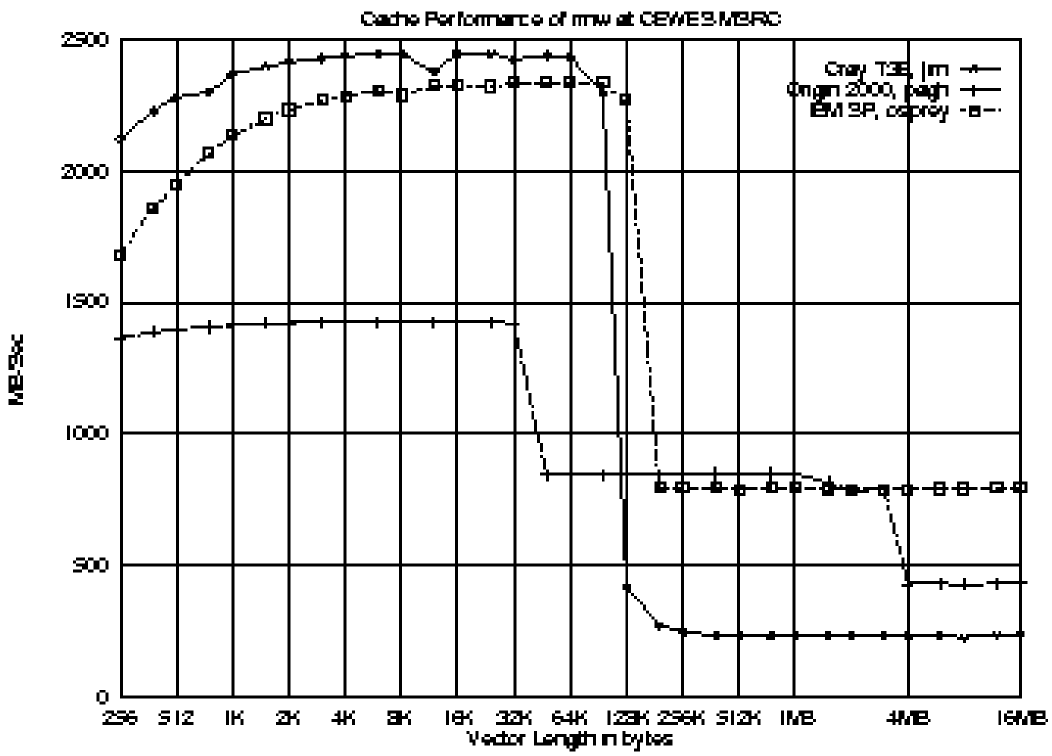
Temporal - If location X is being accessed, it is likely that X will be accessed again *soon.*

Cache Benchmark

http://www.cs.utk.edu/~mucci/cachebench

```
do i = 1,max_length
  start_time
  do j = 1,max_iterations
    do k = 1,i
      A(k) = i
    enddo
  enddo
  stop_time_and_print
enddo
```

Cache Performance



Cache Mapping

- Two major types of mapping
  - Direct Mapped

    Each memory address resides in only one cache line. (constant hit time)
  - N-way Set Associative

    Each memory address resides in one of N cache lines. (variable hit time)
  - Origin is 2-way set associative, 2-way interleaved

2 way Set Associative Cache

*distinct lines = size / line size * associativity*

Line0 Set0	Line1 Set0	Line2 Set0	Line3 Set0
Line0 Set1	Line1 Set1	Line2 Set1	Line3 Set1

Every datum can live in any set

but in only 1 line (computed from its address)

Which class? Least Recently Used

The Register Set

- Register access is almost free.
- Can be considered a level 0 cache.
- # of registers is also limited.
- Many processors contain virtual registers that get renamed to physical registers at execution time.

What is a TLB?

- Fully associative cache of virtual to physical address mappings. Used if data not in cache.
- Number is limited on many systems, usually much less than physical memory.

Contention for Shared Resources

- Most SMP's these days have fewer memory buses than processors.
- Most SMP's share some level of cache.
- Interconnect is also shared among processes.

Performance Metrics and Issues

Performance Metrics

- **Wall Clock** time - Time from start to finish of our program
- MFLOPS - Millions of floating point operations per second
- MIPS - Millions of instructions per second
- Possibly ignore set-up cost

What about MFLOPS?

- Poor measures of comparison because
  - They are dependent on the definition, instruction set and the compiler
- Ok measures of numerical *kernel* performance for a single CPU

EXECUTION TIME

What do we use for evaluation

- For purposes of optimization, we are interested in:
  - Execution time of our code over a range of data sets
  - MFLOPS of our kernel code vs. peak in order to determine *EFFICIENCY*
  - Hardware resources dominating our execution time

Performance Metrics

For the purposes of comparing your codes performance among different architectures **base your comparison on time.**

…*Unless* you are completely aware of all the issues in performance analysis including architecture, instruction sets, compiler technology etc...

Fallacies

- *MIPS is an accurate measure for comparing performance among computers.*
- *MFLOPS is a consistent and useful measure of performance among computers.*
- *Synthetic benchmarks predict performance for real programs.*
- *Peak performance tracks observed performance.*

(Hennessey and Patterson)

Basis for Performance Analysis

- Our evaluation will be based upon:
  - Performance of a single machine on a
  - Single (*optimal*) algorithm using
  - Execution time
- Optimizations are portable

Asymptotic Analysis

- Algorithm X requires O(N log N) time on O(N processors)
- This ignores constants and lower order terms!

$$10N > N \log N \text{ for } N < 1024$$

$$10N*N < 1000N \log N \text{ for } N < 996$$

Amdahl's Law

- The performance improvement is limited by the fraction of time the faster mode can be used.

$$Speedup = Perf.\ enhanced \,/\, Perf.\ standard$$

$$Speedup = Time\ sequential \,/\, Time\ parallel$$

$$Time\ parallel = T_{ser} + T_{par}$$

Amdahl's Law

- Be careful when using speedup as a metric. Ideally, use it only when the code is modified. Be sure to completely analyze and document your environment.
- Problem: This ignores the overhead of parallel reformulation.

Amdahl's Law

- Problem? This ignores scaling of the problem size with number of nodes.
- Ok, what about *Scaled Speedup?*
  - Scale the problem size with the # procs.
  - Results will vary given the nature of the algorithm.
  - Requires O() analysis of communication and run-time operations.

Efficiency

- A measure of code quality?

$$E = \mathit{Time\ sequential} / (P * \mathit{Time\ parallel})$$

$$S = P * E$$

- Sequential time is not a good reference point.

Issues in Performance

- Brute speed (MHz and bus width)
- Cycles per operation (startup + pipelined)
- Number of functional units on chip
- Access to Cache, RAM and storage (local & distributed)

Issues in Performance

- Cache utilization
- Register allocation
- Loop nest optimization
- Instruction scheduling and pipelining
- *Compiler Technology*
- Programming Model (Shared Memory, Message Passing)

Problem Size and Precision

- Necessity
- Density and Locality
- Memory, Communication and Disk I/O
- Numerical representation
  - INTEGER, REAL, REAL*8, REAL*16

Parallel Performance Issues

- *Single node performance*
- Compiler Parallelization
- I/O and Communication
- Mapping Problem - Load Balancing
- Message Passing or Data Parallel Optimizations

What is Optimization?

- Finding **hot spots** *&* **bottlenecks (profiling)**
  - Code in the program that uses a *disproportional* amount of *time*
  - Code in the program that uses system resources *inefficiently*
- Reducing **wall clock** time
- Reducing resource requirements

Types of Optimization

- Hand-tuning
- Preprocessor
- Compiler
- Parallelization

Performance Strategies

- Use profiling tools before you optimize.
- Always use optimal or near optimal algorithms.
  - Be careful of requirements and problem sizes.
- The largest bottleneck first.
- Maintain realistic and consistent input data sets/sizes during optimization.
- Know when to stop.

Considerations when Optimizing

Developer should be familiar with:

- Machine configuration, libraries and tools
- Hardware and Software overheads
- Algorithm and alternatives
- CPU/Resource requirements
- Amdahl's Law
- Communication patterns and load balance

Correctness at Every Step

- Floating point arithmetic is not associative. Which order is correct?
- Think about the following example:

```
sum = 0.0
do i = 1, n
  sum = sum + a(i)
enddo
```

```
sum1 = 0.0
sum2 = 0.0
do i = 1, n-1, 2
  sum1 = sum1 + a(i)
  sum2 = sum2 + a(i+1)
enddo
sum = sum1 + sum2
```

Compiler Technology

Understanding Compilers

- Compilers emphasize correctness rather than performance
- On well recognized constructs, compilers will *usually* do better than the developer
- The idea? To express an algorithm *clearly* to the compiler allows the most optimization.

Compiler Technology

- Ideally, compiler should do most of the work.
- Rarely happens in practice for *real* applications.
- Getting better every day.

Compiler flags

- Many optimizations can be controlled separately from -O<big>
- If possible, it's better to selectively disable optimizations rather than reduce the level of global optimization.

Exceptions

- Numerical computations resulting in undefined results or requiring assistance.
- Exception is generated by the processor.
- Handled in software by the Operating System.
- DENORM's are the worst.

Pointer Aliasing

- The compiler needs to assume that any 2 pointers can point to the same region of memory.
- This removes many optimization opportunities.
- Programmer knows much more about pointer usage than compiler, try to express it with directives.

Advanced Aliasing

- Typed: Only pointers of the same type can point to the same region of memory.
- Restricted: All pointers are assumed to point to non-overlapping regions of memory.
- Disjointed: All pointer expressions are assumed to result in pointers to non-overlapping regions of memory.

Software Pipelining

- Different iterations of a loop are overlapped in time in an attempt to keep all the functional units busy.
- Data needs to be in cache for this to work well.

Interprocedural Analysis

- When analysis is confined to a single procedure, the optimizer is forced to make worst case assumptions about the possible effects.
- IPA analyzes more of the code and feeds that to the other phases.
- Usually, the code is generated at link time.

IPA features

- Inlining across source files
- Common block padding
- Constant propagation
- Dead function/variable elimination
- Library reference optimizations

Inlining

- Replaces a subroutine call with the function itself.
- Useful in loops that have a large iteration count and functions that don't do a lot of work.
- Allows other optimizations.
- Most compilers will do inlining but the decision process is conservative.

Serial Code Optimization

Parallel Performance

"The single most important impediment to good parallel performance is *still* poor single-node performance."

- William Gropp

Argonne National Lab

Guidelines for Performance

- I/O is slow
- System calls are slow
- Use your in-cache data completely
- When looping, remember the pipeline!
  - Branches
  - Function calls
  - Speculation/Out-of-order execution
  - Dependencies

Code Examples

- Many of the examples shown here are canonical.
- In simple benchmarks, modern compilers can optimize them fairly well.
- In a production code, they cannot.
- It is in your best interest, to learn how to write fast (and bug free) code from the beginning.

Array Optimization

- Array Initialization
- Array Padding
- Stride Minimization
- Loop Fusion
- Floating IF's
- Loop Defactorization
- Loop Peeling
- Loop Interchange
- Loop Collapse
- Loop Unrolling
- Loop Unrolling and Sum Reduction
- Outer Loop Unrolling

Array Initialization

- Static initialization requires:
  - Disk space (if non-zero)
  - Demand paging
  - Extra Cache and TLB misses.
- Use only when you have to.
- Really, why use static at all?

Array Initialization

- Static initialization

```
REAL(8) A(100,100) /10000*1.0/
```

- Dynamic initialization

```
DO I=1, DIM1
   DO J=1, DIM2
      A(I,J) = 1.0
```

Memory Access

- Programs should be designed for maximal cache benefit.
  - Stride 1 access patterns
  - Use entire cache lines
  - Reusing data as soon as possible after first reference
- Also, we should minimize page faults and TLB misses.

Array Allocation

- Array's are allocated differently in C and FORTRAN.

1	2	3	4
5	6	7	8
9	10	11	12

C: 1 2 3 4 5 6 7 8 9 10 11 12

Fortran: 1 5 9 2 6 10 3 7 11 4 8 12

Array Referencing

- In C, outer-most index should change fastest.

  [x,**Y**]

- In Fortran, inner-most index should change fastest.

  (**X**,y)

Inter-Array Padding

- Common Block Example: dot product, miss per element on 16KB Direct mapped cache, 4 byte elements

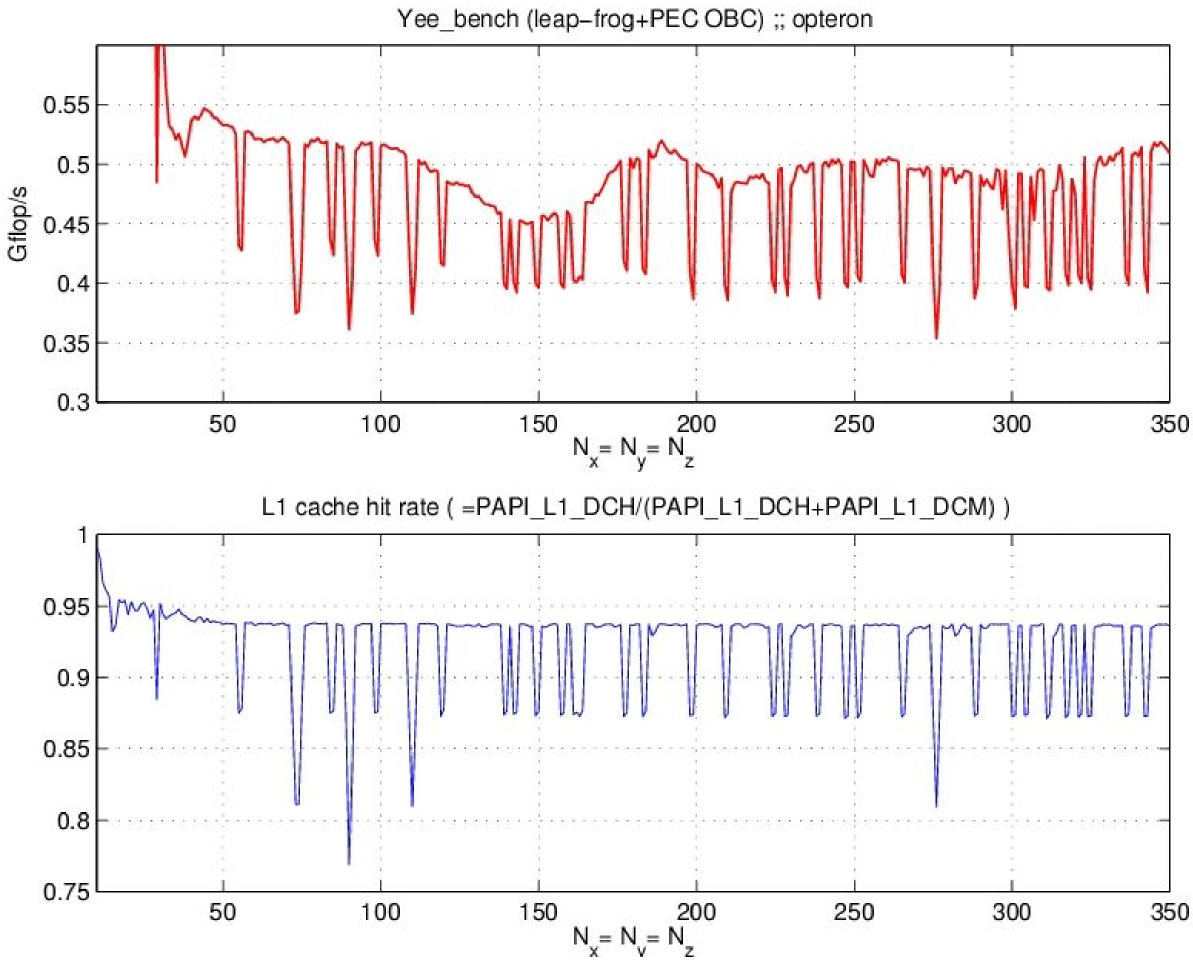
```
common /xyz/ a(2048),b(2048)
common /xyz/ a(2048),pad(16),b(2048)
```

- Allocate is more difficult. Requires allocating additional space and starting from different offset.

Inter-Array Padding

- Data is often allocated in physically contiguous memory and on a page boundary.
- Look for data structures whose size is a powers of two
- Know the associativity of your cache.
- Watch for performance anomalies.

Inter-Array Padding



Inter-Array Padding

*a = a + b * c*

	Tuned	Untuned	Tuned -O3	Untuned -O3
Origin 2000	1064.1	1094.7	800.9	900.3

Intra-Array Padding

- Often required by matrix operations when striding across each dimension.
- C: **Trailing** dimension of a power of two is often a bad choice.
- Fortran: **Leading** dimension of a power of two is often a bad choice.
- This depends on the degree of associativity of the cache.

Intra-Array Padding DGEMM

	Tuned	Untuned
Xeon	2.8	3.3

Stride Minimization

- We must think about spatial locality.
- Effective usage of the cache provides us with the best possibility for a performance gain.
- *Recently* accessed data are likely to be faster to access.
- Tune your algorithm to minimize stride, *innermost index changes fastest*.

Stride Minimization

- Stride 1

```
do y = 1, 1000
  do x = 1, 1000
     c(x,y) = c(x,y) + a(x,y)*b(x,y)
```

- Stride 1000

```
do y = 1, 1000
  do x = 1, 1000
     c(y,x) = c(y,x) + a(y,x)*b(y,x)
```

Stride Minimization

	Untuned -O3	Tuned -O3
Origin 2000	67.24	23.27
IBM SP2	201.07	17.54
Cray T3E	37.61	37.66

Loop Fusion

- Loop overhead reduced
- Better instruction overlap
- Lower cache misses
- Be aware of associativity issues with array’s mapping to the same cache line.

Loop Fusion

- Untuned

```
do i = 1, 50000
  x = x * a(i) + b(i)
enddo
do i = 1, 100000
  y = y + a(i) / b(i)
enddo
```

- Tuned

```
do i = 1, 50000
  x = x * a(i) + b(i)
  y = y + a(i) / b(i)
enddo
do i = 50001, 100000
  y = y + a(i) / b(i)
enddo
```

Loop Fusion

	Untuned -O3	Tuned -O3
Origin 2000	276.37	191.06
IBM SP2	254.96	202.76
Cray T3E	1405.52	1145.91

Loop Interchange

- Swapping the nested order of loops
  - Minimize stride
  - Reduce loop overhead where inner loop counts are small
  - Allows better compiler scheduling

Loop Interchange

- Untuned

```
real*8 a(2,40,2000)

do i=1, 2000
 do j=1, 40
   do k=1, 2
     a(k,j,i) = a(k,j,i)*1.01
   enddo
 enddo
enddo
```

- Tuned

```
real*8 a(2000,40,2)

do i=1, 2
 do j=1, 40
   do k=1, 2000
     a(k,j,i) = a(k,j,i)*1.01
   enddo
 enddo
enddo
```

Loop Interchange

	Untuned -O3	Tuned -O3
Origin 2000	73.85	55.23
IBM SP2	432.39	434.15
Cray T3E	241.85	241.80

Floating IF’s

- IF statements that do not change from iteration to iteration may be moved out of the loop.
- Compilers can usually do this except when
  - Loops contain calls to procedures
  - Variable bounded loops
  - Complex loops

Floating IF's

- Untuned

```
do i = 1, lda
  do j = 1, lda
    if (a(i) .GT. 100) then
      b(i) = a(i) - 3.7
    endif
      x = x + a(j) + b(i)
  enddo
enddo
```

- Tuned

```
do i = 1, lda
  if (a(i) .GT. 100) then
    b(i) = a(i) - 3.7
  endif
  do j = 1, lda
     x = x + a(j) + b(i)
  enddo
enddo
```

Floating IF's

	Untuned –O3	Tuned –O3
Origin 2000	203.18	94.11
IBM SP2	80.56	80.77
Cray T3E	160.86	161.21

Loop Defactorization

- Loops involving multiplication by a *constant* in an array.
- Allows better instruction scheduling.
- Facilitates use of multiply-adds.

Gather-Scatter Optimization

- Untuned

```
do i = 1, n
  if (t(I).gt.0.0) then
    a(I)=2.0*b(I-1)
  end if
enddo
```

- Tuned

```
inc = 0
do i = 1, n
  tmp(inc) = i
  if (t(I).gt.0.0) then
    inc = inc + 1
  end if
enddo
do I = 1, inc
  a(tmp(I))=2.0*b((tmp(I)-1)
enddo
```

Gather-Scatter Optimization

- For loops with branches inside loops
- Increases pipelining
- Often, body of the loop is executed on every iteration, thus no savings
- Solution is to split the loop with a temporary array containing indices of elements to be computed with

IF Statements in Loops

- Solution is to unroll the loop
- Move conditional elements into scalars
- Test scalars at the end of the loop body

```
do I = 1, n, 2
  a = t(I)
  b = t(I+1)
  if (a .eq. 0.0)
  end if
  if (b .eq. 0.0)
  end if
end do
```

Loop Defactorization

- Note that floating point operations are not always associative.

$$(A + B) + C \quad != A + (B + C)$$

- Be aware of your precision
- Always verify your results with unoptimized code first!

Loop Defactorization

- Untuned

```
do i = 1, lda
   A(i) = 0.0
   do j = 1, lda
     A(i)=A(i)+B(j)*D(j)*C(i)
   enddo
enddo
```

- Tuned

```
do i = 1, lda
  A(i) = 0.0
  do j = 1, lda
    A(i) = A(i) + B(j) * D(j)
  enddo
  A(i) = A(i) * C(i)
enddo
```

Loop Defactorization

	Tuned -O3	Untuned -O3
Origin 2000	371.95	559.17
IBM SP2	449.03	591.26
Cray T3E	3201.35	3401.61

Loop Peeling

- For loops which access previous elements in arrays.
- Compiler often cannot determine that an item doesn’t need to be loaded every iteration.

Loop Peeling

- Untuned

```
jwrap = lda
do i = 1, lda
  b(i) = (a(i)+a(jwrap))*0.5
  jwrap = i
enddo
```

- Tuned

```
b(1) = (a(1)+a(lda))*0.5
do i = 2, lda
   b(i) = (a(i)+a(i-1))*0.5
enddo
```

Loop Peeling

	Tuned -O3	Untuned -O3
Origin 2000	61.06	63.33
IBM SP2	25.68	40.50
Cray T3E	72.93	90.05

Loop Collapse

- For multi-nested loops in which the entire array is accessed.
- This can reduce loop overhead and improve compiler vectorization.

Loop Collapse

- Untuned

```
do i = 1, lda
   do j = 1, ldb
      do k = 1, ldc
         A(k,j,i) = A(k,j,i) + B(k,j,i) * C(k,j,i)
      enddo
   enddo
enddo
```

Loop Collapse

- Tuned

```
do i = 1, lda*ldb*ldc
   A(i,1,1) = A(i,1,1) + B(i,1,1) * C(i,1,1)
enddo
```

- More Tuned (declarations are 1D)

```
do i = 1, lda*ldb*ldc
   A(i) = A(i) + B(i) * C(i)
enddo
```

Loop Collapse

	Tuned	Tuned –O3	Tuned 2^{nd}	Tuned 2^{nd} –O3
Origin 2000	400.25	143.01	410.58	77.86
IBM SP2	144.75	31.57	144.18	31.54
Cray T3E	394.19	231.44	394.92	229.86

Loop Unrolling

- Data dependence delays can be reduced or eliminated.
- Reduce loop overhead.
- Usually performed well by the compiler or preprocessor.

Loop Unrolling

- Untuned

```
do i = 1, lda
   do j = 1, lda
      do k = 1, 4
         a(j,i) = a(j,i) + b(i,k) * c(j,k)
      enddo
   enddo
enddo
```

Loop Unrolling

- Tuned (4)

```
do i = 1, lda
   do j = 1, lda
      a(j,i) = a(j,i) +  b(i,1) * c(j,1)
      a(j,i) = a(j,i) +  b(i,2) * c(j,2)
      a(j,i) = a(j,i) +  b(i,3) * c(j,3)
      a(j,i) = a(j,i) +  b(i,4) * c(j,4)
   enddo
enddo
```

Loop Unrolling

	Tuned -O3	Untuned -O3
Origin 2000	61.06	63.33
IBM SP2	11.26	12.65
Cray T3E	36.30	24.41

Loop Unrolling and Sum Reductions

- When an operation requires as input the result of the last output.
- Called a Data Dependency.
- Frequently happens with multi-add instruction inside of loops.
- Introduce intermediate sums. Use your registers!

Loop Unrolling and Sum Reductions

- Untuned

```
do i = 1, lda
   do j = 1, lda
      a = a + (b(j) * c(i))
   enddo
enddo
```

Loop Unrolling and Sum Reductions

- Tuned (4)

```
do i = 1, lda
   do j = 1, lda, 4
      a1 = a1 + b(j) * c(i)
      a2 = a2 + b(j+1) * c(i)
      a3 = a3 + b(j+2) * c(i)
      a4 = a4 + b(j+3) * c(i)
   enddo
enddo
aa = a1 + a2 +a3 + a4
```

Loop Unrolling and Sum Reductions

	Untuned –O3	2 Tuned	2 Tuned –O3	4 Tuned -O3	8 Tuned -O3	16 Tuned -O3
Origin 2000	454	4945	352	350	350	**330**
IBM SP2	281	6490	563	281	281	**263**
Cray T3E	865	10064	564	340	**231**	860

Outer Loop Unrolling

- For nested loops, unrolling outer loop may reduce loads and stores in the inner loop.
- Compiler may perform this optimization.

Outer Loop Unrolling

- Untuned
  - Each flop requires two loads and one store.

```
do i = 1, lda
   do j = 1, ldb
      A(i,j) = B(i,j) * C(j)
   enddo
enddo
```

Outer Loop Unrolling

- Tuned
  - Each flop requires 5/4 loads and one store.

```
do i = 1, lda, 4
   do j = 1, ldb
      A(i,j)   = B(i,j) * C(j)
      A(i+1,j) = B(i+1,j) * C(j)
      A(i+2,j) = B(i+2,j) * C(j)
      A(i+3,j) = B(i+3,j) * C(j)
   enddo
enddo
```

Outer Loop Unrolling

	Tuned -O3	Untuned -O3
Origin 2000	28.85	34.52
IBM SP2	74.67	286.11
Cray T3E	14.33	30.91

Cache Blocking

- Takes advantage of the cache by working with smaller tiles of data
- Only really beneficial on problems with significant potential for reuse
- Merges naturally with unrolling and sum-reduction

Cache Blocking

- Untuned

```
REAL*8 A(M,N)
REAL*8 B(N,P)
REAL*8 C(M,P)

DO J=1,P
 DO I=1,M
  DO K=1,N
    C(I,P) = C(I,P) +
    A(I,K)*B(K,J)
  ENDDO
 ENDDO
ENDDO
```

- Tuned

```
DO JB=1,P,16
 DO IB=1,M,16
  DO KB=1,N
   DO J=JB,MIN(P,JB+15)
    DO I=IB,MIN(M,IB+15)
      C(I,P) = C(I,P) +
      A(I,K)*B(K,J)
     ENDDO
    ENDDO
   ENDDO
  ENDDO
 ENDDO
ENDDO
```

Indirect Addressing

```
XX(I) = XX(I) * Y(A(I))
```

- One of the most difficult constructs to optimize.
- Consider using a sparse solver package.
- Otherwise, consider doing blocks of operations. Instead of sparse degree 1, use blocked sparse format with prefetching.
- Redundant computations are ok.

Loop structure

- IF/GOTO and WHILE loops inhibit some compiler optimizations.
- Some optimizers and preprocessors can perform transforms.
- DO and for() loops are the most highly tuned.

Strength Reduction

- Reduce cost of mathematical operation with no loss in precision, compiler might do it.
  - Integer multiplication/division by a constant with shift/adds
  - Exponentiation by multiplication
  - Factorization and Horner's Rule
  - Floating point division by inverse multiplication

Strength Reduction
Horner's Rule

- Polynomial expression can be rewritten as a nested factorization.

```
Ax^5 + Bx^4 + Cx^3 + Dx^2 + Ex + F =
((((Ax + B) * x + C) * x + D) * x + E) * x + F.
```

- Also uses multiply-add instructions
- Eases dependency analysis

Strength Reduction
Horner's Rule

	Tuned -O3	Untuned -O3
Origin 2000	74.20	74.09
IBM SP2	40.69	74.71
Cray T3E	61.70	160.05

Strength Reduction
Integer Division by a Power of 2

- Shift requires less cycles than division.
- Both dividend and divisor must both be unsigned or positive integers.
- Divides are often costly.
  - Consider also multiplying times the inverse.

Strength Reduction
Integer division by a Power of 2

- Untuned

```
IL = 0
DO I=1,ARRAY_SIZE
  DO J=1,ARRAY_SIZE
    IL = IL + A(J)/2
  ENDDO
  ILL(I) = IL
ENDDO
```

- Tuned

```
IL = 0
ILL = 0
DO I=1,ARRAY_SIZE
  DO J=1,ARRAY_SIZE
    IL = IL + ISHFT(A(J),-1)
  ENDDO
  ILL(I) = IL
ENDDO
```

Strength Reduction

Integer division by a Power of 2

	Tuned -O3	Untuned -O3
Origin 2000	210.71	336.44
IBM SP2	422.65	494.05
Cray T3E	771.28	844.17

Strength Reduction
Factorization

- Allows for better instruction scheduling.
- Compiler can interleave loads and ALU operations.
- Especially benefits compilers able to do software pipelining.

Strength Reduction
Factorization

- Untuned

```
XX = X*A(I) + X*B(I) + X*C(I) + X*D(I)
```

- Tuned

```
XX = X*(A(I) + B(I) + C(I) + D(I))
```

Strength Reduction
Factorization

	Tuned -O3	Untuned -O3
Origin 2000	51.65	48.99
IBM SP2	57.43	57.40
Cray T3E	387.77	443.45

Subexpression Elimination
Parenthesis

- Parenthesis can help the compiler recognize repeated expressions.
- Some preprocessors and aggressive compilers will do it.
- Might limit aggressive optimizations

Subexpression Elimination
Parenthesis

- Untuned

```
XX = XX + X(I)*Y(I)+Z(I) + X(I)*Y(I)-Z(I) + X(I)*Y
   (I) + Z(I)
```

- Tuned

```
XX = XX + (X(I)*Y(I)+Z(I)) + X(I)*Y(I)-Z(I) + (X
   (I)*Y(I)+Z(I))
```

Subexpression Elimination
Type Considerations

- Changes the type or precision of data.
  - Reduces resource requirements.
  - Avoid type conversions.
  - Processor specific performance.
- Do you really need 8 or 16 bytes of precision?

Subexpression Elimination
Type Considerations

- Consider which elements are used together?
  - Should you be merging your arrays?
  - Should you be splitting your loops for better locality?
  - For C, are your structures packed tightly in terms of storage and reference pattern?

F90 Considerations

- WHERE statements
- ARRAY syntax
- ALLOCATE placement
- OO complication
  - Class dependencies
  - Code fragmentation
  - Operator overloading
  - Inlining

F90 WHERE

- This construct is basically a masking operator for array operations.
- It results in an IF statement for every operation.
- Consider copying to temporary and then multiplying by mask array.

F90 ARRAY

- Be aware that specifying sections of arrays often implies a copy.
- Often this is done more than once in your code.
- Consider doing it yourself and saving the result for reuse.

F90 ALLOCATE

- Recent experiments have shown that ALLOCATE often returns data on a page boundary.
- Very dangerous for caches with low associativity.

C/C++ Considerations

- Use STL and the C++ operators.
- Dynamic typing and polymorphism isn't free.
- Use `inline`, `const` and `restrict` keywords.
- Easy to become memory/pointer bound with operator overloading.
- OO complication as before.

STL and C++

- The goal of STL is to export more of the author's intent to the compiler.
- Many classes run much faster than handwritten code in applications
  - Strong typing
  - The compiler can tell what you're doing vs. just making a function call on a pointer.

Parallel Optimization

Parallel Performance

"The single most important impediment to good parallel performance is *still* poor single-node performance."

- William Gropp

Argonne National Lab

What is Good Parallel Performance?

- Single CPU performance is high.
- The code is scalable out to more than a few nodes.
- The network is not the bottleneck.
- In parallel computation, algorithm design is the key to good performance.
- You must reduce the amount of data that needs to be sent around.

Beware The Fallacy Linear Scalability

- But what about per/PE performance?
- With a slow code, overall performance of the code is not vulnerable to other system parameters like communication bandwidth, latency.
- Very common on tightly integrated systems where you can simple add PE's for performance.

Parallel Optimization

- Two programming models.
  - Message Passing
  - Shared Memory

Parallel Performance

- Architecture is characterized by
  - Number of CPU's
  - Connectivity
  - I/O capability
  - Single processor performance

MPP Optimization

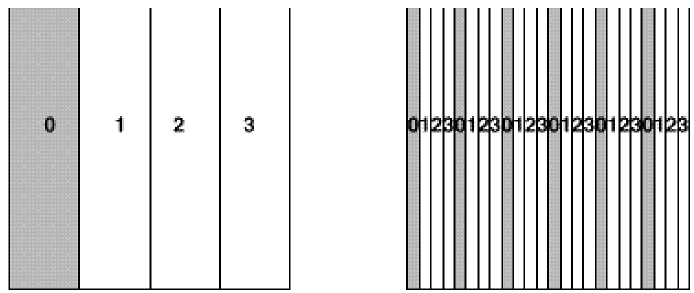
- Programming
  - Message passing (MPI, MPI-2, Shmem)
  - Shared memory (OpenMP directive based)
- Algorithms
  - Data or Functional Parallelism
  - SIMD, MIMD
  - Granularity (fine, medium, coarse)
  - Master/Worker or Hostless

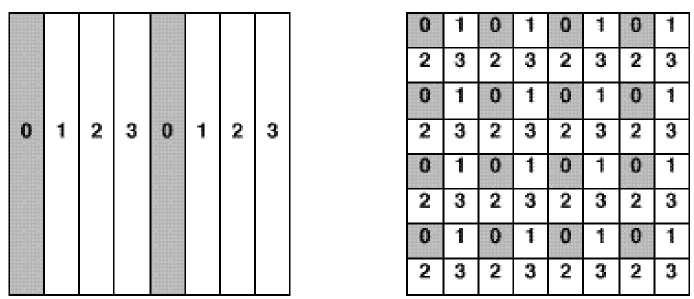
Choosing a Data Distribution

- The main issue in choosing a data layout for dense matrix computations is:
  - **load balance**, or splitting the work reasonably evenly among the processors throughout the algorithm

Possible Data Layouts

- 1D block and cyclic column distributions





- 1D block-cyclic column and 2D block-cyclic distribution used in ScaLAPACK

Two-dimensional Block-Cyclic Distribution

- **Ensure good load balance --> Performance and scalability**,
- Encompasses a large number of (but not all) data distribution schemes,
- Need redistribution routines to go from one distribution to the other.

Load Balancing

- Static
  - Data/tasks are partitioned among existing processors.
  - Problem of finding an efficient mapping
- Dynamic
  - Master/Worker model
  - Synchronization and data distribution problems

Traditional Message Passing

- Node 1 needs X bytes from node 0
- Node 0 calls a send function (X bytes from address A)
- Node 1 calls a receive function (X bytes into address B)

Remote DMA

- Node 1 needs X bytes to addr. A from node 0 at addr. B
- Either:
  - Node 0 sends RDMA PUT (X bytes from addr. A to Node 1 addr. B)
  - Node 1 sends RDMA GET to Node 0 (X bytes from addr. A to Node 1 addr. B)

Memory Window's

- Node 0: Declare comm. region between addr. A and B.
- Node 1: Declare comm. region between addr. C and D.
- Either node issues a PUT or GET.

MPI Optimization

Communication Issues

- Startup time, latency or overhead
- Bandwidth
- Network contention and congestion
- Bidirectionality
- Communication API
- Dedicated Channels

Communication Issues

- Startup time and bandwidth
  - Startup time is higher than the time to actually transfer a *small* message.
  - Send larger messages fewer times, but try to keep everyone busy.
- Contention can be reduced by uniformly distributing messages.

Message Passing Interface

- Provides numerous send/recv modes.
  - Asynchronous
  - One-sided
- Provides optimized collective operations.
- Supports customized data types.
- Is a standard and is highly portable.

Message Passing

- Upon message arrival
  - If node B has not **posted** a receive the data is **buffered** until the receive function is called.
  - Else the data is delivered directly to the address given to the receive function. No copy!
  - The amount of buffering is implementation dependent.

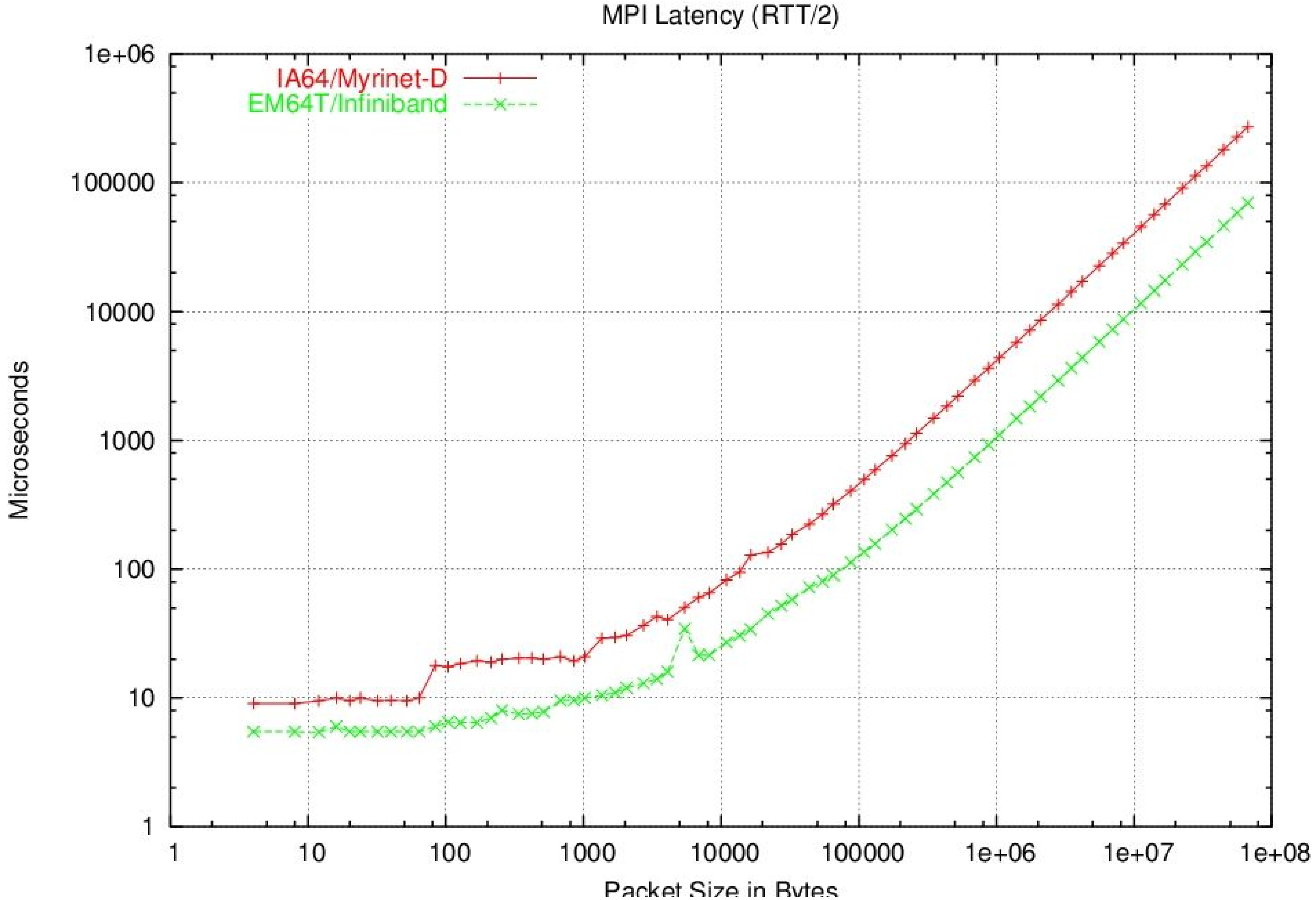
Posting a Receive

- Means that the application has informed the communication layer about a message to be received (soon).
- Matching done in software, not hardware:
  - context, rank and tag.
- User should provide as much information as possible to MPI to reduce matching operation.

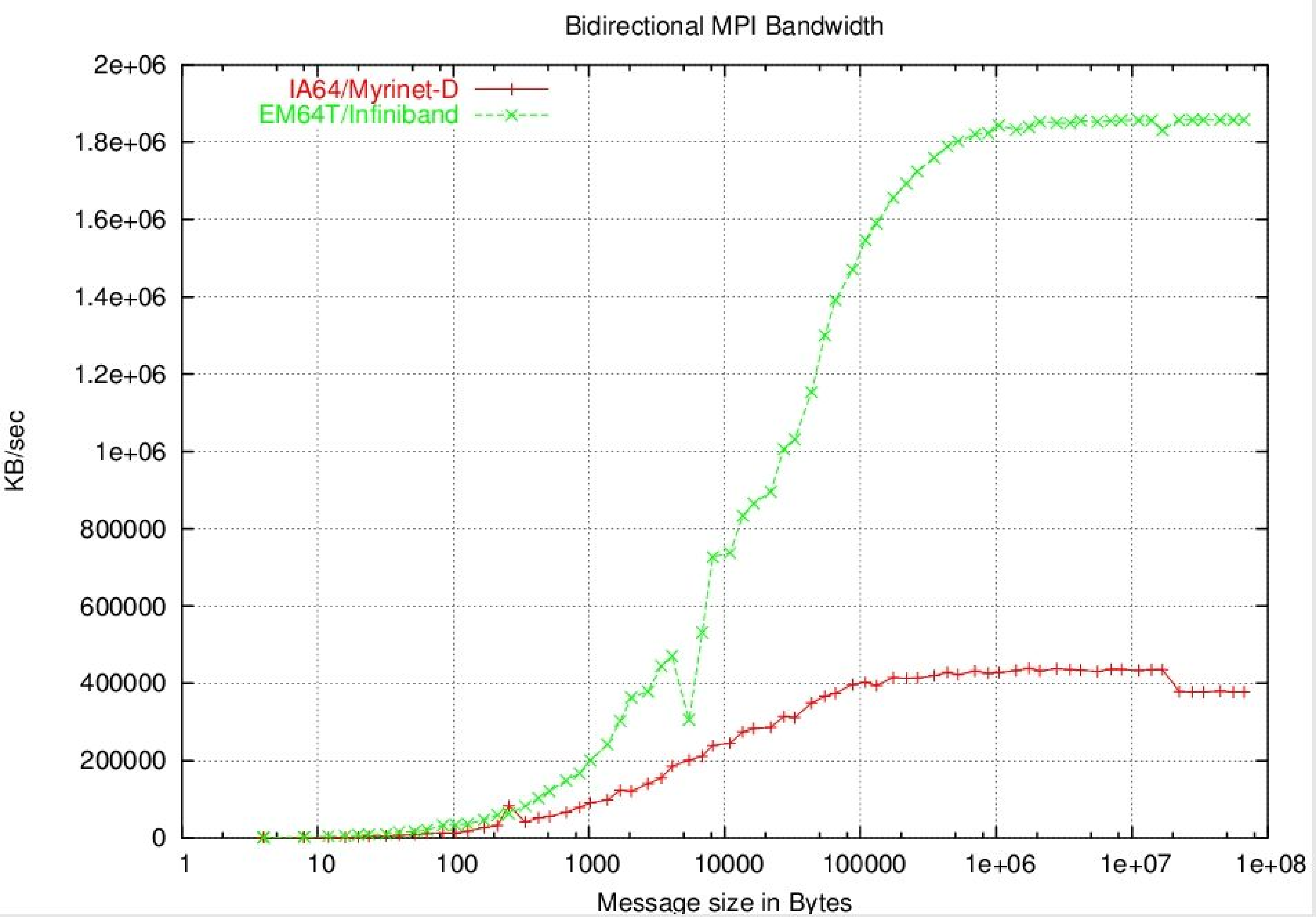
MPI Protocol

- Often 2 or 3 message size ranges.
- Short messages:
  - Send right away, buffer, match and copy at receiver.
- Medium messages.
  - Send first chunk, ask for more space or match, return with dest. addr. or wait.
- Long
  - Send first chunk, return with dest. addr.

MPI Latency Infiniband vs. Myrinet



MPI Bidirectional Bandwidth Infiniband vs. Myrinet



Message Passing

- It is possible for sends and receives to be
  - Nonblocking(send) or Posted(receive)
  - Synchronous(send)
  - Buffered
  - Blocking

Message Passing

Buffering - Temporary storage of data.

Posting - Temporary storage of an address.

Nonblocking - Refers to an function A that initiates an operation B and returns to the caller before the completion of B.

Blocking - The function A does not return to the caller until the completion of operation B.

Polling/Waiting - Testing for the completion of a nonblocking operation.

MPI Message Passing

- MPI introduces communication **modes** dictating semantics of completion of send operations.
  - **B**uffered - When transmitted or buffered, space provided/limited by application, else error.
  - **R**eady - Only if receive is posted, else error.
  - **S**ynchronous - Only when receive begins to execute, else wait. Useful for debugging.

MPI Message Passing

- In addition

  standard - MPI will decide if/how much outgoing data is buffered. If space is unavailable, completion will be delayed until data is transmitted to receiver. (Like PVM)

  Immediate - nonblocking, returns to the caller ASAP. May be used with any of the above modes.

MPI Message Passing

- Ready sends can remove a handshake for large messages.
- There is only one receive mode, it matches any of the send modes.

MPI Optimizations

- We are primarily interested in

  `MPI_ISEND, MPI_IRECV, MPI_IRSEND`

- Why? Because your program could be doing something useful while sending or receiving! You can hide much of the cost of these communication operations.

MPI Message Passing

- To test for the completion of a message use

  `MPI_WAITxxx` and `MPI_TESTxxx`

  where `xxx` is all, any, some or NULL.

- Remember you must test ISEND’s as well as IRECV’s before you can reuse the argument.

MPI Data Types

- For array transfers MPI has user defined data types to gather and scatter data to/from memory.
- Try to use `MPI_TYPE_[H]VECTOR()` or `MPI_TYPE_[H]INDEXED()`
- Avoid `MPI_TYPE_STRUCT()`

MPI Performance Tips

- Send big messages, infrequently.
- Avoid, small frequent messages.
- Think about the actual communication pattern.
  - Use a collective operation.

MPI Performance Tips

- Reduce number of unexpected, unmatched messages.
- Always post receives as early as possible.
- Take advantage of bidirectionality in the communication link.
  - MPI_sendrecv()

MPI Performance Tips

- Avoid data translation and derived data types unless necessary for good performance.
- Avoid wildcard receives.
- Align application buffers to double words and page sizes.

MPI Performance Tips

- Pipeline communication/computation.
  - On most systems, the data can move without CPU intervention.
  - Take advantage of this fact!
  - Avoid constructions like:
    - MPI_IRECV()
    - MPI_ISEND()
    - MPI_WAIT()
  - Here, no useful work is done while waiting!

MPI Collective Communication

- Unlike PVM, with MPI you should use the collective operations. They are likely to be highly tuned for the architecture.
- These operations are very difficult to optimize and are often the bottlenecks in parallel applications.

MPI Collective Communication

```
MPI_Barrier()
MPI_Bcast()
MPI_Gather[v]() MPI_Scatter[v]()
MPI_Allgather[v]()
MPI_Alltoall[v]()
MPI_Reduce()
MPI_AllReduce()
MPI_Reduce_Scatter()
MPI_Scan()
```

Message Passing Optimization
Nearest Neighbor Example 1

N slave processors available plus Master, M particles each having (*x*,*y*,*z*) coordinates.

1) Master reads and distributes all coordinates to N processors.

2) Each processor calculates its subset of M/N and sends it back to the master.

3) Master processor receives and outputs information.

Message Passing Optimization
Nearest Neighbor Example 2

1) Master reads and scatters M/N coordinates to N processors.
2) Each processor receives its own subset and makes a replica.
3) Each processor calculates its subset of M/N coordinates versus the replica.
4) Each processor sends to the next processor its replica of M/N coordinates.
5) Each processor receives the replica. Goto 3) N-1 times.
6) Each processor sends its info back to the Master

Message Passing Optimization
Nearest Neighbor Example

- Example 1 works better only when:
  - There are a small number of particles
  - You have an super efficient broadcast
- Example 2 works better more often because:
  - Computation is pipelined. Note that slave processor 0 is already busy before processor 1 even gets its input data.

OpenMP Optimization

Thread Level Parallelism

- **Data parallelism:** different processors running the same code on different data. (SPMD)
- **Task parallelism** means different processors are running different procedures. (MPMD)

OpenMP

- Designed for quick and easy parallel programming for SMP (and NUMA) machines.
- Insert compiler directives in code that implicitly spawn threads.
- Usually placed around loops but can work for any piece of structured code.
  - One entry, one exit.

OpenMP Data Parallelism

```
  j = 0
c$omp parallel do shared(j),private(i)
  do i=1,n
    j += i
  end do
```

OpenMP Task Parallelism

```
c$omp parallel private(i)
  do i=1,n
   if (i=1) call sub1(...)
   if (i=2) call sub2(...)
   if (i=3) call sub3(...)
   if (i=4) call sub4(...)
  end do
```

Parallel Overhead

- Creating/Scheduling threads
- Communication
- Synchronization
- Partitioning

Parallel Overhead

- For data parallel programming we can estimate some of the parallel overhead.
- Time the code with only one thread
  - OMP_NUM_THREADS environment variable.
- Compare with code compiled without OpenMP turned on.

Reducing Parallel Overhead

- Don’t parallelize ALL the loops.
- Parallelize the big loops.
- Privatize variables where possible
  - Create per thread temporaries with
    - PRIVATE, FIRSTPRIVATE, THREADPRIVATE

Reducing Parallel Overhead

- Use task parallelism.
  - Lower overhead
  - More code runs in parallel
  - Requires a parallel algorithm

Improving Load Balance

- Change the way loop iterations are allocated to threads.
  - Change the scheduling type
  - Change the chunk size

Improving Load Balance

- Scheduling

```
setenv OMP_SCHEDULE <type>
c$omp schedule(<type>)
```

  - STATIC,[<chunk> - default, iterations equally and sequentially allocated per processor.
  - RUNTIME – use the OMP_SCHEDULE environment variable. Default, static.

Improving Load Balance

- Scheduling
  - DYNAMIC,[<chunk>] - iterations are allocated per processor during run-time. When the amount of work is unknown.
  - GUIDED,[<chunk>] - guided self scheduling. Each processor starts with a large number and finishes with a small number.

OpenMP Gotcha's

- False sharing
  - Shared variables that ping-pong between processors cache lines
- Hyperthreading
  - Conflicting over shared resources
  - OMP_NUM_THREADS to physical number of CPU's if doing data-parallel.
- Locking

Automatic Parallelization

- Let the compiler do the work.
- Advantages
  - It’s easy
- Disadvantages
  - Only does loop level parallelism.
  - It wants to parallelize every loop iteration in your code.

Numerical Libraries

Optimized Arithmetic Libraries

- Advantages:
  - Subroutines are quick to code and understand.
  - Routines provide *portability.*
  - Routines perform well.
  - Comprehensive set of routines.
- Disadvantages
  - Can lead to vertical code structure
  - May mask memory performance problems

Think you can do it yourself?

- 512x512 Matrix Multiply
- Naïve (next page)
  - ~200 Mflops (gcc 3.4)
- Advanced (next page)
  - ~1000 Mflops (gcc 3.4)
- ATLAS
  - ~2500 Mflops (gcc 3.4)

```
A(i,j) = A(i,j) + B(i,k) * C(k,j)
```

```
do kb = 1,kk,blk
   ke = min(kb+blk-1,kk)
   do ib = 1,ii,blk
      ie = min(ib+blk-1,ii)
      do i = ib,ie
         do k = kb,ke
            TB(k-kb+1,i-ib+1) = B(i,k)
         end do
      end do
      do jb = 1,jj,blk
         je = min(jb+blk-1,jj)
         do j = jb,je,2
            do i = ib,ie,2
               T1 = 0.0d0
               T2 = 0.0d0
               T3 = 0.0d0
               T4 = 0.0d0
               do k = kb,ke
                  T1 = T1 + TB(k-kb+1,i-ib+1)*C(k,j)
                  T2 = T2 + TB(k-kb+1,i-ib+2)*C(k,j)
                  T3 = T3 + TB(k-kb+1,i-ib+1)*C(k,j+1)
                  T4 = T4 + TB(k-kb+1,i-ib+2)*C(k,j+1)
               enddo
               A(i,j) = A(i,j)+T1
               A(i+1,j) = A(i+1,j)+T2
               A(i,j+1) = A(i,j+1)+T3
               A(i+1,j+1) = A(i+1,j+1)+T4
            enddo
         enddo
      enddo
   enddo
enddo
```

Optimized Arithmetic Libraries

- BLAS: Basic Linear Algebra Subroutines
  - PBLAS: Parallel version
- LAPACK: Linear Algebra Package
  - ScaLAPACK: Parallel version

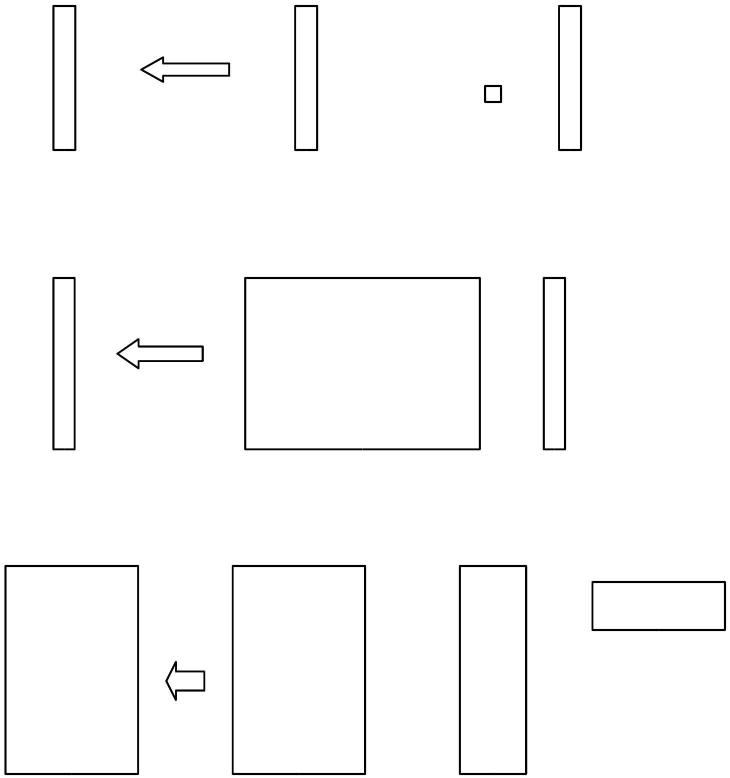
BLAS

- Common Matrix/Matrix, Matrix-Vector, Vector-Vector. REAL/DOUBLE/COMPLEX
- Reference version available from UT.
- Vendor versions offer high performance.
  - MKL on Intel
  - ACML on AMD
- Multithreaded are usually available.

`http://www.netlib.org/blas/index.html`

Level 1, 2 and 3 BLAS

- Level 1 BLAS Vector-Vector operations
- Level 2 BLAS Matrix-Vector operations
- Level 3 BLAS Matrix-Matrix operations



Goto/ATLAS BLAS

- If you don't have a vendor BLAS:
  - K. Goto has hand coded many BLAS routines.
  - Near peak performance
- ATLAS: Automatic Tuned Linear Algebra Software
  - Generates near optimal BLAS and a few LAPACK routines for ANY architecture by brute force.

LAPACK

- F77 routines for solving
  - systems of simultaneous linear equations and eigenvalue problems
  - matrix factorizations (LU, Cholesky, QR, SVD, Schur, generalized Schur)
  - Related computations such as reordering and conditioning.
  - Built on the level 1, 2 3 BLAS Single, Double, Complex, Double Complex

`http://www.netlib.org/lapack/index.html`

LAPACK -- Release 3.0

- Add functionality
  - divide and conquer SVD,
  - error bounds for GLM and LSE,
  - new expert drivers for GSEP,
  - faster QRP,
  - faster solver for the rank-deficient LS (xGELSY),
  - divide and conquer least squares
  - ...

ScaLAPACK Functionality

- Orthogonal/unitary transformation routines
- Prototypes
  - Packed Storage routines for LLT, SEP, GSEP
  - Out-of-Core Linear Solvers for LU, LLT, and QR
  - Matrix Sign Function for Eigenproblems
  - SuperLU and SuperLU_MT
  - HPF Interface to ScaLAPACK

ScaLAPACK Documentation

- Documentation
  - ScaLAPACK Users' Guide
    http://www.netlib.org/scalapack/slug/scalapack_slug.html
  - Installation Guide for ScaLAPACK
  - LAPACK Working Notes
- Test Suites for ScaLAPACK, PBLAS, BLACS
- Example Programs
  http://www.netlib.org/scalapack/examples/
- Prebuilt ScaLAPACK libraries on netlib

Parallelism in ScaLAPACK

- Level 3 BLAS block operations
  - All the reduction routines
- Pipelining
  - QR Algorithm, Triangular Solvers, classic factorizations
- Redundant computations
  - Condition estimators
- Static work assignment
  - Bisection
- Task parallelism
  - Sign function eigenvalue computations
- Divide and Conquer
  - Tridiagonal and band solvers, symmetric eigenvalue problem and Sign function
- Cyclic reduction
  - Reduced system in the band solv

Narrow Band and Tridiagonal Matrices

- The ScaLAPACK routines solving **narrow-band** and **tridiagonal** linear systems assume
  - the narrow band or tridiagonal coefficient matrix to be distributed in a block-column fashion, and
  - the dense matrix of right-hand-side vectors to be distributed in a block-row fashion.
- Divide-and-conquer algorithms have been implemented because they offer greater scope for exploiting parallelism than the corresponding adapted dense algorithms.

PETSc

- Generalized sparse solver package for solution of PDEs.
- Multiple preconditioners and explicit and implicit methods.
- Highly optimized for compressed block storage.
- Serial and Parallel versions.

SuperLU

- LU factorization sparse solver package.
- Highly optimized for compressed block storage.
- Serial and Parallel versions.

FFTW and UHFFT

- 1,2,3D FFT's on a variety of data types.
- Very good performance.
- Serial and Parallel versions.

VSIPL

- Vector Signal Image Processing Library
- Filters
- Stencils
- Convolutions
- Wavelet
- Serial and Parallel versions.

EISPACK

- LAPACK for Eigenvalue problems
- Serial and Parallel versions.

Performance Analysis Tools

Performance Evaluation

- Traditionally, performance evaluation has been somewhat of an art form:
  - Limited set of tools (time & -p/-pg)
  - Major differences between systems
  - Lots of guesswork as to what was 'behind the numbers'
- Today, the situation is different.
  - Hardware support for performance analysis
  - A wide variety of Open Source tools to choose from.

Why Performance Analysis?

- 2 reasons: Economic & Qualitative
- Economic: TIME IS MONEY
  - Average lifetime of these large machines is 4 years before being decommissioned.
  - Consider the cost per day of a 4 Million Dollar machine, with annual maintenance/electricity cost of $300,000 (US). That's $1500.00 (US) per hour of compute time.

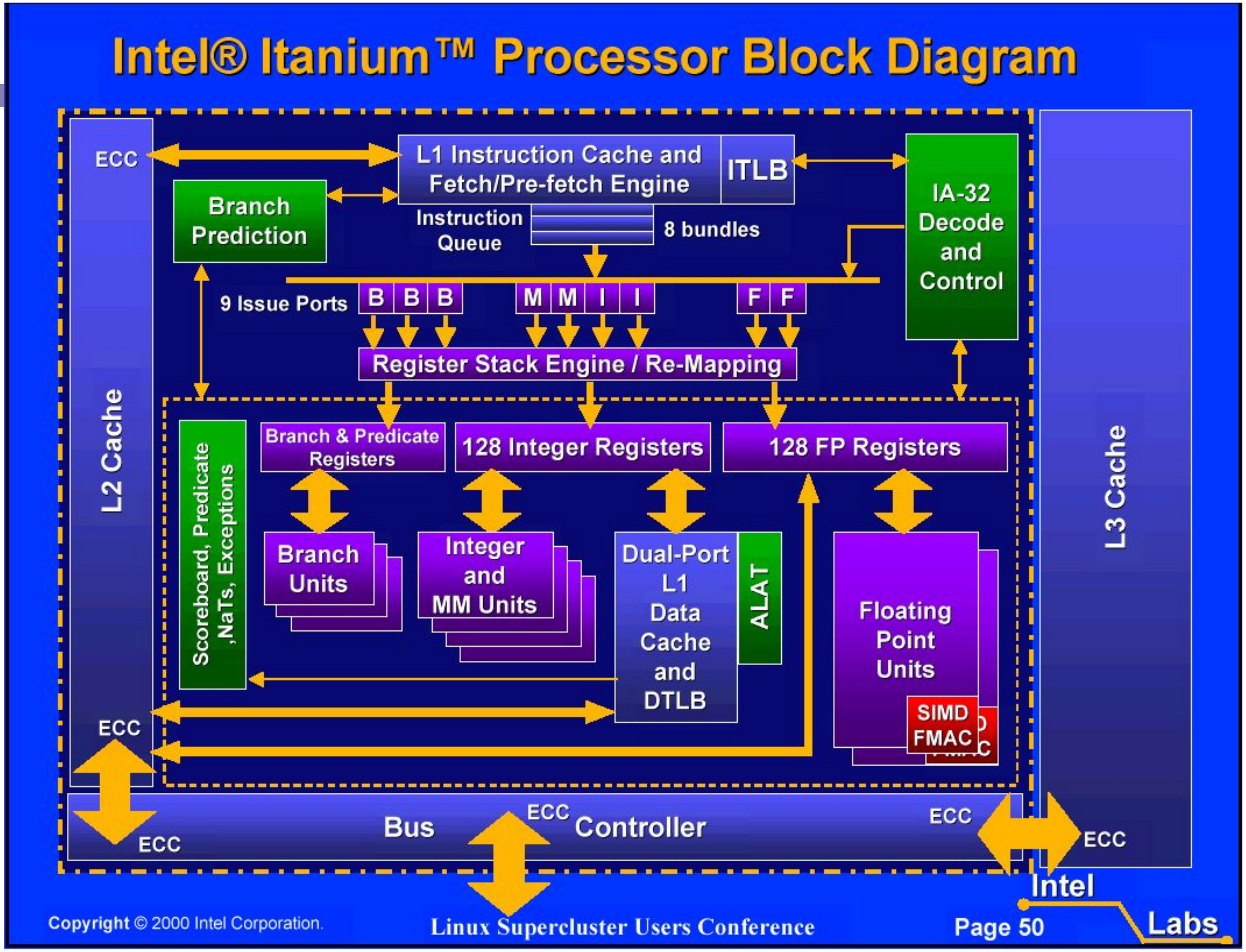
Why Performance Analysis 2?

- Qualitative Improvements in Science
  - Consider: Poorly written code can easily run 10 times worse than an optimized version.
  - Consider a 2-dimension domain decomposition of a Finite Difference formulation simulation.
  - For the same amount of time, the code can do 10 times the work. 400x400 elements vs. 1300x1300 elements
  - Or it can do 400x400 for 10 times more time-steps.

Why Performance Analysis 3?

- So, we must strive to evaluate how our code is running.
- Learn to think of performance during the entire cycle of your design and implementation.

Processor Complexity



Rising Processor Complexity

- No longer can we easily trace the execution of a segment of code.
  - Static/Dynamic Branch Prediction
  - Prefetching
  - Out-of-order scheduling
  - Predication
- So, just a measure of 'wallclock' time is not enough. Need to know what's really happening under the hood.

Direct Measurement Methods

- Instrumentation based
  - Tracing
    - Generate a record for each measured event.
    - Useful only when evidence of performance anomalies is present due to the large volume of data generated.
  - Aggregate
    - Reduce data at run-time avg/min/max measurements.
    - Useful for application and architecture characterization and optimization.

Measurement Methods 2

- Indirect methods requires no instrumentation and can be used on unmodified applications.
- The reality is that the boundary between indirect and direct is somewhat fuzzy.
  - gprof (no source mods, but requires relink or recompile)

Statistical Profiling

- At a defined interval (interrupts), record WHERE in the program the CPU is.
- Data gathered represents a probabilistic distribution in the form of a histogram.
- Interrupts can be based on time or hardware counter events with the proper infrastructure like...

External Timers

- `/usr/bin/time <command>` returns 3 kinds.
  - Real time: Time from start to finish
  - User: CPU time spent executing your code
  - System: CPU time spent executing system calls
- Warning! The definition of CPU time is different on different machines.

External Timers

- Sample output (from Linux)

```
0.56user 0.12system 0:03.80elapsed 18%CPU
  (0avgtext+0avgdata 0maxresident)k
0inputs+0outputs (55major+2684minor)pagefaults
  0swaps
```

1) User
2) System
3) Real
4) Percent of time spent on behalf of this process, not including waiting.
5) Text size, data size, max memory
6) 0 input, 0 output operations
7) Page faults (major, minor), swaps.

Internal Timers

- `gettimeofday()`, part of the C library obtains seconds and microseconds since Jan 1, 1970.
- `second()`, Fortran 90.
- Latency is not the same as resolution.
  - Many calls to this function will affect your wall clock time.

Internal Timers

- `clock_gettime()` for POSIX, usually implemented as `gettimeofday()`.
- `MPI_Wtime`() returns elapsed wall clock time in seconds as a double.

Hardware Performance Counters

- On/off chip registers that count hardware events
- Many different events.
- OS accumulates counts into 64-bit quantities.
- Both user and kernel modes can be measured.
- Explicit counting or statistical histograms based on counter overflow.

Performance Counters

- Most high performance processors include hardware performance counters.
  - AMD Athlon and Opteron
  - Compaq Alpha EV Series
  - CRAY T3E, X1
  - IBM Power Series
  - Intel Itanium, Itanium 2, Pentium
  - SGI MIPS R1xK Series
  - Sun UltraSparc II, III, IV
  - IBM Blue Gene
  - And many others...

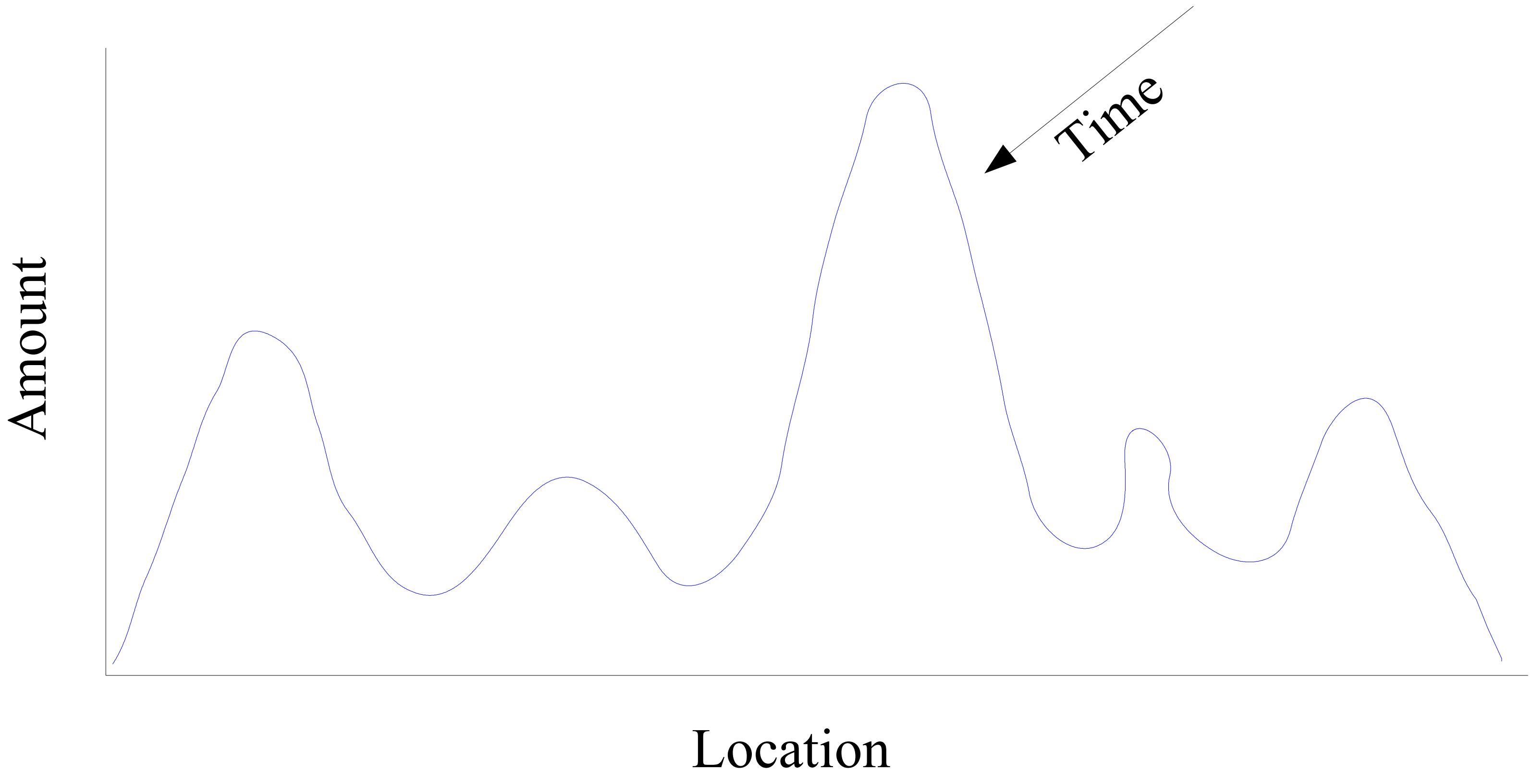
Performance Counters

- Performance Counters are hardware registers dedicated to counting certain types of events within the processor or system.
  - Usually a small number of these registers (2,4,8)
  - Sometimes they can count a lot of events or just a few
  - Symmetric or asymmetric
- Each register has an associated control register that tells it what to count and how to do it.
  - Interrupt on overflow
  - Edge detection (cycles vs. events)
  - User vs. kernel mode

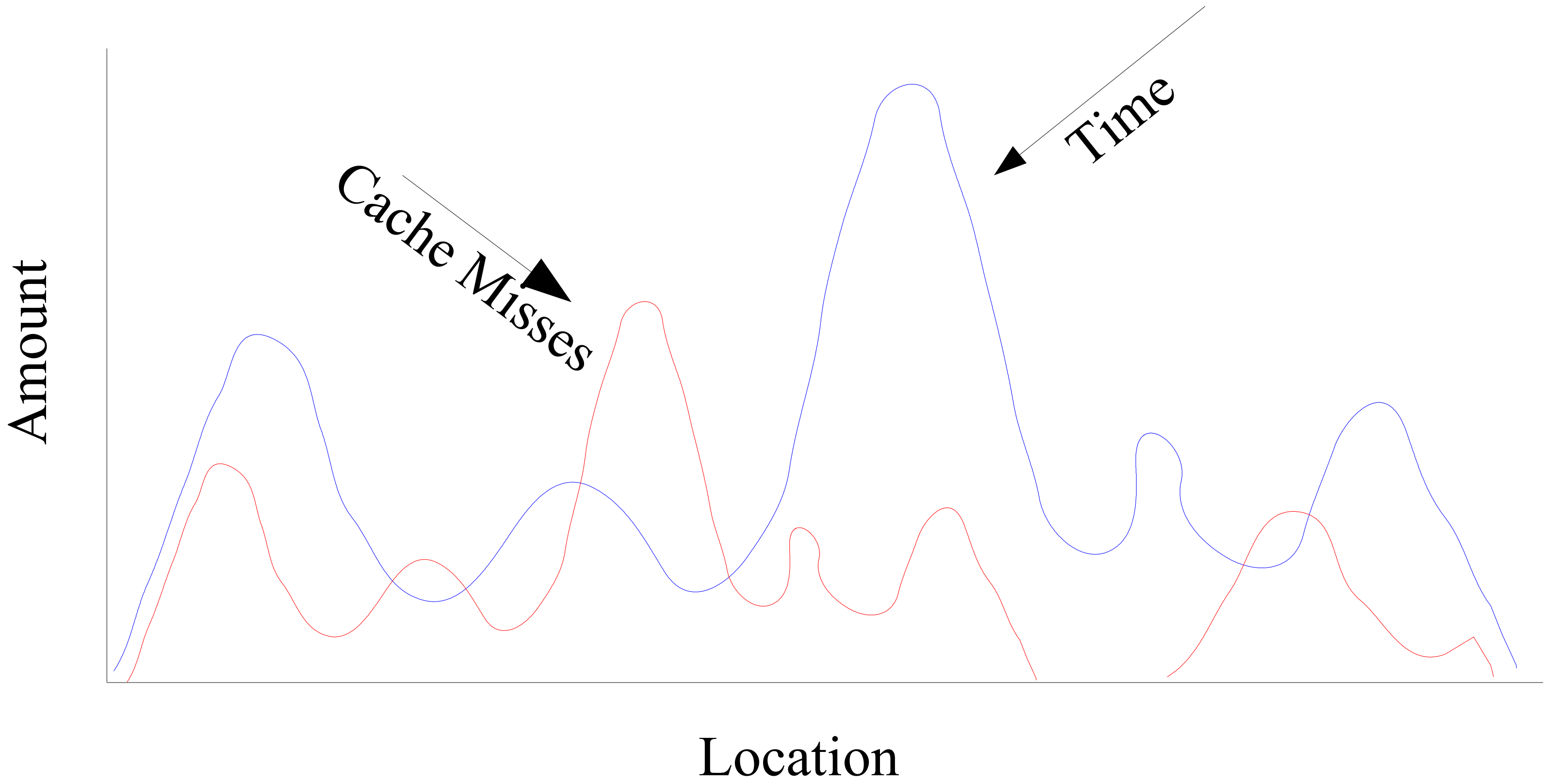
Some Hardware Performance Counter Events

- Cycle count
- Instruction count
  - All instructions
  - Floating point
  - Integer
  - Load/store
- Branches
  - Taken / not taken
  - Mispredictions
- Pipeline stalls due to
  - Memory subsystem
  - Resource conflicts
- Cache
  - I/D cache misses for different levels
  - Invalidations
- TLB
  - Misses
  - Invalidations

Statistical Profiling



Hardware Statistical Profiling



PAPI

- **P**erformance **A**pplication **P**rogramming **I**nterface
- The purpose of PAPI is to implement a standardized portable and efficient API to access the hardware performance monitor counters found on most modern microprocessors.
- The goal of PAPI is to facilitate the optimization of parallel and serial code performance by encouraging the development of cross-platform optimization tools.

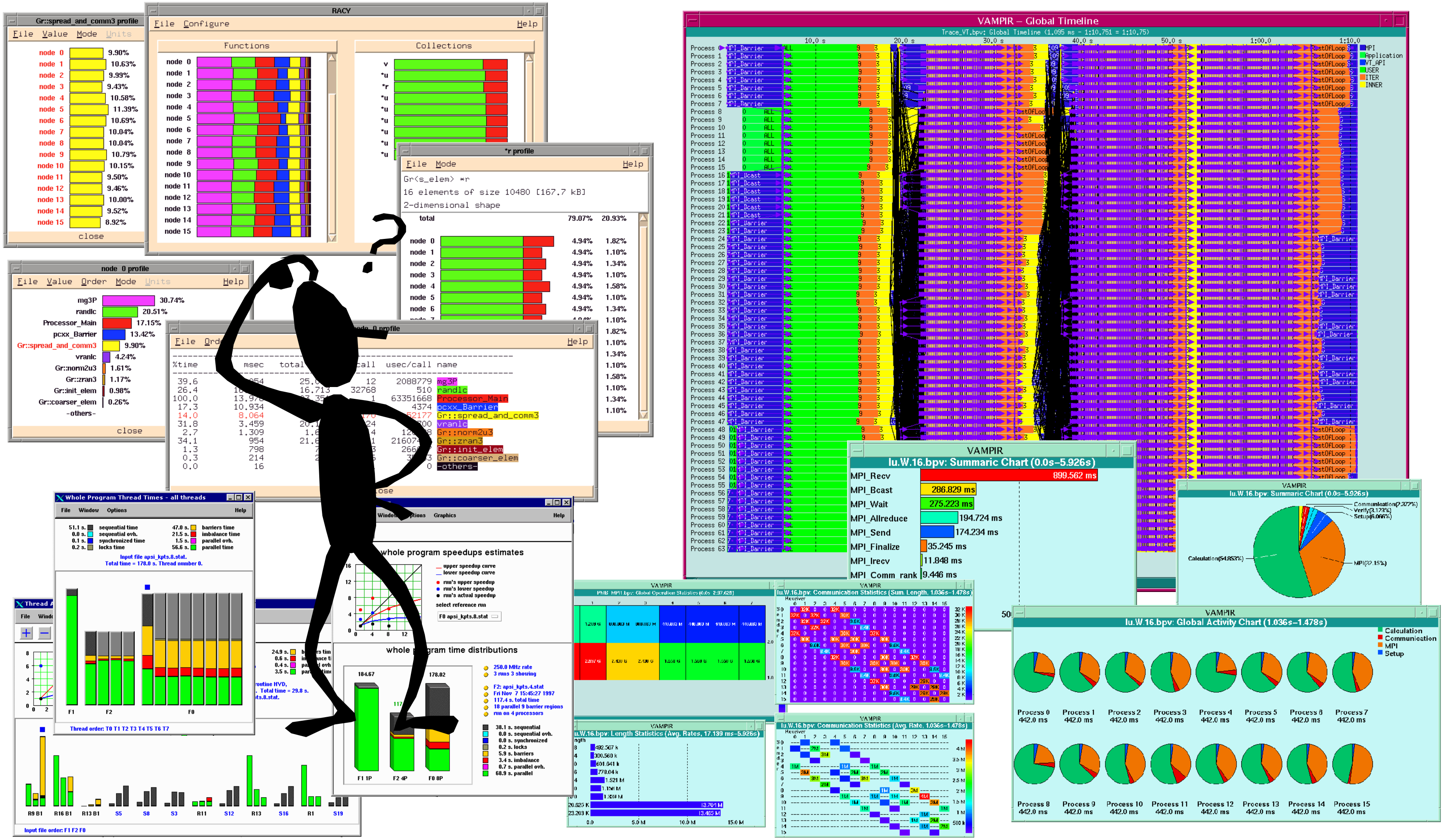
PAPI Preset Events

- PAPI supports around preset events
- Proposed set of events deemed most relevant for application performance tuning
- Preset events are mappings from symbolic names to machine specific definitions for a particular hardware resource.
  - Total Cycles is PAPI_TOT_CYC
- Mapped to native events on a given platform
- PAPI also supports presets that may be derived from the underlying hardware metrics

Linux Performance Tools

- Contrary to popular belief, the Linux infrastructure is well established.
- PAPI is 8 years old.
- Wide complement of tools from which to choose.
- Some are production quality.
- Sun, IBM and HP are now focusing on Linux/HPC which means a focus on performance.

Which Tool?



The Right Performance Tool

- What are your needs? Things to consider:
  - User Interface
    - Complex Suite
    - Quick and Dirty
  - Data Collection Mechanism
    - Aggregate
    - Trace based
    - Statistical

The Right Performance Tool 2

- Performance Data
  - Communications (MPI)
  - Synchronization (Threads and OpenMP)
  - External Libraries
  - User code
- Data correlation
  - Task Parallel (MPI)
  - Thread Parallel
- Instrumentation Mechanism
  - Source/Binary/Library interposition

The Right Performance Tool 3

- Data Management
  - Performance Database
  - User (Flat file)
- Data Visualization
  - Run Time
  - Post Mortem
  - Serial/Parallel Display
  - ASCII

Hardware Profiling and Papiex

- A simple tool that generates performance measurements for the entire run of a code.
- Requires no recompilation.
- Monitors all subprocesses/threads.
- Output goes to stderr or a file.
- Try running your code under papiex to measure IPC or MFLOPS (the default).

Papiex v0.9 Example

```
> module load perftools/1.1
> papiex <application>
> papiex -e PAPI_TOT_CYC -e PAPI_TOT_INS
  -- <application>
> mpirun -np 4 `which papiex` -f --
  <application>
```

papiex v0.9 Output

```
Executable:               /afs/pdc.kth.se/home/m/mucci/mpiP-2.7/testing/a.out
Parent Process ID:        18115
Process ID:               18116
Hostname:                 h05n05.pdc.kth.se
Start:                    Tue Aug 17 17:45:36 2004
Finish:                   Tue Aug 17 17:45:40 2004
Domain:                   User
Real usecs:               3678252 (3s.)
Real cycles:              3310413694
Proc usecs:               16592 (0s.)
Proc cycles:              14932800
PAPI_TOT_CYC:             13962873
PAPI_FP_INS:              285847

Event descriptions:
Event: PAPI_TOT_CYC
        Derived: No
        Short: Total cycles
        Long: Total cycles
        Vendor Symbol: CPU_CYCLES
        Vendor Long: CPU_CYCLES
Event: PAPI_FP_INS
        Derived: No
        Short: FP instructions
        Long: Floating point instructions
        Vendor Symbol: FP_OPS_RETIRED
        Vendor Long: FP_OPS_RETIRED
```

Papiex v0.9 Usage

Usage: papiex [-lLihvtmnukord] [-f [prefix]] [-e event]... -- <cmd> <cmd options>

-l	**List the available events.**
-L	**List all information about the available events.**
-i	**Print information about the host machine.**
-h	**Print this message.**
-v	**Print version information.**
-t	**Enable monitoring of multiple threads.**
-m	**Enable multiplexing of hardware counters.**
-n	**Do not follow fork()'s.**
-u	**Monitor user mode events. (default)**
-k	**Monitor kernel mode events.**
-f[prefix]	**Output to <prefix><cmd>.papiex.<host>.<pid>.<tid>.**
-e event	**Monitor this hardware event.**

Parallel Profiling

- Often we want to see how much time we are spending communicating.
- Many tools to do this via “Tracing” the MPI calls.
- A very good and simple tool available on Lucidor is mpiP v2.7, it does online trace reduction.

MpiP v2.7 Example

```
> module load perftools/1.1
> module show perftools
```

- Follow the instructions to link your C/C++/F77/F90 codes with mpiP.
- Run your code and examine the output in <*.mpiP>.

MpiP v2.7 Output

```
@--- MPI Time (seconds) ---------------------------------------------------
Task    AppTime    MPITime     MPI%
   0      0.084     0.0523    62.21
   1     0.0481      0.015    31.19
   2      0.087     0.0567    65.20
   3     0.0495     0.0149    29.98
   *      0.269      0.139    51.69

@--- Aggregate Time (top twenty, descending, milliseconds) ----------------
Call                 Site       Time    App%    MPI%
Barrier                 1        112   41.57   80.42
Recv                    1       26.2    9.76   18.89
Allreduce               1      0.634    0.24    0.46
Bcast                   1        0.3    0.11    0.22
Send                    1      0.033    0.01    0.02

@--- Aggregate Sent Message Size (top twenty, descending, bytes) ----------
Call                 Site      Count      Total       Avrg  Sent%
Allreduce               1          8    4.8e+03        600  46.15
Bcast                   1          8    4.8e+03        600  46.15
Send                    1          2        800        400   7.69
```

MpiP v2.7 Output 2

```
@--- Callsite Time statistics (all, milliseconds): 16 Name             Site Rank
Count      Max     Mean      Min   App%   MPI%
Allreduce          1    0      2    0.105    0.087    0.069   0.21   0.33
Allreduce          1    1      2    0.118     0.08    0.042   0.33   1.07
Allreduce          1    2      2     0.11    0.078    0.046   0.18   0.27
Allreduce          1    3      2    0.102    0.072    0.042   0.29   0.97
Barrier            1    0      3     51.9     17.3    0.015  61.86  99.44
.
.
.
@--- Callsite Message Sent statistics (all, sent bytes) Name             Site
Rank   Count       Max      Mean       Min       Sum
Allreduce          1    0       2       800       600       400      1200
Allreduce          1    1       2       800       600       400      1200
Allreduce          1    2       2       800       600       400      1200
Allreduce          1    3       2       800       600       400      1200
Bcast              1    0       2       800       600       400      1200
Bcast              1    1       2       800       600       400      1200
Bcast              1    2       2       800       600       400      1200
Bcast              1    3       2       800       600       400      1200
Send               1    0       1       400       400       400       400
Send               1    2       1       400       400       400       400
Send               1    *      18       800     577.8       400  1.04e+04
---------------------------------------------------------------------------
@--- End of Report --------------------------------------------------------
```

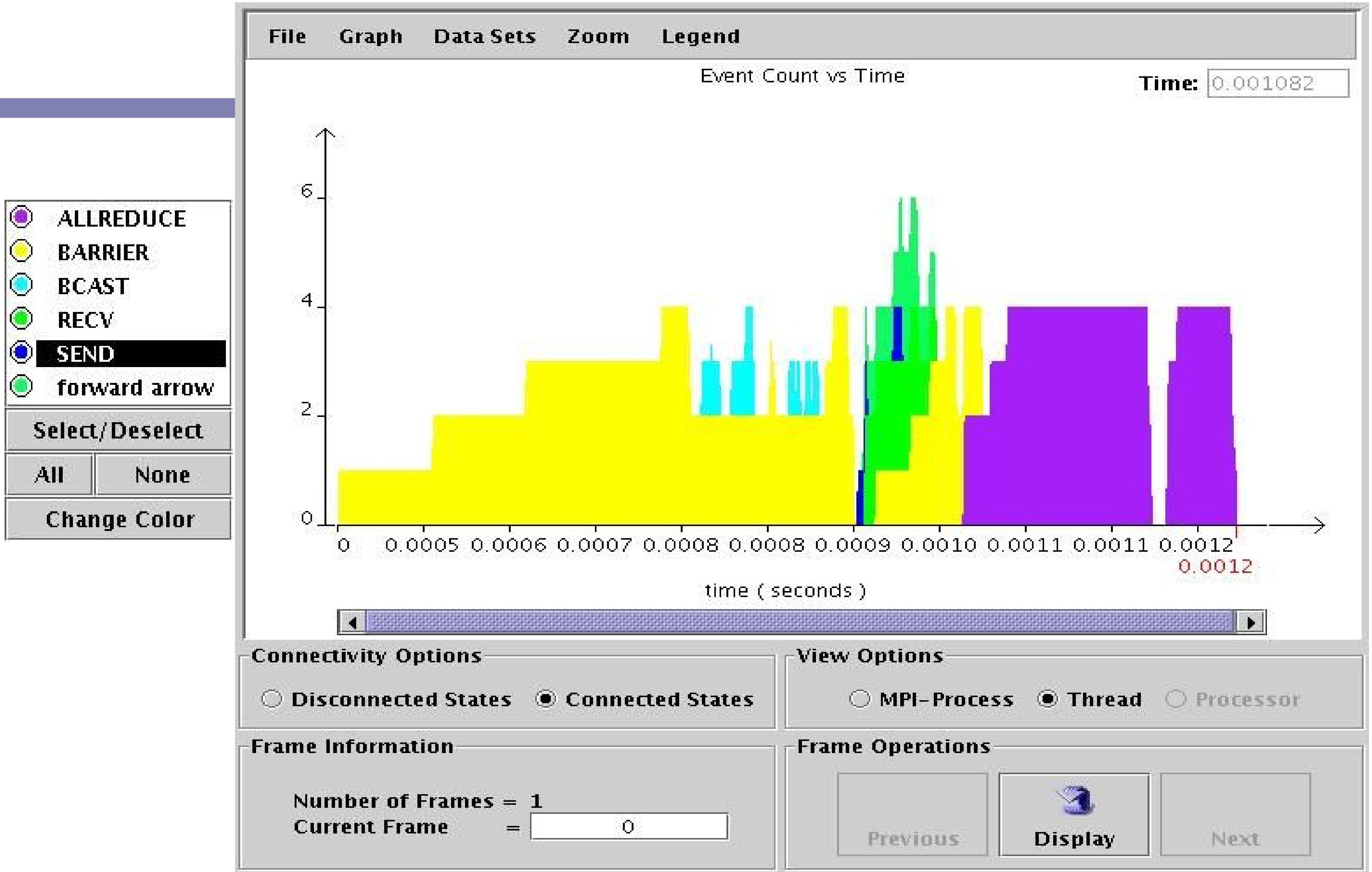
MPI Tracing and Jumpshot

- Sometimes we need to see the exact sequence of messages exchanged between processes.
- For this, we can enable MPI tracing by relinking our application and using the Jumpshot tool.
- Works with any MPI by linking with the Jumpshot MPI tracing library.

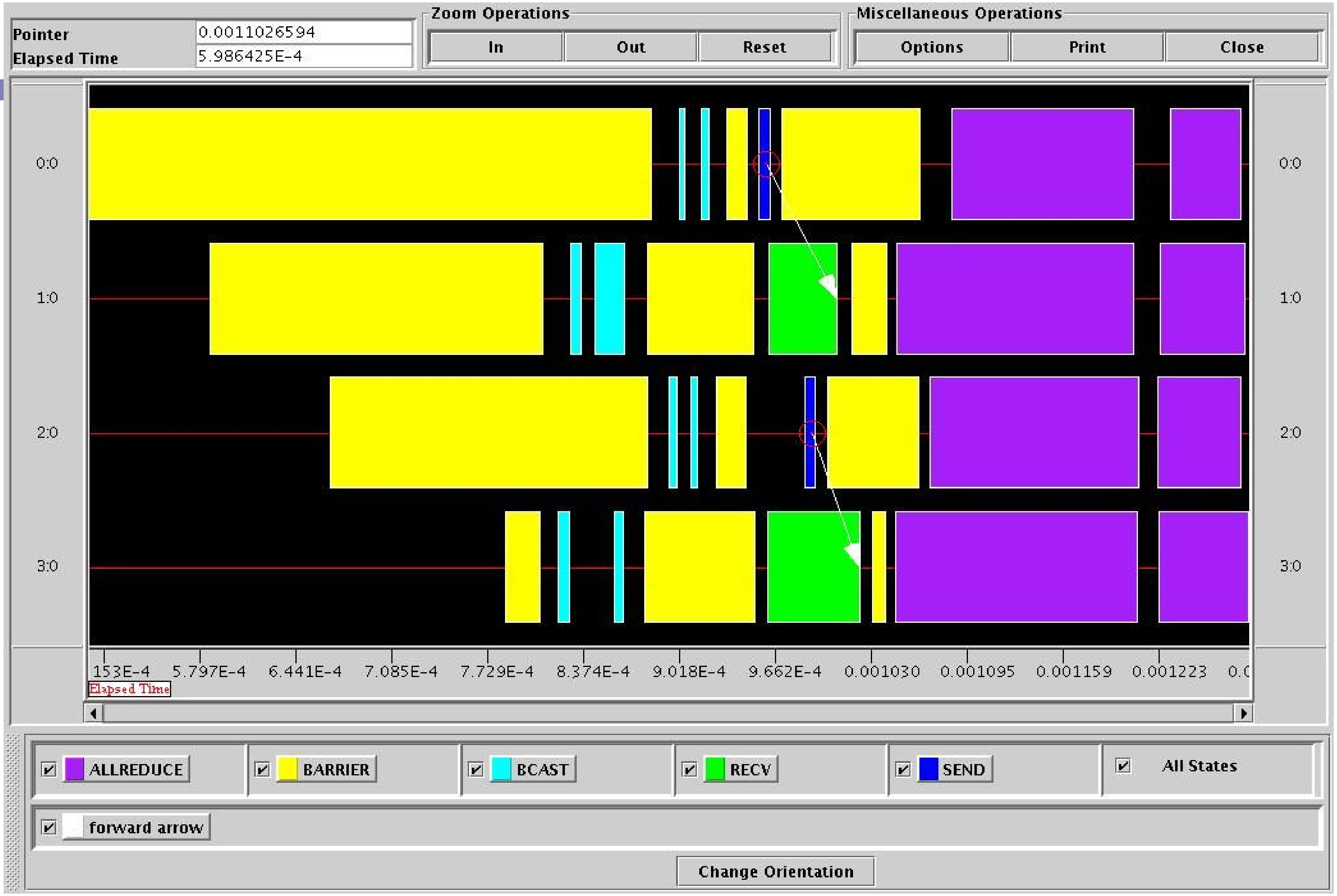
Jumpshot 3 Example

```
> module load perftools/1.1
> mpicc -mpilog example.c -o example
> mpirun -np 4 example
> clog2slog example.clog
> jumpshot example.slog
```

Jumpshot Main Window



Jumpshot Timeline



PerfSuite from NCSA

- Command line tool similar to IRIX's perfex command.
- Does aggregate counting of the entire run. Also provides statistical profiling.
- Uses library preloading.
- Output is XML or Plain Text.
  - Machine information
  - Raw counter values
  - Derived metrics

PSRUN Sample Output

```
Index Description                                                                Counter Value
==============================================================================================

  1 Conditional branch instructions mispredicted.....................          4831072449
  2 Conditional branch instructions correctly predicted..............         52023705122
  3 Conditional branch instructions taken............................         47366258159
  4 Floating point instructions......................................         86124489172
  5 Total cycles.....................................................        594547754568
  6 Instructions completed...........................................       1049339828741
  7 Level 1 data cache accesses......................................         30238866204
  8 Level 1 data cache hits..........................................           972479062
  9 Level 1 data cache misses........................................         29224377672
 10 Level 1 instruction cache reads..................................        221828591306
 11 Level 1 cache misses.............................................         29312740738
 12 Level 2 data cache accesses......................................        129470315862
 13 Level 2 data cache misses........................................         15569536443
 14 Level 2 data cache reads.........................................        110524791561
 15 Level 2 data cache writes........................................         18622708948
 16 Level 2 instruction cache reads..................................           566330907
 17 Level 2 store misses.............................................          1208372120
 18 Level 2 cache misses.............................................         15401180750
 19 Level 3 data cache accesses......................................          4650999018
 20 Level 3 data cache hits..........................................           186108211
 21 Level 3 data cache misses........................................          4451199079
 22 Level 3 data cache reads.........................................          4613582451
 23 Level 3 data cache writes........................................            38456570
 24 Level 3 instruction cache misses.................................             3631385
 25 Level 3 instruction cache reads..................................            17631093
 26 Level 3 cache misses.............................................          4470968725
 27 Load instructions................................................        111438431677
 28 Load/store instructions completed................................        130391246662
 29 Cycles Stalled Waiting for memory accesses.......................        256484777623
 30 Store instructions...............................................         18840914540
 31 Cycles with no instruction issue.................................         61889609525
 32 Data translation lookaside buffer misses.........................             2832692
```

PSRUN Sample Output

```
Statistics
==========================================================================================
Graduated instructions per cycle.......................................          1.765
Graduated floating point instructions per cycle........................          0.145
% graduated floating point instructions of all graduated instructions..          8.207
Graduated loads/stores per cycle.......................................          0.219
Graduated loads/stores per graduated floating point instruction........          1.514
Mispredicted branches per correctly predicted branch...................          0.093
Level 1 data cache accesses per graduated instruction..................          2.882
Graduated floating point instructions per level 1 data cache access....          2.848
Level 1 cache line reuse (data)........................................          3.462
Level 2 cache line reuse (data)........................................          0.877
Level 3 cache line reuse (data)........................................          2.498
Level 1 cache hit rate (data)..........................................          0.776
Level 2 cache hit rate (data)..........................................          0.467
Level 3 cache hit rate (data)..........................................          0.714
Level 1 cache miss ratio (instruction).................................          0.003
Level 1 cache miss ratio (data)........................................          0.966
Level 2 cache miss ratio (data)........................................          0.120
Level 3 cache miss ratio (data)........................................          0.957
Bandwidth used to level 1 cache (MB/s).................................       1262.361
Bandwidth used to level 2 cache (MB/s).................................       1326.512
Bandwidth used to level 3 cache (MB/s).................................        385.087
% cycles with no instruction issue.....................................         10.410
% cycles stalled on memory access......................................         43.139
MFLOPS (cycles)........................................................        115.905
MFLOPS (wallclock).....................................................        114.441
MIPS (cycles)..........................................................       1412.190
MIPS (wallclock).......................................................       1394.349
CPU time (seconds).....................................................        743.058
Wall clock time (seconds)..............................................        752.566
% CPU utilization......................................................         98.737
```

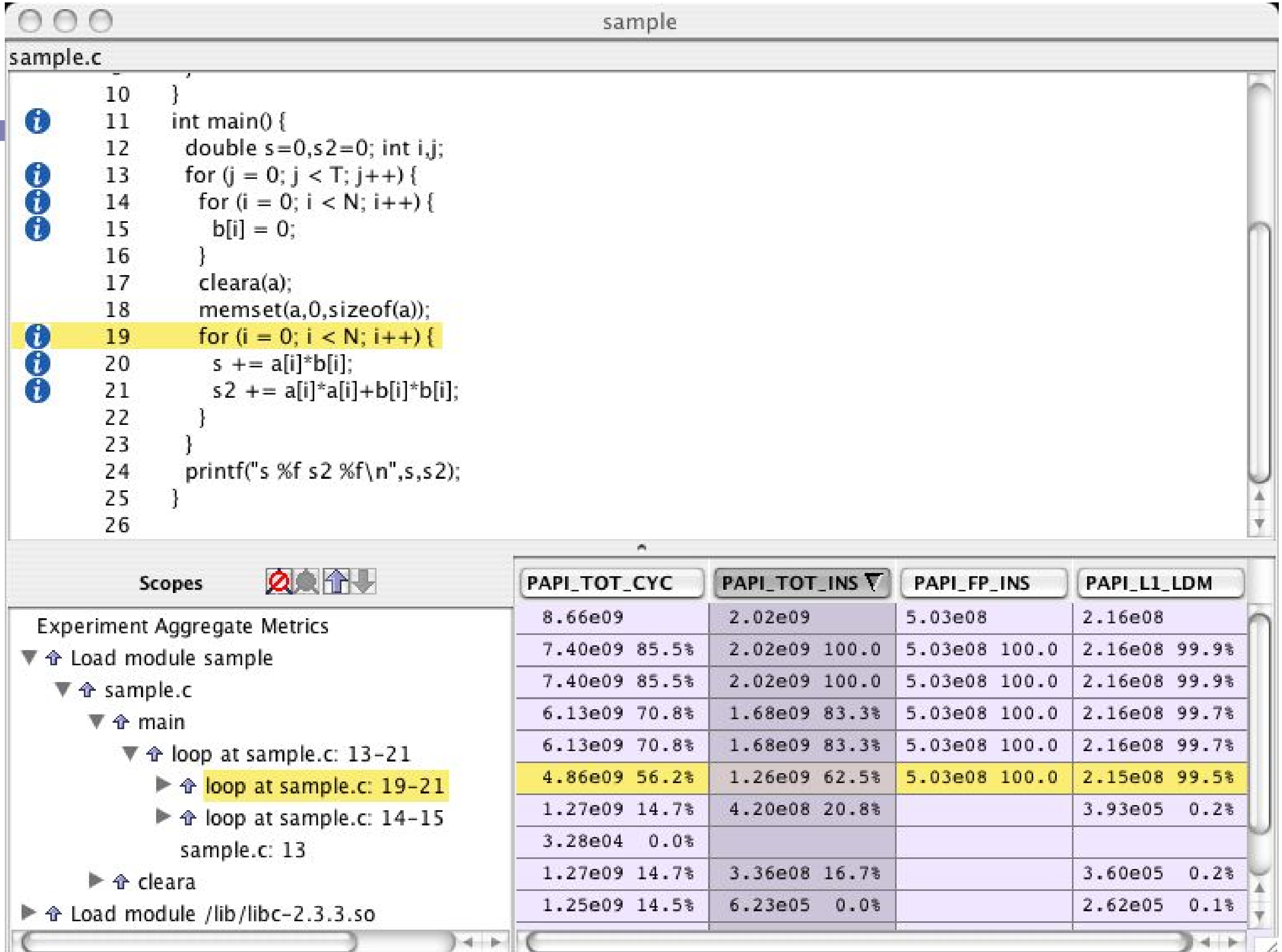
HPCToolkit from Rice U.

- Use event-based sampling and statistical profiling to profile unmodified applications: hpcrun
- Interpret program counter histograms: hpcprof
- Correlate source code, structure and performance metrics: hpcprof/hpcquick
- Explore and analyze performance databases: hpcviewer

HPCToolkit Goals

- Support large, multi-lingual applications
  - Fortran, C, C++, external libraries (possibly binary only) with thousands of procedures, hundreds of thousands of lines
  - Avoid
    - Manual instrumentation
    - Significantly altering the build process
    - Frequent recompilation
- Collect execution measurements scalably and efficiently
    - Don't excessively dilate or perturb execution
    - Avoid large trace files for long running codes
- Support measurement and analysis of serial and parallel codes
- Present analysis results effectively
  - Top down analysis to cope with complex programs
  - Intuitive enough for physicists and engineers to use
  - Detailed enough to meet the needs of compiler writers
- Support a wide range of computer platforms

HPCToolkit Sample Output



TAU from U. Oregon

- Integrated toolkit for parallel and serial performance instrumentation, measurement, analysis, and visualization
- Open software approach with technology integration
- Robust timing and hardware performance support using PAPI
- TAU supports both profiling and tracing models.

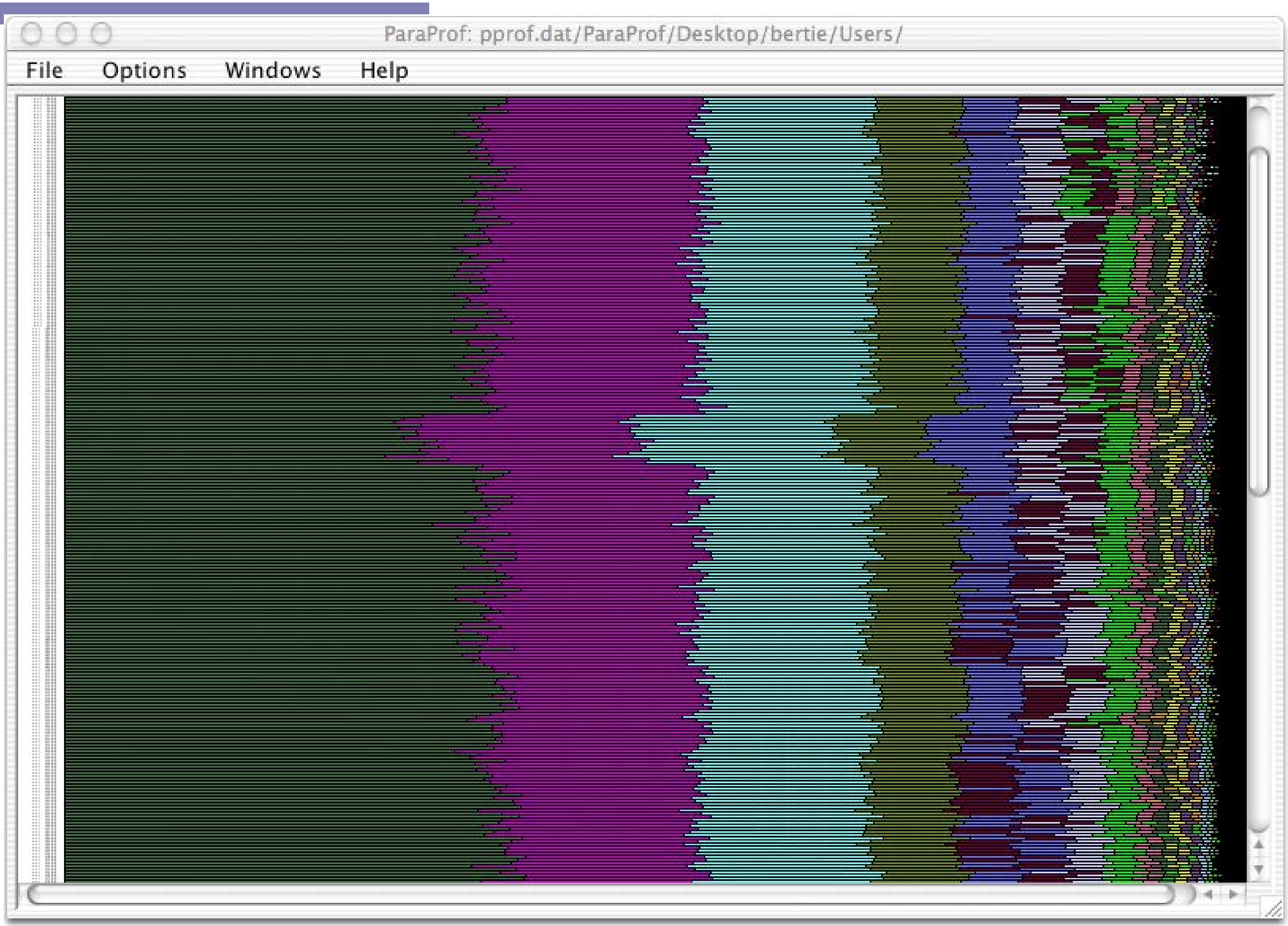
Some TAU Features

- Function-level, block-level, statement-level
- Support for callgraph and callpath profiling
- Parallel profiling and Inter-process communication events
- Supports user-defined events
- Trace merging and format conversion

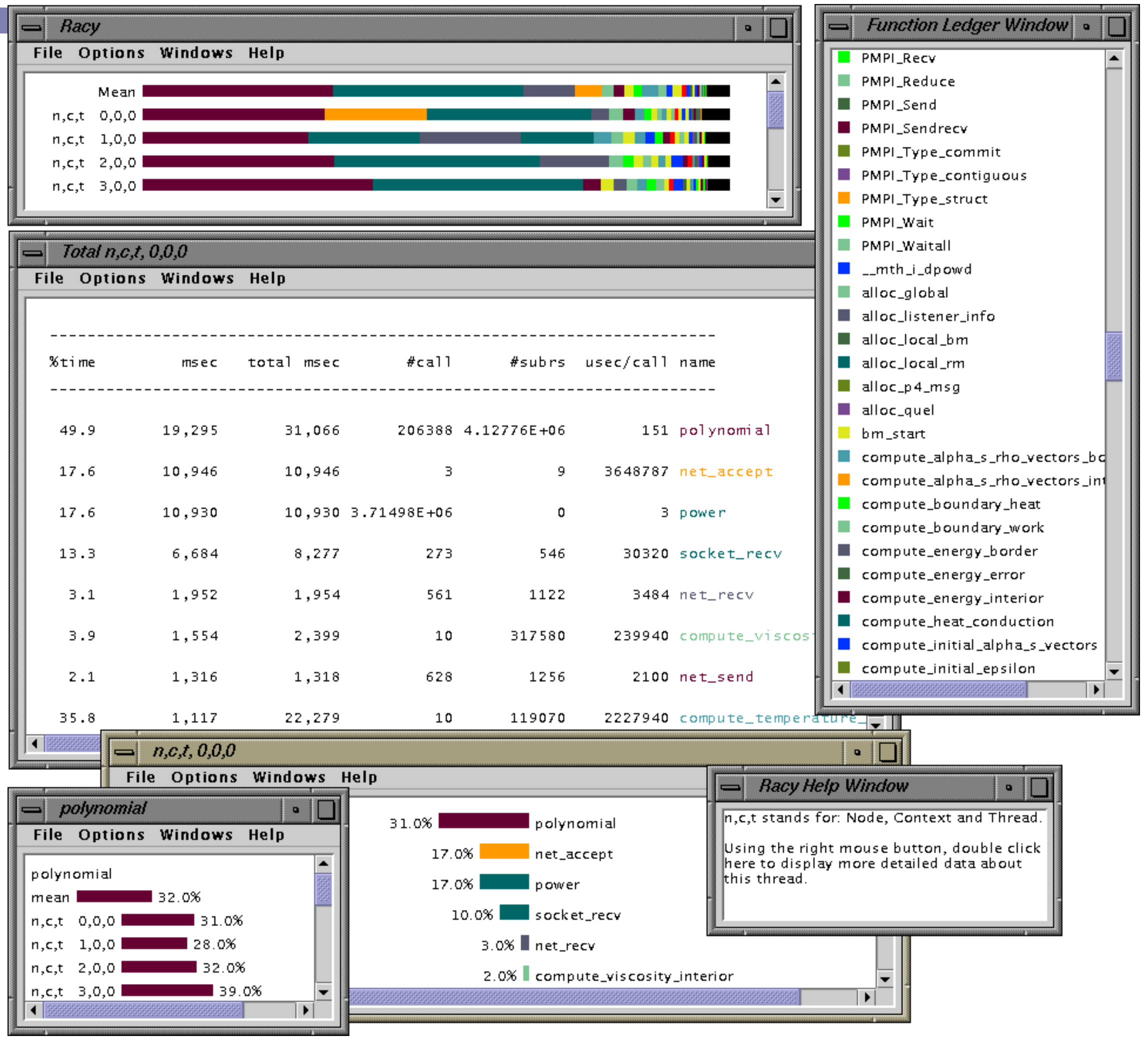
TAU Instrumentation

- Source code both manual and automatic.
  - C, C++, F77/90/95 (Program Database Toolkit (PDT))
  - OpenMP (directive rewriting (Opari), POMP spec)
- Object code
  - pre-instrumented libraries (e.g., MPI using PMPI)
- Executable code
  - dynamic instrumentation (pre-execution) (DynInstAPI)

TAU Parallel Display



TAU Program Display



More Performance Tools

- KOJAK (Juelich, UTK)
  - Instrumentation, tracing and analysis system for MPI, OpenMP and Performance Counters.
  - Provides automated diagnosis of many common parallel performance problems.
- Q-Tools (HP) (non-PAPI, IA64 only)
  - Statistical profiling of system and user processes
- DynaProf (Me)
  - Dynamic instrumentation tool.

Conclusion

5 Ways to Avoid Performance Problems: Number 1

***Never, ever**, write your own code unless you absolutely have to.*

- Libraries, libraries, libraries!
- Spend time to do the research, chances are you will find a package that suits your needs.
- Often you just need to do the glue that puts the application together.
- The 80/20 Rule! 80% of time is spent in 20% of code.

5 Ways to Avoid Performance Problems: Number 2

Never *violate the usage model of your environment.*

- If something seems impossible to accomplish in your language or programming environment, you're probably doing something wrong.
- Consider such anomalies as:
  - Matlab in parallel on a cluster of machines.
  - High performance(?!) Java.
- There probably is a better way to do it, ask around.

5 Ways to Avoid Performance Problems: Number 3

Always *let the compiler do the work.*

- The compiler is much better at optimizing most code than you are.
- Gains of 30-50% are reasonably common when the 'right' flags are thrown.
- Spend some time to read the manual and ask around.

5 Ways to Avoid Performance Problems: Number 4

***Never** use more data than absolutely necessary.*

- C: float vs. double.
- Fortran: REAL*4, REAL*8, REAL*16
- Only use 64-bit precision if you NEED it.
- A reduction in the amount of data the CPU needs ALWAYS translates to a increase in performance.
- Remember that the memory subsystem and the network are the ultimate bottlenecks.

5 Ways to Avoid Performance Problems: Number 5

Always *make friends with a computer scientist!*

- Learning just a little about modern computer architecture will result in much better code.

Questions?

- Email: mucci@cs.utk.edu
- For those here at KTH, many on the PDC staff are well versed in the art of performance. Use them!

HTTP References

http://www.openmp.org

http://www.netlib.org

http://http://www-unix.mcs.anl.gov/petsc/petsc-2/

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http://www.cs.utk.edu/~mucci/dynaprof

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Thanks