Center for Scalable Application Development Software

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SciDAC Scientific Discovery through Advanced Computing

Goals

- Provide open source software systems, tools, and components that address a spectrum of needs
  - directly usable by application experts
  - provided to the CS community to enable development of other tools
- Engage directly with DOE application teams
- Target architectures of critical interest to DOE
  - Cray XT
  - Blue Gene/P
  - multicore processors in general
- Outreach

Outline

☞ Community engagement

- Research and open source software development
  - system software and language runtime systems
  - communication for partitioned global address space languages
  - math libraries for multicore
  - performance tools
  - compilers
  - applications
- FY09 plans

Community Engagement

CScADS Summer Workshop Series

- Goals
  - identify challenges and open problems for leadership computing
  - brainstorm on promising approaches
  - foster collaborations between computer and application scientists
  - engage the broader community of enabling technology researchers
- Workshops to engage SciDAC and INCITE application teams
  - Leadership class machines, petascale applications, and performance
  - Scientific data analysis and visualization for petascale computing
- Workshops to foster development of enabling technologies
  - Autotuning for petascale systems
  - Performance tools for petascale computing
  - Libraries and algorithms for petascale applications

2009 Workshops at Granlibakken

Some Workshop Outcomes

- Leadership class machines, applications, and performance
  - introduced developers to changes in the leadership platforms
  - introduced developers to OpenMP, advanced MPI, parallel I/O, & tools
  - hands-on: ET researchers assisted developers with platforms and tools
- Performance tools
  - create an international community to share ideas and software
  - foster development of tool components rather than monolithic tools
  - “performance tool dating”
    - unstripping tool looking for symbol table info & an x86 instruction cracker
- Autotuning
  - bring together experts on architecture, libraries, and compilers
  - brainstorm on how to broaden reach of autotuning approaches
  - share experiences and ideas; explore opportunities for collaboration
  - identify common tools and benchmarks

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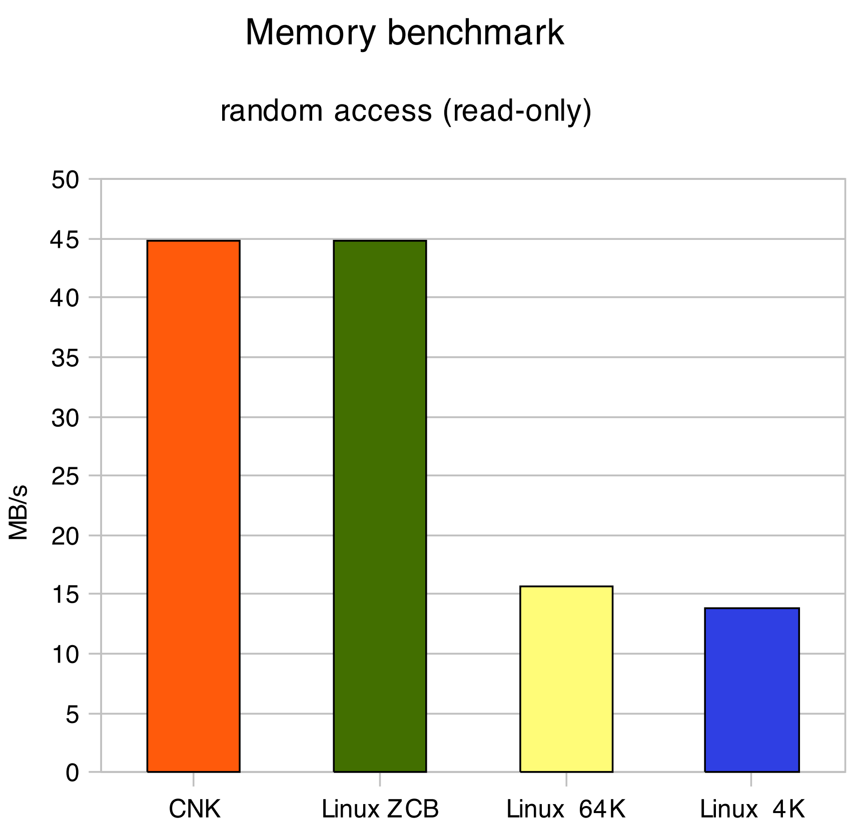
CScADS ZeptoOS Research

- Exploring performance improvements for system software on leadership-class multicore platforms
- Focus
  - memory management
  - I/O forwarding and job control
  - communication software stack
- Benefits
  - foster software research on leadership computing platforms
  - extend the usage of leadership computing platforms

Memory Management on BG/P

- General purpose OS loses memory performance
  - worst case: standard Linux on ppc450 achieves only 25% of the theoretical memory bandwidth due to high cost of TLB misses

- Solution
  - introduced flat memory management to Linux
  - enables a compute task to access memory without TLB misses

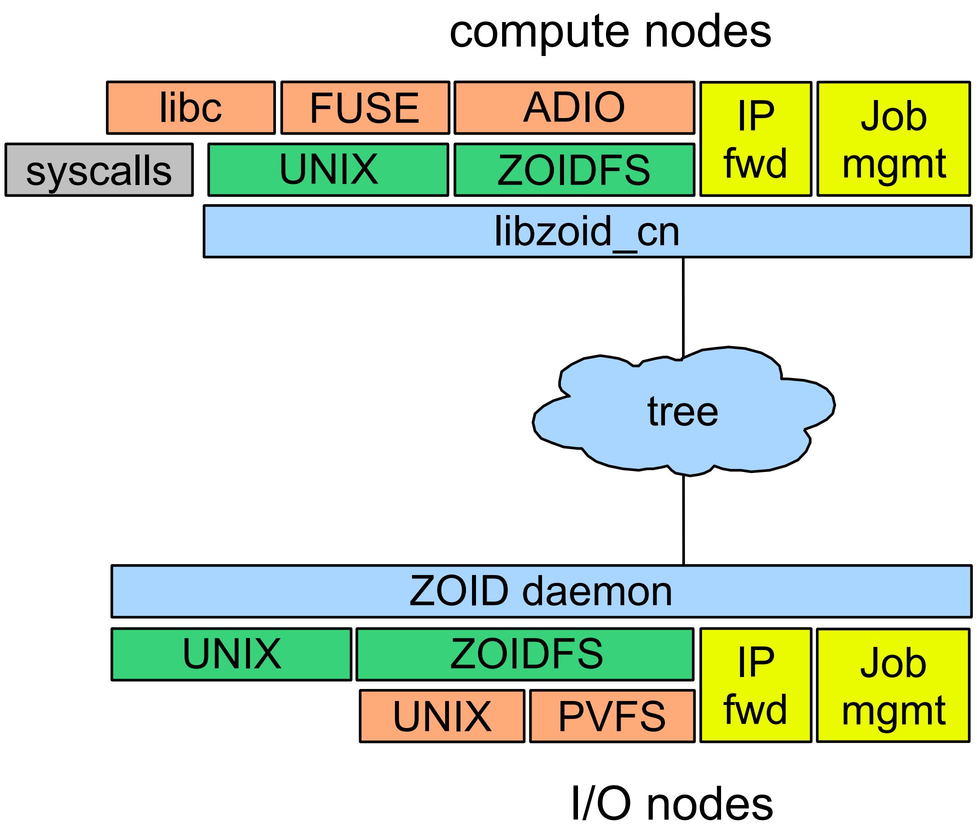


I/O Forwarding and Job Control

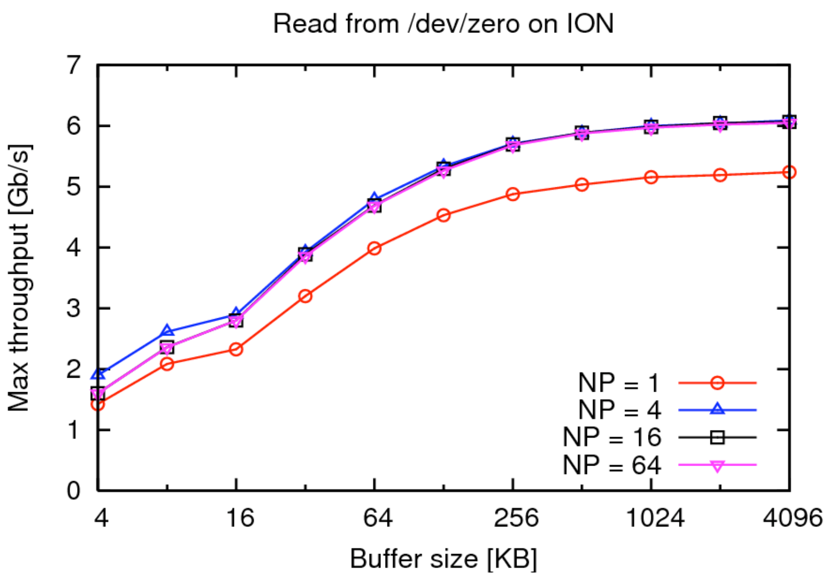
- ZOID (ZeptoOS I/O Daemon) provides
  - complete job management
  - file I/O and IP forwarding for Zepto Compute Node Linux
- Extensible through plugins
  - custom I/O forwarding APIs
    - e.g. file system client, communication layer
- Open, full source code available
  - enables independent computer science research
- Optimized performance
  - multithreading to hide latency
  - reduced context switching

ZeptoOS I/O Daemon (ZOID)

Architecture



Performance



(raw link bandwidth is 6.8 Gb/s)

ZeptoOS Results

Blue Gene/P Compute Node OS and I/O layer operational

- Supports High Performance Computing (HPC) on BG/P
  - BG/P compute node software stack has been ported
  - MPICH is ready to use
- Supports High Throughput Computing (HTC) on BG/P
  - Falkon task execution framework has been ported

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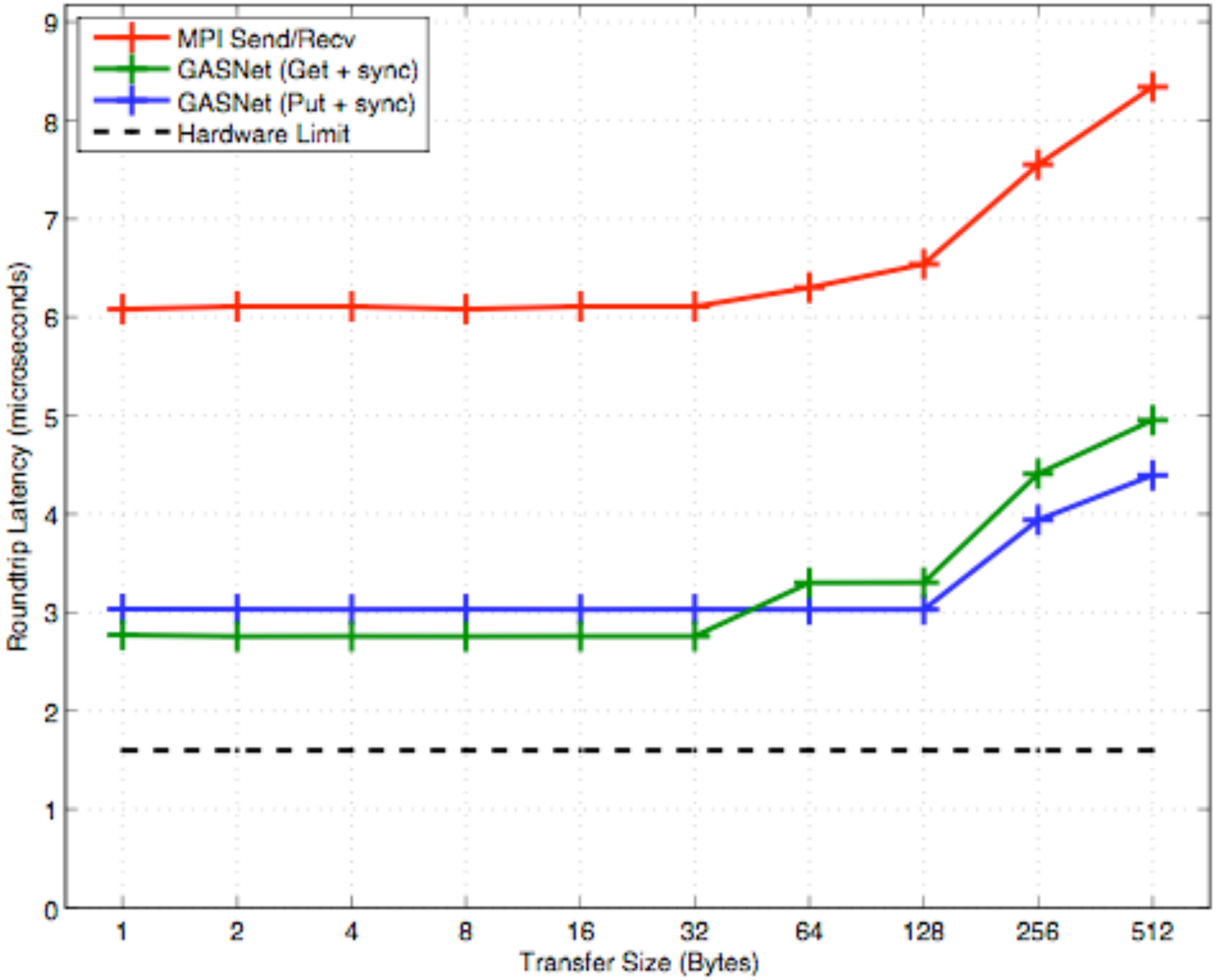
CScADS PGAS Communication

- Planned SC08 release of GASNet and Berkeley UPC
  - updated Portals conduit for Cray XT3/4/5 platforms with “firehose”
    - avoids pin/unpin costs with caching of registration table entries
  - new BG/P conduit based on low level DCMF layer
  - updated Infiniband conduit using new OpenIB/OpenFabrics verbs API
  - LAPI conduit for IBM Power uses RDMA
  - jointly funded by PModels and others
- Implementation goals
  - low latency for small to medium transfers
  - high bandwidth transfers
  - efficient collective communication

GASNet is being used in the upcoming Chapel release

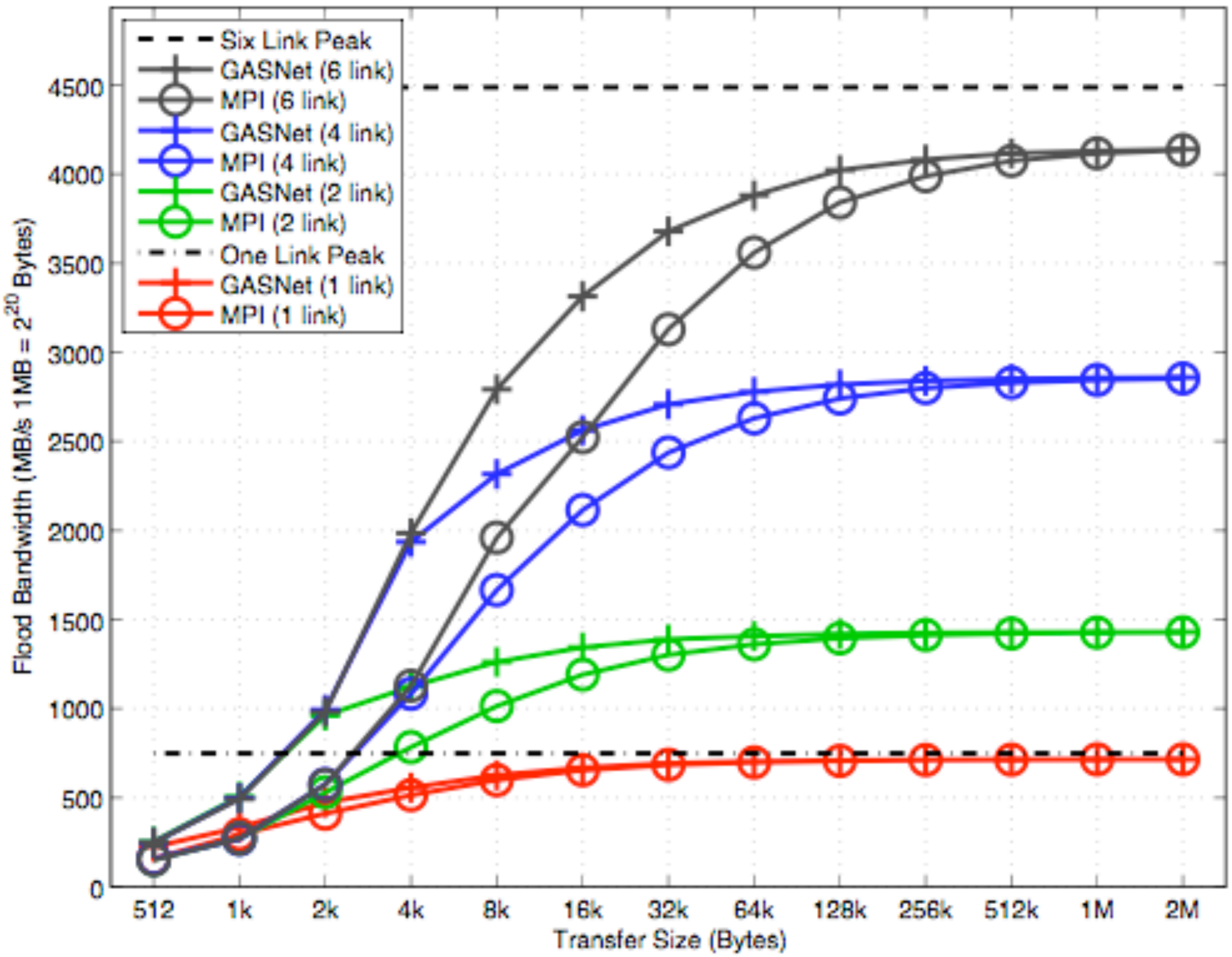
GASNet vs MPI Latency on BG/P



(lower is better)

- Recent work on DCMF Conduit for GASNet
- Jointly funded by PModels and CScADS

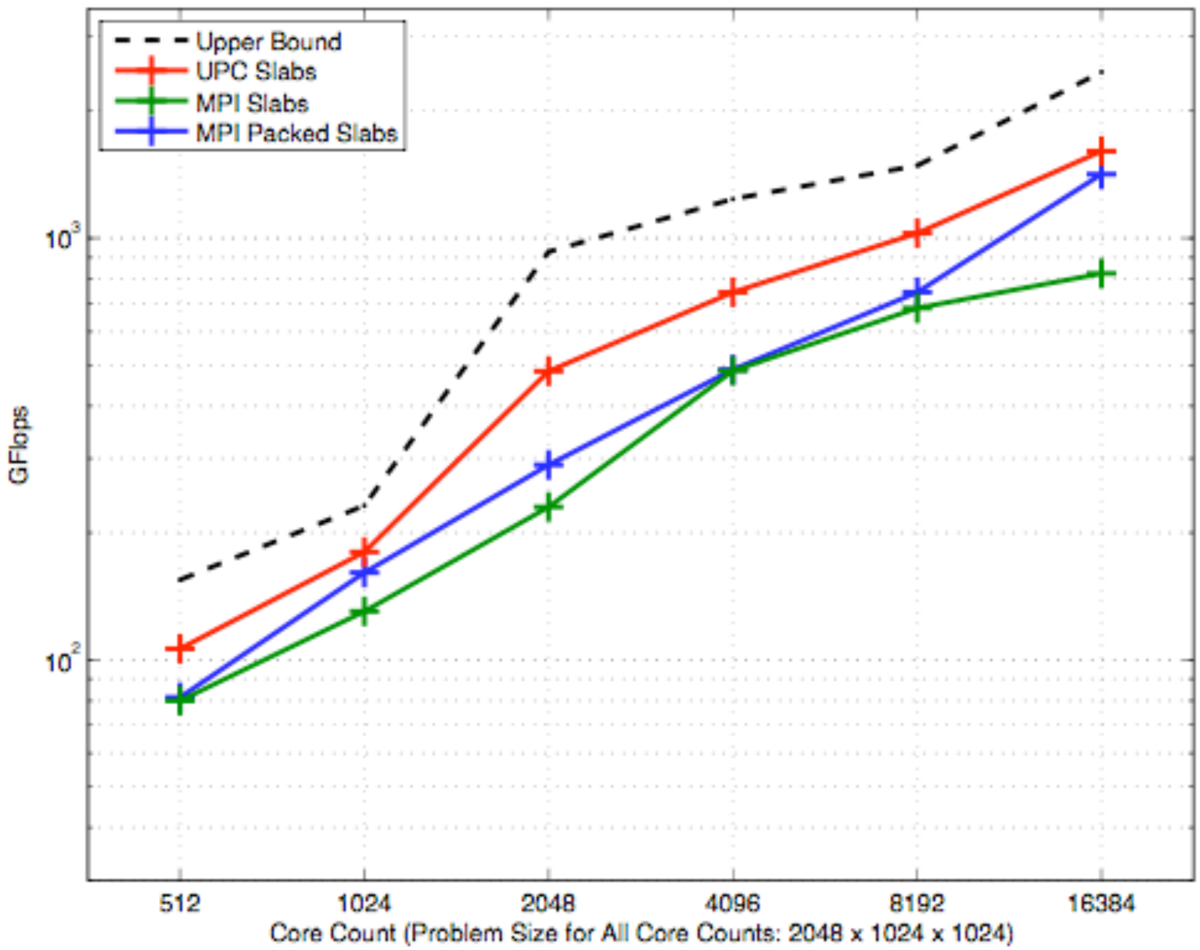
GASNet vs. MPI Bandwidth on BG/P



(higher is better)

GASNet outperforms MPI on small to medium messages, especially when multiple links are used

3D FFT Performance on BG/P



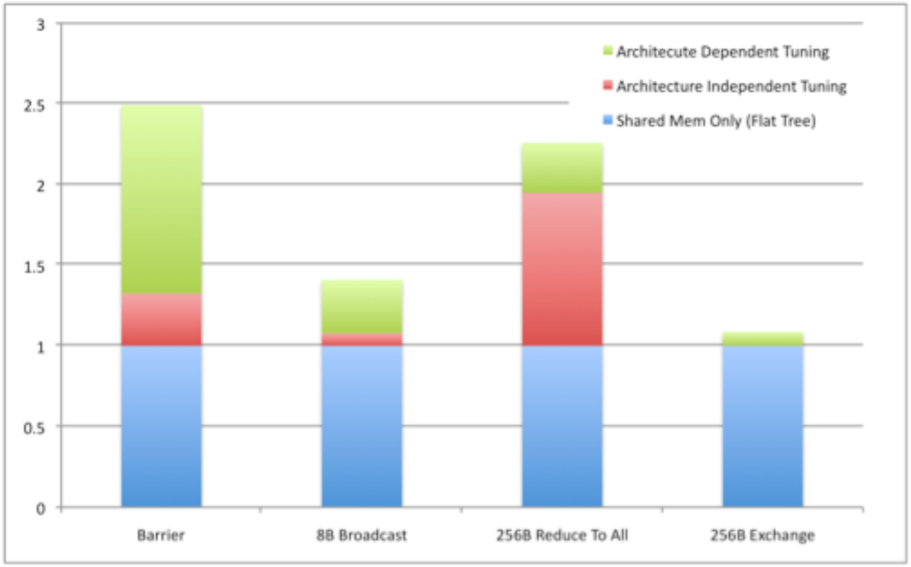
Upper bound is based on performance model of torus and bandwidth

(higher is better)

Strong scaling: good performance up to 16K cores

UPC Collectives on Multicore

- Collective communication is important for many algorithms
- Technology trends encourage sharing on multicore chips
- Many factors affect performance
  - tree structure: balanced vs. binomial
  - collective routine
  - data size
- Exploring use of autotuning on collectives for multicore nodes
- Study different architectures
  - Intel Cloverton
  - Sun Niagara2



Autotuning collectives for Niagara2

(lower is better)

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Linear Algebra for Parallel Systems

- Multicore is a disruptive technology for software
- Must rethink and rewrite applications, algorithms and software
  - as before with cluster computing and message passing
- Numerical libraries, e.g. LAPACK and ScLAPACK, need to change

- CScADS research
  - pOSKI: extend OSKI to autotune sparse matrix kernels for multicore
  - event-driven DAG scheduled computations
    - direct solvers (LU) on distributed memory using UPC
    - PLASMA software framework dense linear algebra for multicore
  - mixed precision

PLASMA: Parallel Linear Algebra s/w for Multicore

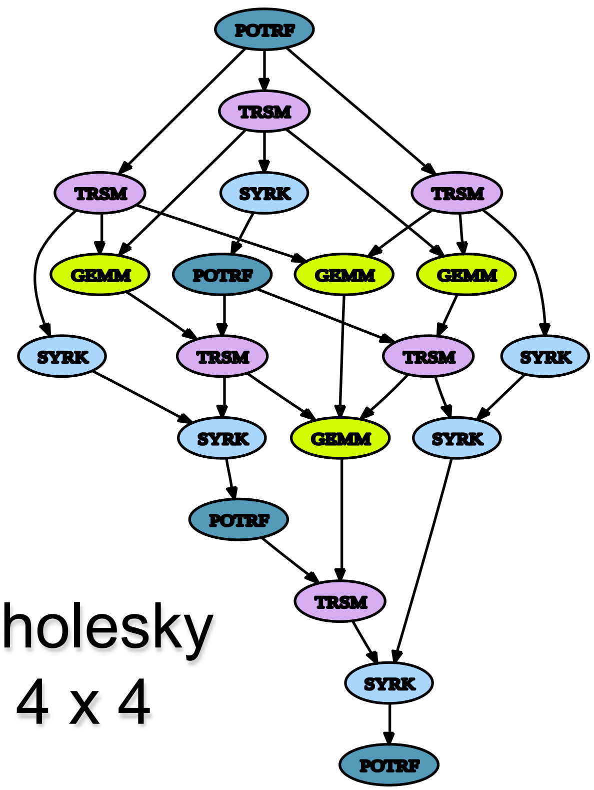
- Objectives
  - parallel performance
    - high utilization of each core
    - scaling to large numbers of cores
  - any memory model
    - shared memory: symmetric or non-symmetric
    - distributed memory
    - GPUs
- Solution properties
  - asychronicity: avoid fork-join (bulk synchronous design)
  - dynamic scheduling: out-of-order execution
  - fine granularity: independent block operations
  - locality of reference: store data using block data layout

A community effort led by Tennessee and Berkeley
(similar to LAPACK/ScaLAPACK)

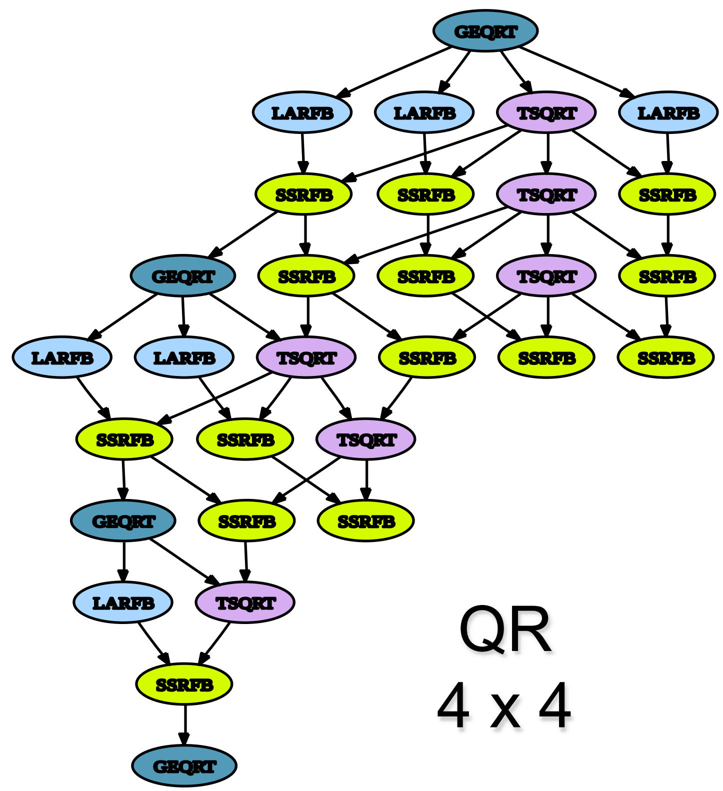
PLASMA Methodology

Computations as DAGs

Reorganize algorithms and software to work on tiles that are scheduled based on the directed acyclic graph of the computation

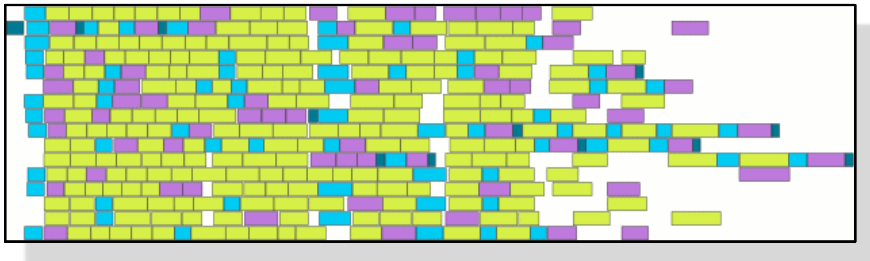


Cholesky
4 x 4



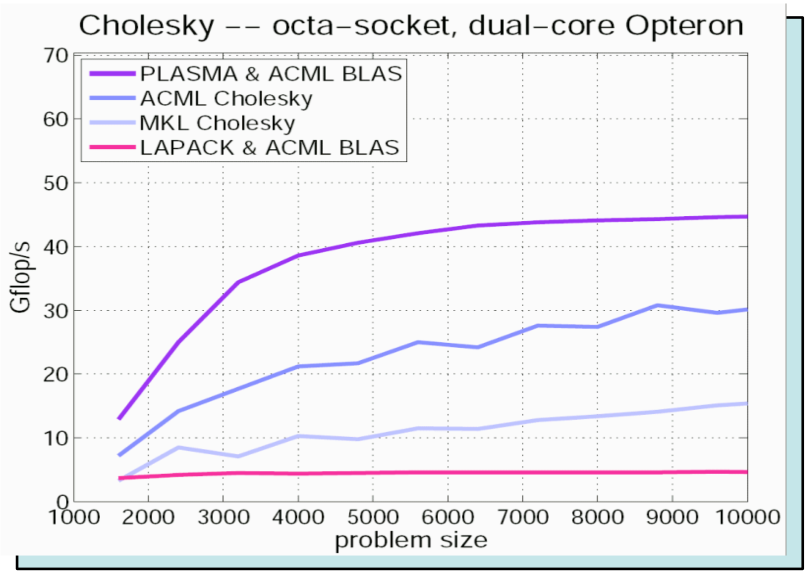
QR
4 x 4

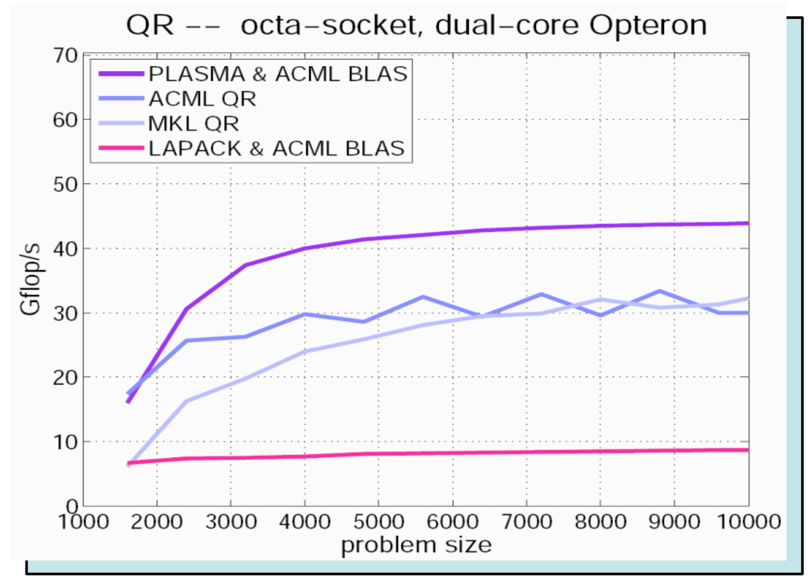
Cholesky using PLASMA

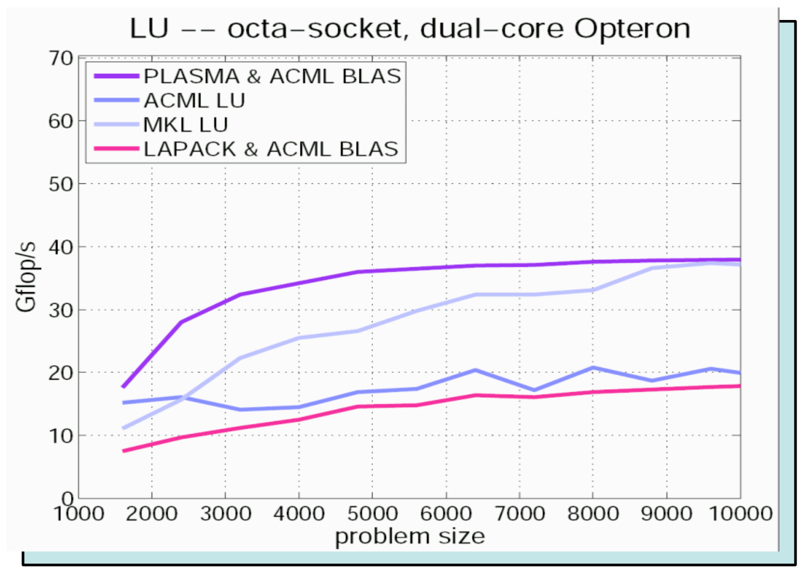


PLASMA
Arbitrary DAG
Fully dynamic scheduling

PLASMA Provides Highest Performance







Leveraging Mixed Precision

- Why use single precision as part of the computation? Speed!
  - higher parallelism within vector units
    - 4 ops/cycle (usually) instead of 2 ops/cycle
  - reduced data motion
    - 32-bit vs. 64-bit data
  - higher locality in cache
    - more data items in cache
- Approach
  - compute a 32-bit result
  - calculate a correction for 32-bit results using 64-bit operations
  - update of 32-bit results with the correction using high precision

Mixed-Precision Iterative Refinement

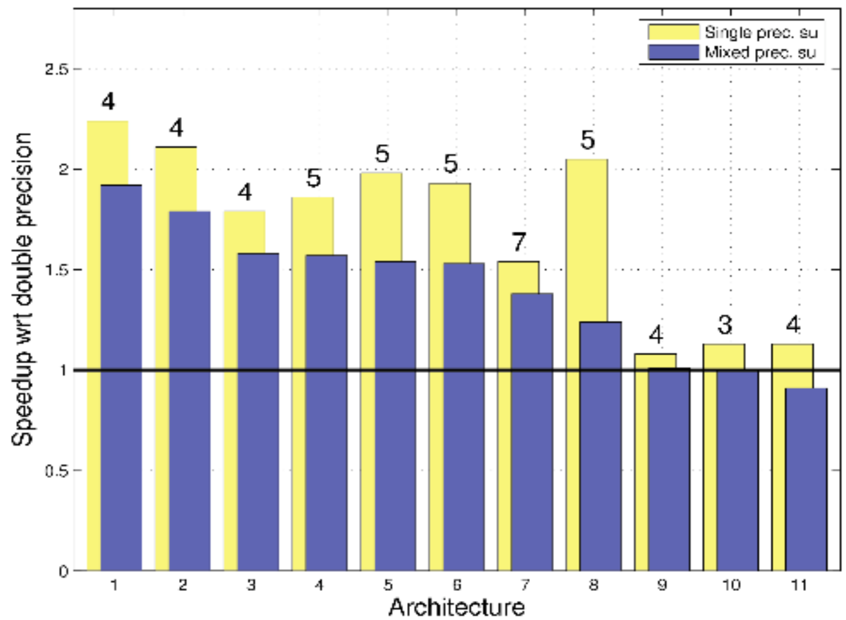
- Iterative refinement for dense systems, $Ax = b$, can work this way:

```
L U = lu(A)                                      O(n^3)
x = L\(U\b)                                      O(n^2)
r = b - Ax                                       O(n^2)
WHILE || r || not small enough
      z = L\(U\r)                                O(n^2)
      x = x + z                                  O(n^1)
      r = b - Ax                                 O(n^2)
END
```

- Wilkinson, Moler, Stewart, & Higham provide error bound for SP floating point results when using DP floating point
- Using this, we can compute the result to 64-bit precision

Results for Mixed Precision

Iterative Refinement for Dense $Ax = b$



	Architecture (BLAS)
1	Intel Pentium III Coppermine (Goto)
2	Intel Pentium III Katmai (Goto)
3	Sun UltraSPARC IIe (Sunperf)
4	Intel Pentium IV Prescott (Goto)
5	Intel Pentium IV-M Northwood (Goto)
6	AMD Opteron (Goto)
7	Cray X1 (libsci)
8	IBM Power PC G5 (2.7 GHz) (VecLib)
9	Compaq Alpha EV6 (CXML)
10	IBM SP Power3 (ESSL)
11	SGI Octane (ATLAS)

Architecture (BLAS-MPI)	# procs	*n*	DP Solve /SP Solve	DP Solve /Iter Ref	# iter
AMD Opteron (Goto – OpenMPI MX)	32	22627	1.85	1.79	6
AMD Opteron (Goto – OpenMPI MX)	64	32000	1.90	1.83	6

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Toward Ubiquitous Tools for Binaries

Infrastructure for performance tools

- Abstract interfaces
  - provide portability and multiplatform support
- Component-based approach
  - enable sharing, rapid prototyping, co-development, development of best-of-breed algorithms and representations
- Extensible data representations
  - support layered library development
- Open source
  - support the above goals and allow broader adoption

Component-based Approach

Benefits

- Increases sharing and reuse
  - reduces redundant development
- Large research tool groups can focus on their priority missions without having to develop all parts of an end-to-end solution
- Small research groups (young investigators!) can explore focused research topics with a software code base comparable to that of the larger groups

Collaborations with internal (Rice, Wisconsin) and external (LLNL, Cray, Intel, Berkeley, Oregon, Jülich) groups on various APIs

workshop discussions are a critical part of the design process

The Deconstruction of DynInst

Realizing our push towards tool components

- InstructionAPI
  - abstract representation of instruction decode and address modes.
- SymtabAPI
  - abstraction of symbols, debug and dynamic linkage information
  - updating to support binary rewriting
- StackwalkerAPI
  - walk stacks: first or third party, standard vs. optimized frames, custom frames (from instrumentation or exceptions)
  - uses a variety of techniques from full symbols and libunwind to stripped binaries requiring control-flow analysis
- ControlFlowAPI
  - platform independent representation of CFG, associated query routines, and extensible data structures

CScADS funded components are underlined

libmonitor

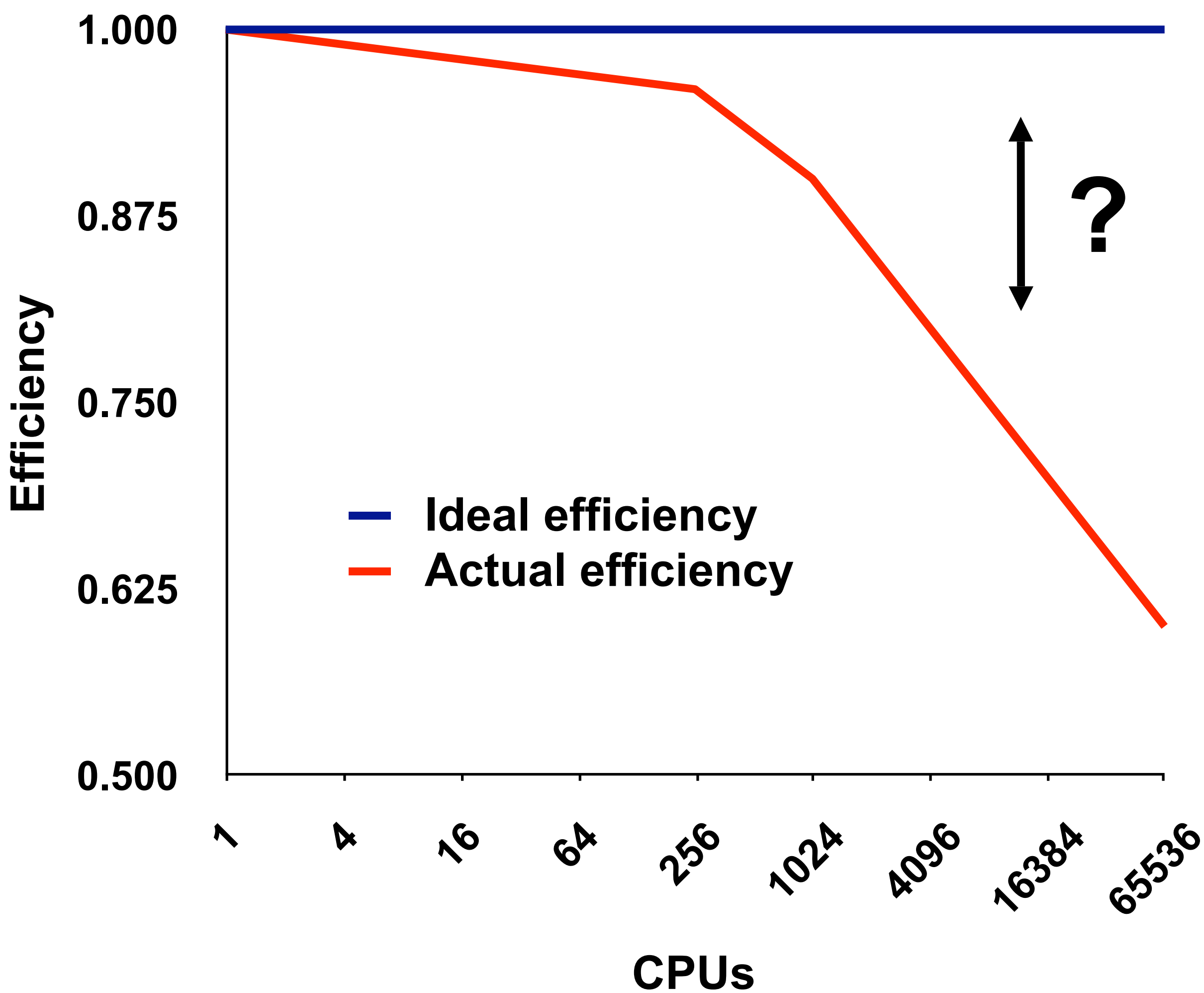
An interface between OS and first-party tools

- Processes
  - parent: pre_fork, post_fork
  - child: init_process, fini_process
- Threads
  - parent: init_thread_support, thread_pre_create, thread_post_create
  - child: init_thread, fini_thread
- Signals
  - selectively catch signals before or instead of delivering to application
- Intercept functions to maintain control
  - e.g. dlopen, sigmask, pthread_sigmask, exit, signal
- Stack unwinding support
  - stack_bottom; identification of PC for bottommost frame

A Few Component Consumers

- Rice: using SymtabAPI and libmonitor in HPCToolkit
- Krell Institute (Open|SpeedShop) Using SymtabAPI to get symbols for their offline collectors. Using libmonitor to manage first-party tools
- UNC and LLNL: using SymtabAPI and StackwalkerAPI for PnMPI project.
- LLNL (STAT project): using SymtabAPI and StackwalkerAPI.
- SiCortex: porting SymtabAPI to Linux/MIPs; uses libmonitor underneath HPCToolkit
- Cray: started work using StackwalkerAPI and SymtabAPI for new APT (Abnormal Process Termination) system
- Univ. of Oregon: using binary rewriter as part of TAU instrumentation
- Forschungszentrum Jülich: using SymtabAPI for Scalasca
- Berkeley (BitBlaze): APIs for binary processing (security tools)

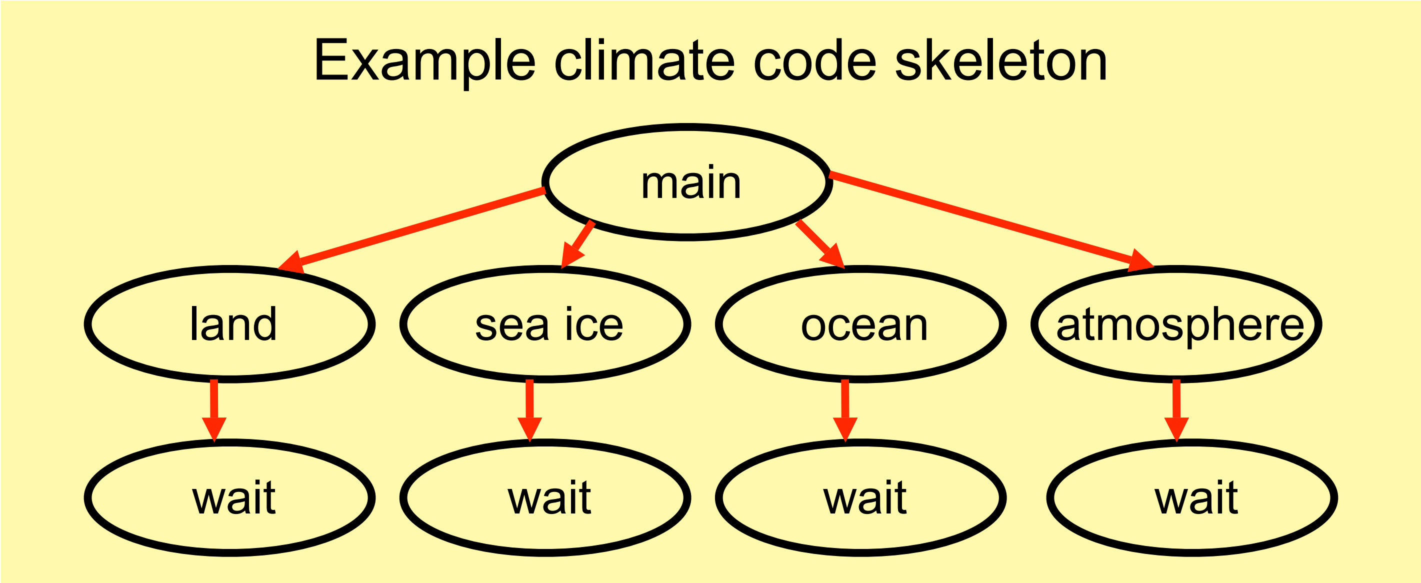
Pinpointing Scalability Bottlenecks



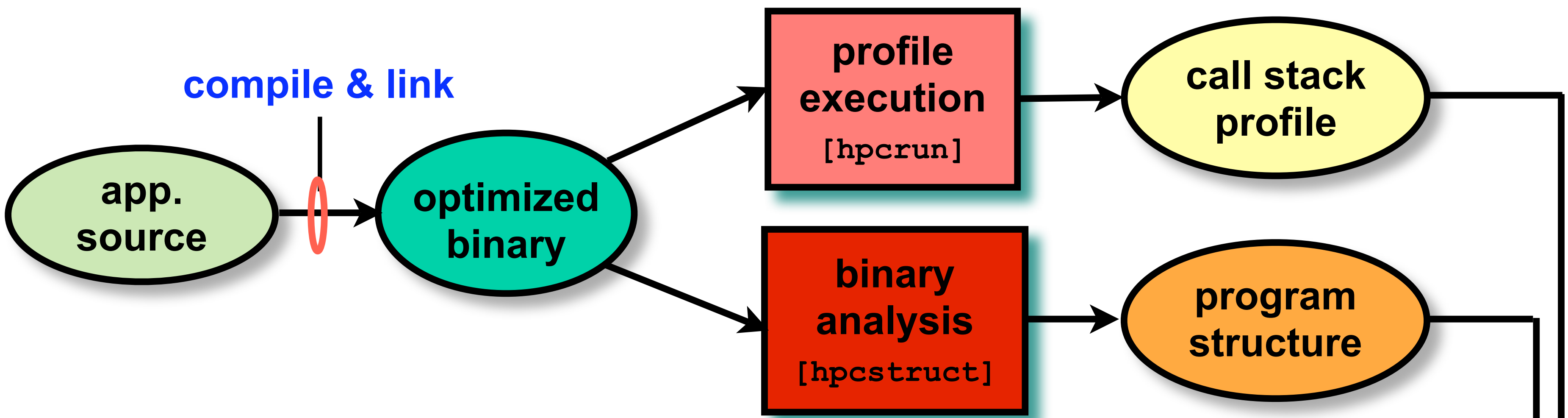
Note: higher is better

Bottleneck Analysis Challenges

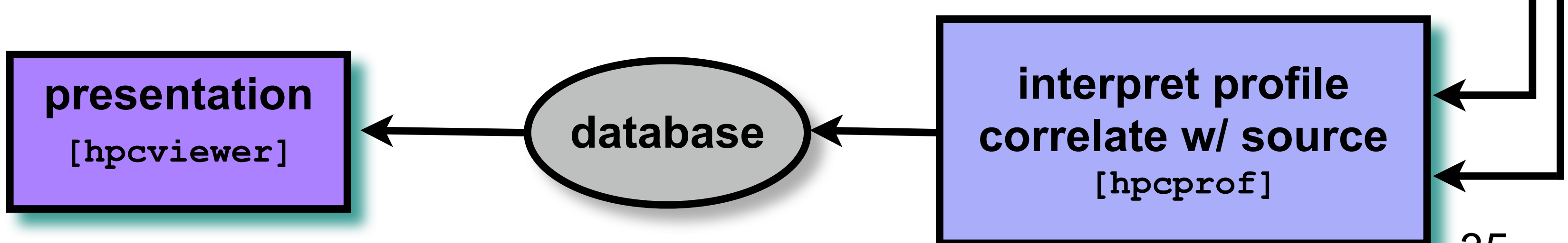
- Parallel applications
  - modern software uses layers of libraries
  - performance is often context dependent
- Monitoring
  - bottleneck nature: computation, data movement, synchronization?
  - size of petascale platforms demands acceptable data volume
  - low perturbation for use in production runs



HPCToolkit Performance Tools



- Measurement, analysis, attribution, and presentation of application performance
- Pinpoint and quantify performance bottlenecks
  - — across scalable parallel systems
  - — within multicore nodes
  - — independent of programming model or cause

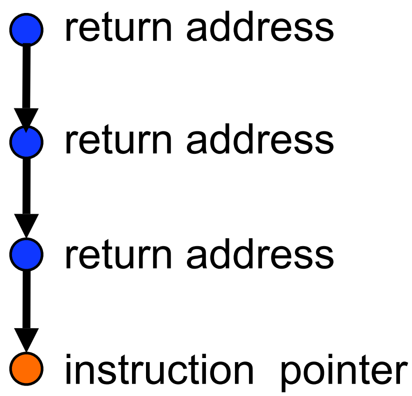


Call Path Profiling

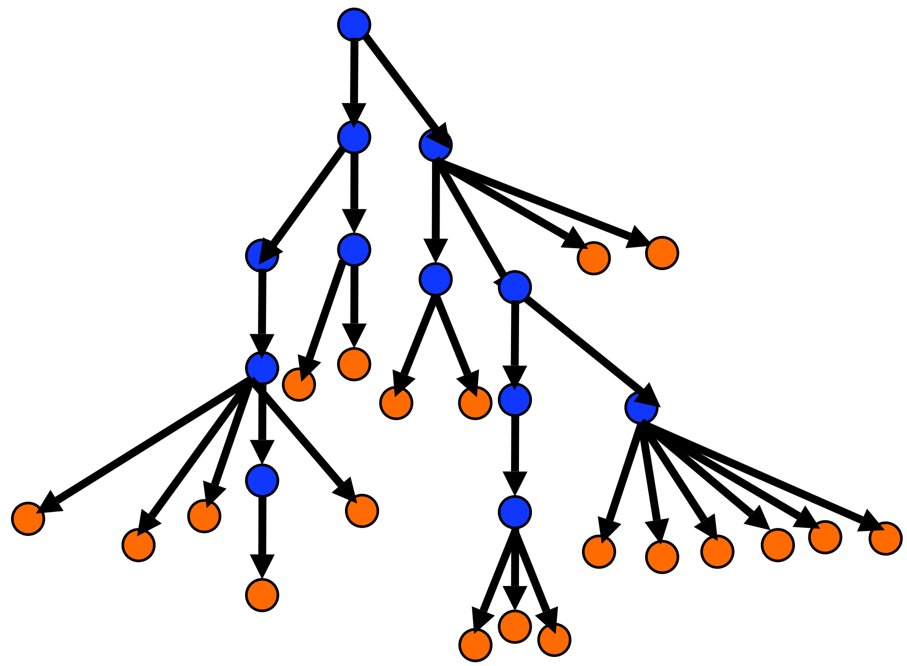
Measure and attribute costs in context

- Sample timer or hardware counter overflows
- Gather calling context using stack unwinding

Call path sample

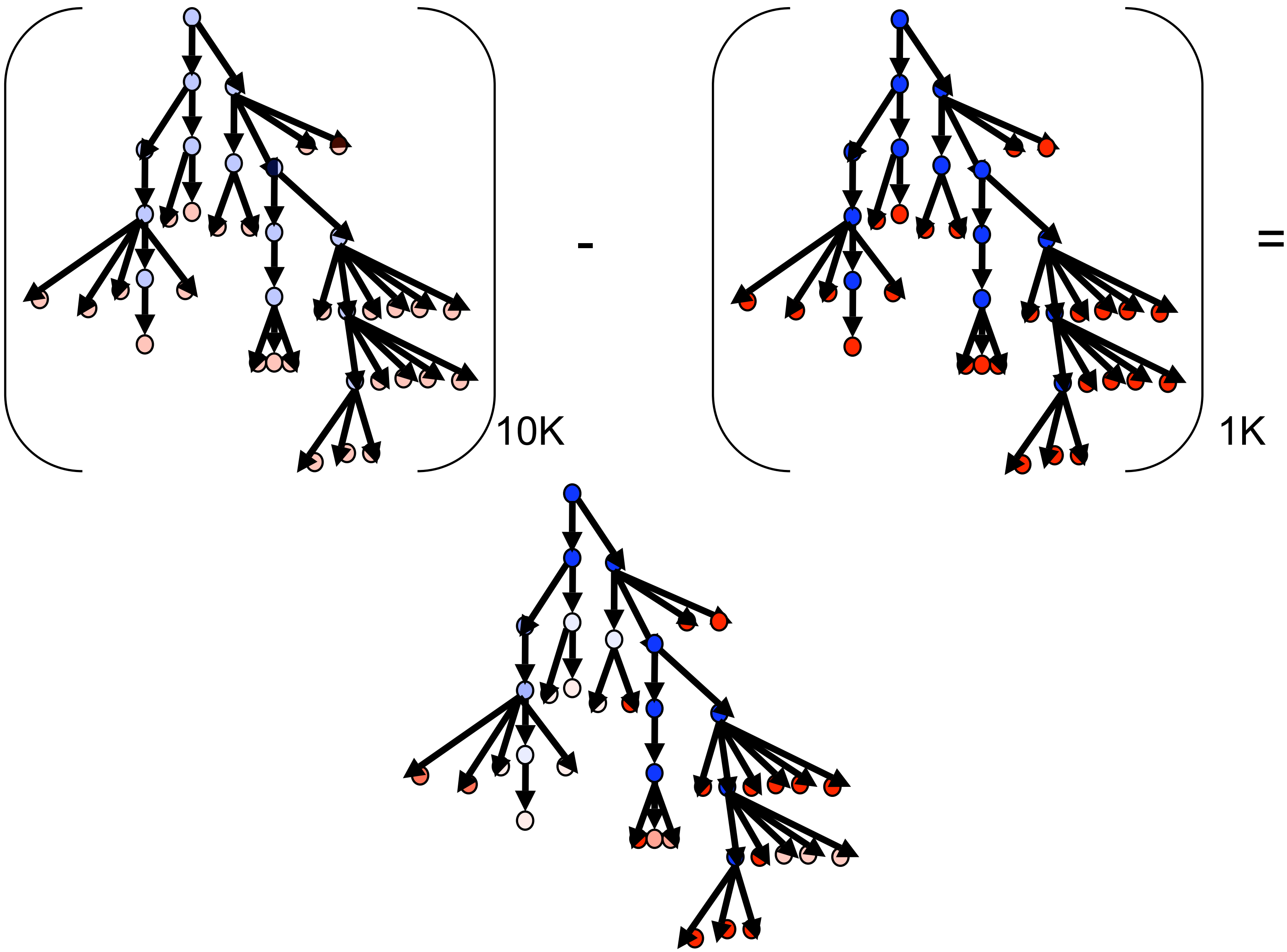


Calling Context Tree (CCT)



Overhead proportional to sampling frequency...
...not call frequency

Weak Scaling: 1K to 10K processors



S3D Multicore Losses at the Loop Level

hpcviewer: [Profile Name]

getrates.f | rhsf.f90 | diffflux_gen_uj.f

```
     *ge. 2) then
             l__ujUpper30 = (3 - 1 + 1) / 3 * 3 + 1 - 1
              do m = 1,l__ujUpper30, 3
                do n = 1, n_spec - 1
                  do lt__2 = 1, nz
                    do lt__1 = 1, ny
                      do lt__0 = 1, nx
                        diffflux(lt__0, lt__1, lt__2, n, m) = -ds_mixavg
     *(lt__0, lt__1, lt__2, n) * (grad_ys(lt__0, lt__1, lt__2, n, m) + y
     *s(lt__0, lt__1, lt__2, n) * grad_mixmw(lt__0, lt__1, lt__2, m))
                        diffflux(lt__0, lt__1, lt__2, n_spec, m) = difff
     *lux(lt__0, lt__1, lt__2, n_spec, m) - diffflux(lt__0, lt__1, lt__2
     *, n, m)
                        diffflux(lt__0, lt__1, lt__2, n, m + 1) = -ds_mi
     *xavg(lt__0, lt__1, lt__2, n) * (grad_ys(lt__0, lt__1, lt__2, n, m
     *+ 1) + ys(lt__0, lt__1, lt__2, n) * grad_mixmw(lt__0, lt__1, lt__2
```

highlighted loop is 2.84x slower on 8 cores in a weak scaling study

Calling Context View | Callers View | Flat View

Scope	1-core (ms) (I)		1-core (ms) (E)		8-core(1) (ms) (I)		8-core(1) (ms) (E)...		Multicore ...ss	
loop at diffflux_gen_uj.f: 197-22	2.86e06	2.6%	2.86e06	2.6%	8.12e06	4.3%	8.12e06	4.3%	5.27e06	6.9%
loop at integrate_erk_jstage_lt_ge	1.09e08	98.1%	1.25e06	1.1%	1.84e08	97.9%	5.94e06	3.2%	4.70e06	6.1%
loop at variables_m.f90: 88-99	1.49e06	1.3%	1.49e06	1.3%	6.08e06	3.2%	6.08e06	3.2%	4.60e06	6.0%
loop at rhsf.f90: 516-536	2.70e06	2.4%	1.31e06	1.2%	6.49e06	3.5%	3.72e06	2.0%	2.41e06	3.1%
loop at rhsf.f90: 538-544	3.35e06	3.0%	1.45e06	1.3%	7.06e06	3.8%	3.82e06	2.0%	2.36e06	3.1%
loop at rhsf.f90: 546-552	2.56e06	2.3%	1.47e06	1.3%	5.86e06	3.1%	3.42e06	1.8%	1.96e06	2.6%
loop at thermchem_m.f90: 127-1	8.00e05	0.7%	8.00e05	0.7%	2.28e06	1.2%	2.28e06	1.2%	1.48e06	1.9%
loop at heatflux_lt_gen.f: 5-132	1.46e06	1.3%	1.46e06	1.3%	2.88e06	1.5%	2.88e06	1.5%	1.41e06	1.8%
loop at rhsf.f90: 576	6.65e05	0.6%	6.65e05	0.6%	1.87e06	1.0%	1.87e06	1.0%	1.20e06	1.6%
loop at getrates.f: 504-505	8.00e06	7.2%	8.00e06	7.2%	8.74e06	4.7%	8.74e06	4.7%	7.35e05	1.0%
loop at derivative_x.f90: 213-690	1.78e06	1.6%	1.78e06	1.6%	2.47e06	1.3%	2.47e06	1.3%	6.95e05	0.9%

Multicore Loss
(Multicore time - single core time)

Moab: Integrated Static and Dynamic Info

hpcviewer: mbperf_iMesh 200 B / intel -O3

mbperf_iMesh.cpp | stl_tree.h | TypeSequenceManager.hpp | iMesh_MOAB.cpp

```
25  class SequenceCompare {
26    public: bool operator()( const EntitySequence* a, const EntitySequence* b ) const
27      { return a->end_handle() < b->start_handle(); }
28  };
```

Calling Context View | Callers View | Flat View

Scope	PAPI_TOT_CYC (I)	PAPI_TOT_CYC (E)	PAPI_L2_DCM (I)	PAPI_RES_STL (E)	PA
Experiment Aggregate Metrics	1.13e11 100 %	1.13e11 100 %	3.01e08 100 %	7.62e10 100 %	
main	1.13e11 100 %	2.75e09 2.4%	3.01e08 100 %	2.59e09 3.4%	
testB(void*, int, double const*, int const*)	1.10e11 97.6%	4.71e09 4.2%	2.71e08 90.0%	4.09e09 5.4%	
inlined from mbperf_iMesh.cpp: 261	9.71e10 85.9%	1.04e09 0.9%	2.34e08 77.8%	7.05e08 0.9%	
loop at mbperf_iMesh.cpp: 336-349	6.42e10 56.7%	1.75e08 0.2%	1.30e08 43.3%	2.72e07 0.0%	
imesh_getentadj_	6.36e10 56.3%	9.00e07 0.1%	1.30e08 43.3%	4.00e05 0.0%	
imesh_getentarradj_	6.35e10 56.2%	2.29e09 2.0%	1.30e08 43.3%	2.26e08 0.3%	
loop at iMesh_MOAB.cpp: 1010-1024	6.23e10 55.1%	1.82e09 1.6%	1.30e08 43.3%	1.29e08 0.2%	
MBCore::get_adjacencies(unsigned long const*, int, int, bool, std::vector<unsig	5.60e10 49.5%	3.75e08 0.3%	1.30e08 43.3%	3.52e07 0.0%	
AEntityFactory::get_adjacencies(unsigned long, unsigned int, bool, std::vec	5.56e10 49.2%	2.70e08 0.2%	1.30e08 43.2%	3.78e07 0.0%	
AEntityFactory::create_vert_elem_adjacencies()	4.32e10 38.2%	1.72e09 1.5%	1.11e08 37.0%	1.29e09 1.7%	
loop at AEntityFactory.cpp: 513-530	4.32e10 38.2%	1.72e09 1.5%	1.11e08 37.0%	1.29e09 1.7%	
loop at AEntityFactory.cpp: 522-530	4.32e10 38.2%	1.72e09 1.5%	1.11e08 37.0%	1.29e09 1.7%	
loop at AEntityFactory.cpp: 529-530	4.28e10 37.8%	1.60e09 1.4%	1.11e08 37.0%	1.24e09 1.6%	
AEntityFactory::add_adjacency(unsigned long, unsig	4.13e10 36.5%	1.11e10 9.9%	1.08e08 36.0%	8.38e09 11.0%	
AEntityFactory::get_adjacencies(unsigned long,	2.29e10 20.2%	2.22e10 19.6%	7.58e07 25.2%	1.78e10 23.4%	
inlined from stl_tree.h: 466	1.10e10 9.8%	1.10e10 9.8%	5.94e07 19.8%	8.96e09 11.8%	
loop at stl_tree.h: 1370	1.10e10 9.7%	1.10e10 9.7%	5.94e07 19.8%	8.95e09 11.8%	
inlined from TypeSequenceManager.h	1.02e10 9.0%	1.02e10 9.0%	5.80e07 19.3%	8.35e09 11.0%	
TypeSequenceManager.hpp: 27	1.02e10 9.0%	1.02e10 9.0%	5.80e07 19.3%	8.35e09 11.0%	
inlined from stl_tree.h: 485	6.20e08 0.5%	6.20e08 0.5%	9.00e05 0.3%	4.81e08 0.6%	
stl_tree.h: 1370	1.50e08 0.1%	1.50e08 0.1%	5.00e05 0.2%	1.18e08 0.2%	
stl_tree.h: 477	2.00e07 0.0%	2.00e07 0.0%		8.96e06 0.0%	

Outline

- Community engagement
- Research and open source software development
  - system software and language runtime systems
  - communication for partitioned global address space languages
  - math libraries for multicore
  - performance tools
  - ☞ compilers
  - applications
- FY09 plans

Compilers: Runtime Re-optimization

- A source of inefficiency in large-scale applications is the “glue” that holds together code from different sources
  - library code, code cribbed from other applications
  - often different languages with different programming models
    - e.g., call object-oriented code from inside imperative C program

- Classic compilers cannot improve this kind of code
  - compiler never sees all the pieces
    - limits the scope of analysis and transformation
    - could build link-time optimizer, but would miss dynamically linked code
  - good application for runtime re-optimization
    - monitor execution, notice inefficiency, rewrite code to avoid it

Runtime Re-optimization

Opportunities for improvement

- Classic answers
  - straighten hot paths to avoid jumps
  - fold constants from input data
  - reschedule long-latency ops to reflect actual behavior

- Opportunities in large-scale applications
  - improve procedure calls & chains of calls (libraries, CCA)
    - Runtime inlining and specialization of calls
  - fold constants from distribution of work and data
  - runtime selection of library components
    - e.g., choose communication routines based on actual distribution

Runtime Re-optimization

Current work

- Experimental
  - we are running a series of small-scale experiments to look at opportunities for improvement and magnitude of potential benefits
  - we have worked with both PIN (x86-specific tool) and LLVM
- Analytical
  - compile-time analysis to predict how much improvement we might find, given some set of runtime-knowable facts
  - compile-time analysis in support of the actual transformations and techniques to encode the results in the executable image

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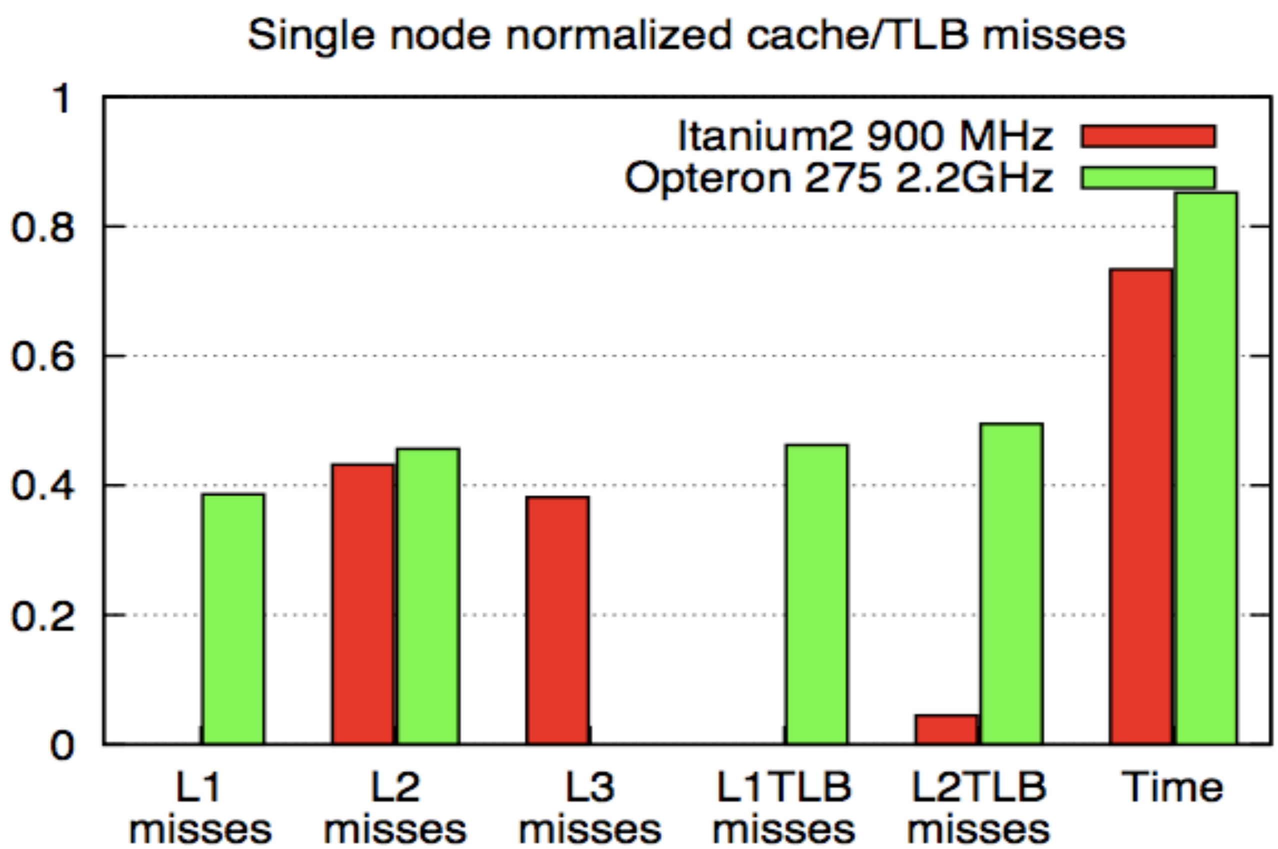
Application Engagement: GTC

- GTC: simulates turbulent plasma in tokamak reactors
  - 3D particle-in-cell code; 1D decomposition along toroidal direction
    - charge: deposit charge from particles to grid points
    - solve: compute the electrostatic potential and field on grid points
    - push: compute the force on each particle from nearby grid points
- Extend performance analysis work of PERI Tiger team
- Used measurement and modeling tools developed at Rice with CScADS support to pinpoint performance losses
  - poor spatial locality due to vector of structures representation for ions
  - unrealized opportunities for temporal reuse between loops over ions
- Code optimization
  - manually transform to structure of vectors
  - manually apply fusion and blocking to improve temporal reuse
  - transmit improvements back to GTC code team

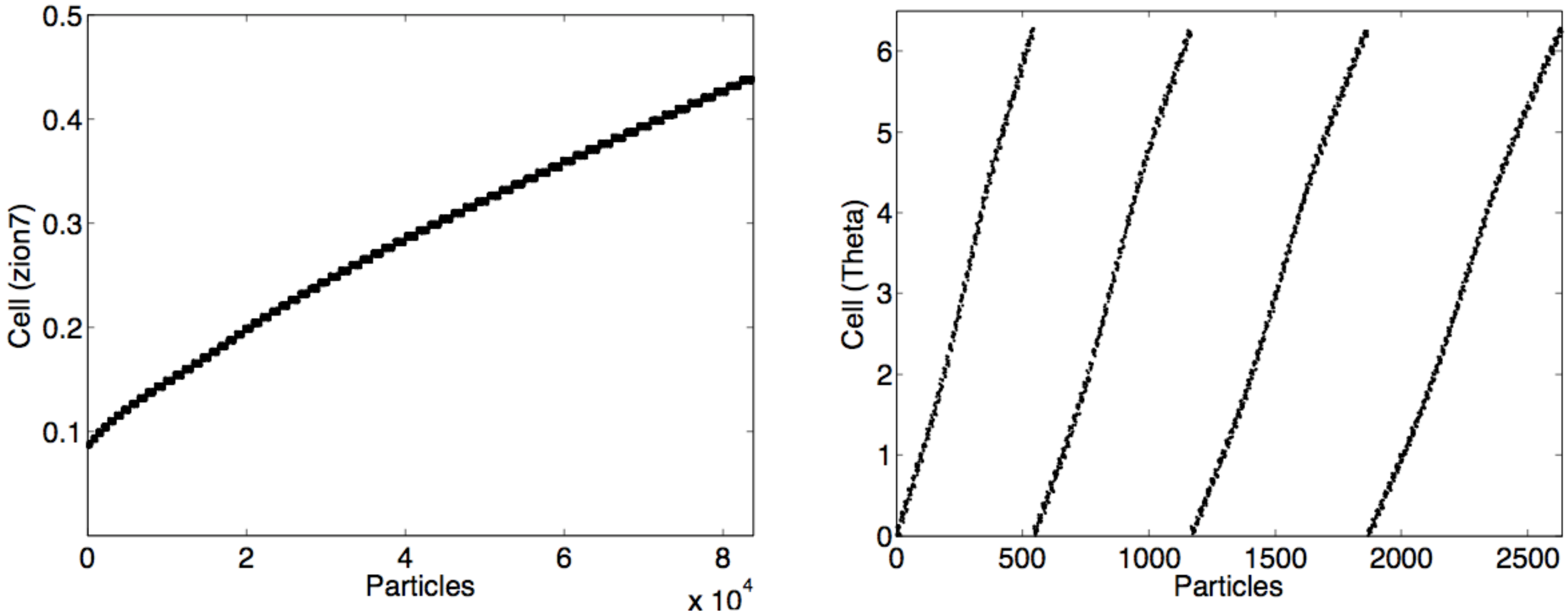
GTC: Node Performance Improvements



- Metrics normalized to measurements of original code
- Lower is better

GTC: Locality Degrades as Ions Swirl

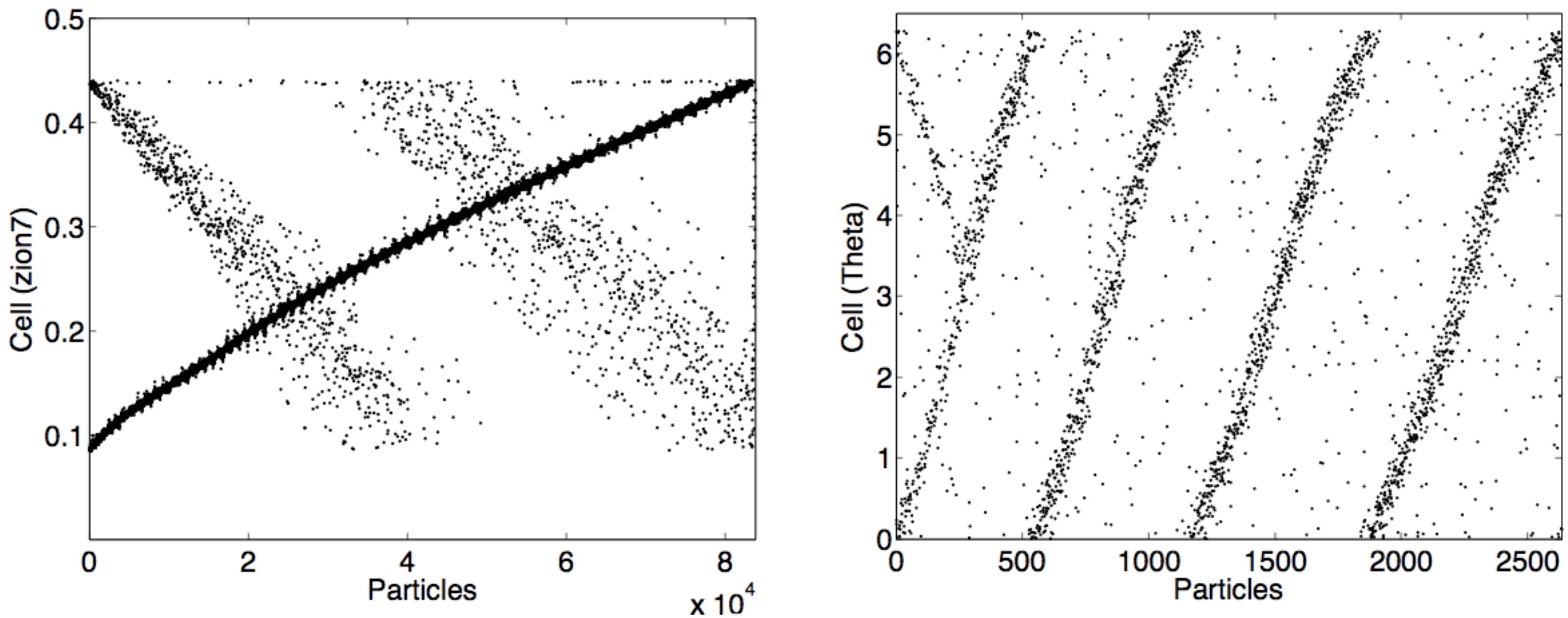
- Locality is best when particles are sorted in cell order
  - —potential computation uses cell data only
  - —charge deposition and particle pushing involve interactions between particles and cells
- <u>Initially particles are uniformly distributed in cell order</u>



Time step 0

GTC: Locality Degrades as Ions Swirl

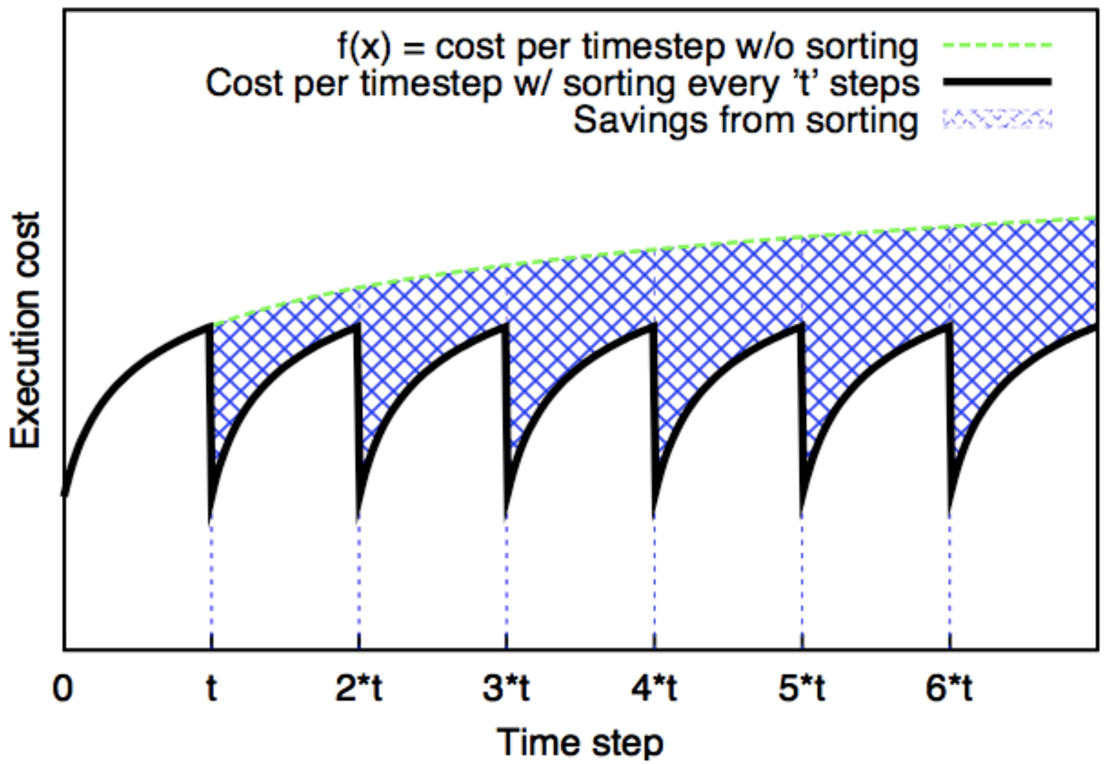
- Locality is best when particles are sorted in cell order
  - —potential computation uses cell data only
  - —charge deposition and particle pushing involve interactions between particles and cells
- Over time, the particle distribution diverges from cell order



Time step 20

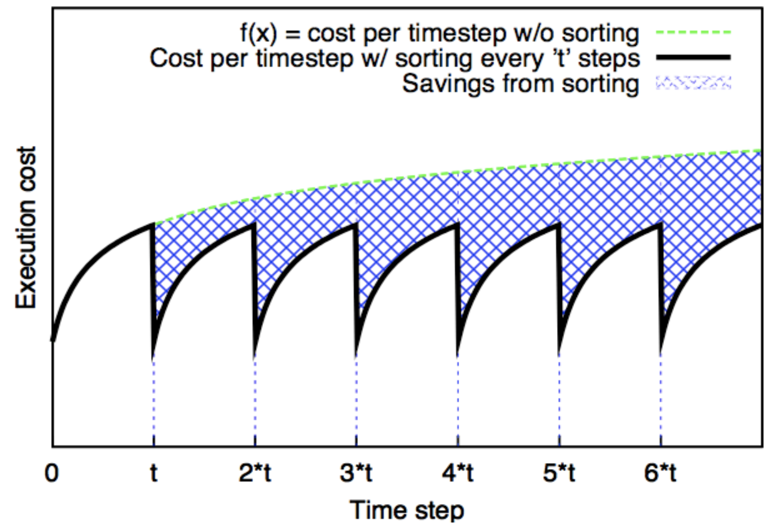
GTC: Potential Improvement from Reordering

- Locality degrades gradually at run-time
- Assumptions:
  - —periodic particle reordering restores locality and performance
  - —performance degrades at similar rate after each sorting step



GTC: Compute Optimal Sorting Interval

- Notations
  - f(x) = time step cost function
  - C = cost of sorting
  - G(t) = gain from sorting every ***t*** time steps



- Find ***t*** that maximizes ***G(t)*** over N steps

$$G(t) = \sum_{k=1}^{\frac{N}{t}-1} \left(\int_{kt}^{(k+1)t} f(x)\,dx - \int_0^t f(x)\,dx - C \right)$$

terms constant in ***t***

$$G(t) = \boxed{\int_0^N f(x)\,dx} - \frac{N}{t}\int_0^t f(x)\,dx - \frac{N}{t}C + \boxed{C}$$

- Find ***t*** that minimizes $h(t) = \frac{1}{t}\left(\int_0^t f(x)\,dx + C \right)$
  - ***h(t)*** = average time step cost with sorting

Adaptive Particle Sorting Algorithm

Step 0: *Compute C*. Measure cost of sorting after program executed a fixed number of time steps. Start initialization at step 1.

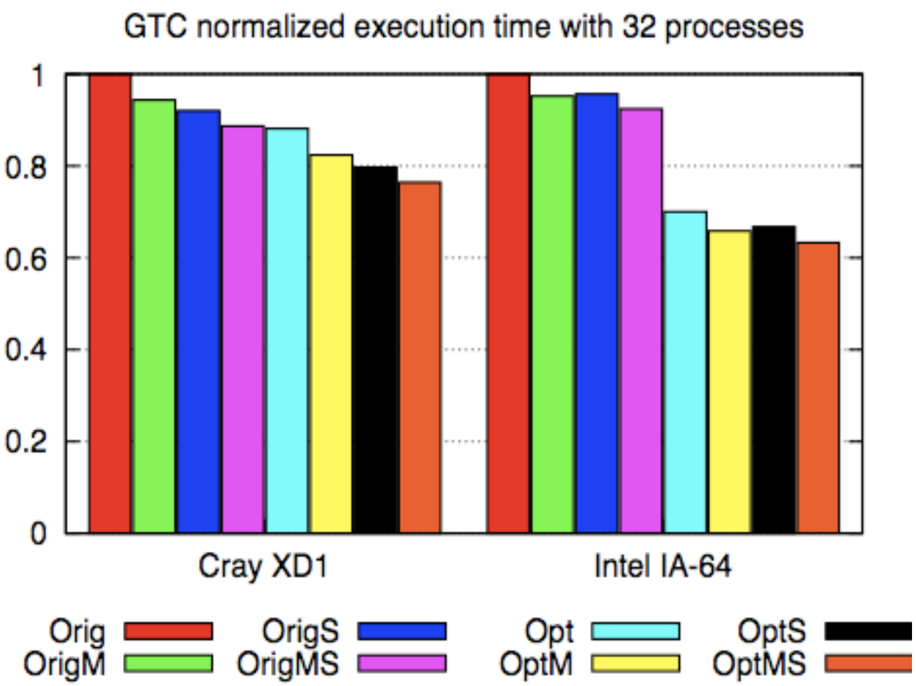
Step 1: *Evaluate h(t)*. At each time step compute the value of the integral incrementally, evaluate $h(t)$, and update h_{min} as needed.

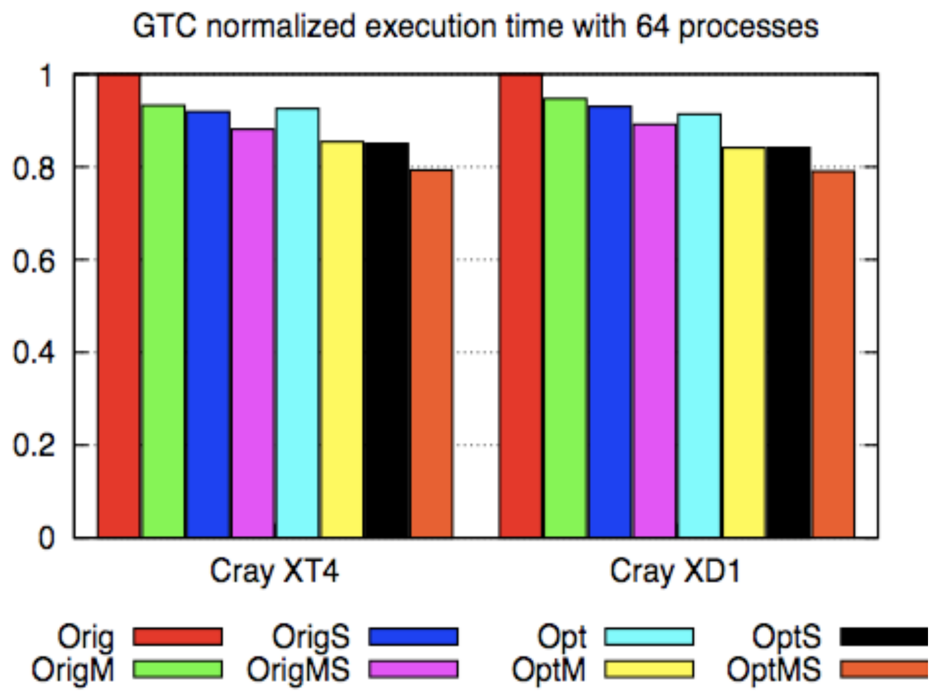
Step 2: *Compute local optimum*. If last $h(t) > h_{min}$, local optimum $\tau_{local} = t-1$

Step 3: *Compute global optimum*. Apply reduction with MAX operator across all processors. Global optimum $\tau = \max(\tau_{local})$

Step 4: *Provide confidence in the global optimum*. Continue initialization (steps 1 to 3) while $t < 2\tau$.

Parallel Performance Results





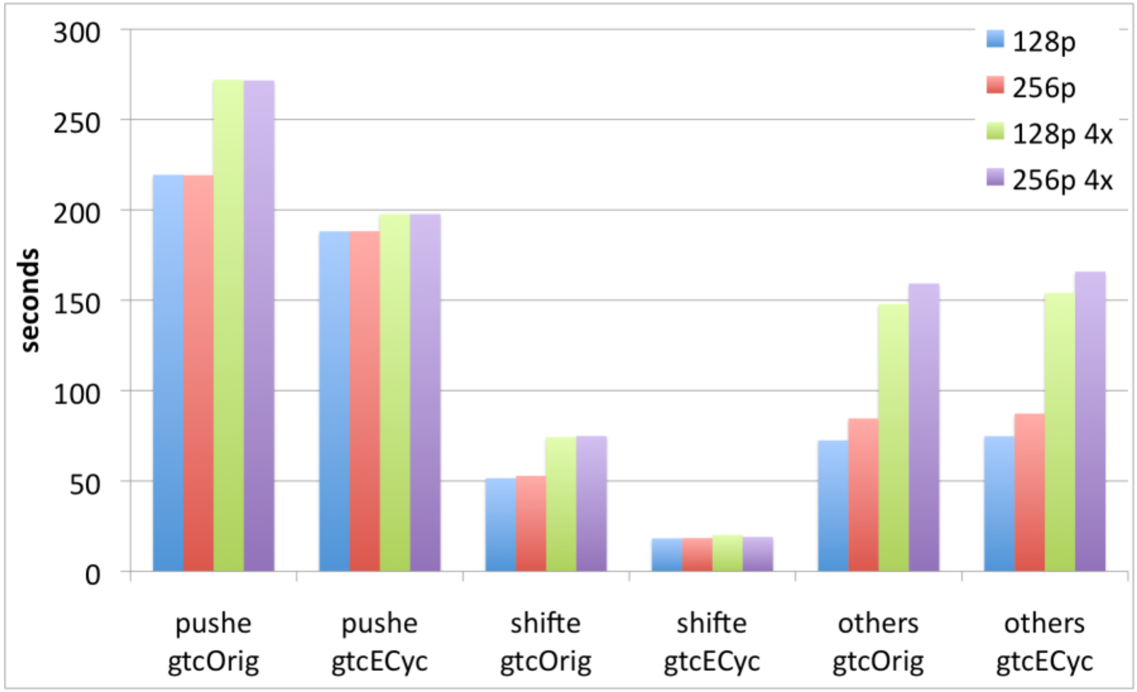
- Combined optimizations reduce GTS execution time by
  - —37% on Itanium2 cluster
  - —21% on Cray XT and Cray XD1

GTC: Electron Sub-Cycle Loop

- GTC simulates ions + trapped electrons
- GTS transformations still apply to ion simulation
- Electrons move much faster than ions
  - execute multiple sub-cycle steps in each time step
  - electron sub-cycle loop dominates simulation cost
  - electron data reused in each sub-step; reuse distance large
- Locality improvements
  - each electron simulated for multiple sub-steps at a time
    - electron data reused with a short distance
    - electron migration accomplished with fewer, larger messages
    - better locality to grid data when electrons become disordered

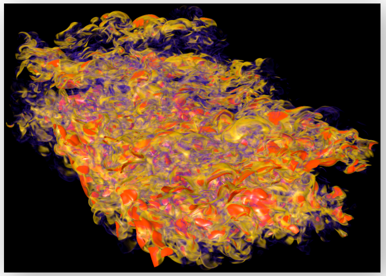
GTC: Electron Sub-Cycle Loop Results

- Evaluate code with restructured electron sub-cycle loop
  - —GTS transformations not applied
  - —128p = 32 poloidal planes x 4 particle domains
  - —256p = 32 poloidal planes x 8 particle domains
  - —4x = four times more grid points, # particles in tokamak unchanged



Application Engagement: S3D

- Direct numerical simulation (DNS) of turbulent combustion
  - state-of-the-art code developed at CRF/Sandia
    - PI: Jaqueline H. Chen, SNL
  - 2007/2008 INCITE awards at NCCS
  - pioneering application for 250TF system



- Extend performance analysis work of PERI Tiger team
  - use HPCToolkit to locate single-core performance bottlenecks
    - compiler inserted array copies
    - streaming calculations with low data reuse
    - loop nests with recurrences
  - identified opportunities for compiler-based improvement
  - enhanced LoopTool for addressing S3D's needs
  - improved loop nests with LoopTool's semi-automatic transforms
    - transformed code is now part of S3D's source base
  - used HPCToolkit to assess multicore scaling issues

S3D: What Opportunities Exist?

5D loop nest:
2D explicit loops
3D F90 vector syntax

mixavg_transport_m.f90

```
diffFlux(:,:,:,n_spec,:) = 0.0
DIRECTION: do m=1,3
 SPECIES: do n=1,n_spec-1

   if (baro_switch) then
     ! driving force includes gradient in mole fraction and baro-diffusion:
     diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                    + Ys(:,:,:,n) * ( grad_mixMW(:,:,:,m)    &
                    + (1 - molwt(n)*avmolwt) * grad_P(:,:,:,m)/Press))
   else
     ! driving force is just the gradient in mole fraction:
     diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                    + Ys(:,:,:,n) * grad_mixMW(:,:,:,m) )
   endif

   ! Add thermal diffusion:
   if (thermDiff_switch) then
     diffFlux(:,:,:,n,m) = diffFlux(:,:,:,n,m)    &
         - Ds_mixavg(:,:,:,n) * Rs_therm_diff(:,:,:,n) * molwt(n) &
         * avmolwt * grad_T(:,:,:,m) / Temp
   endif

   ! compute contribution to nth species diffusive flux
   ! this will ensure that the sum of the diffusive fluxes is zero.
   diffFlux(:,:,:,n_spec,m) = diffFlux(:,:,:,n_spec,m) - diffFlux(:,:,:,n,m)

 enddo SPECIES
enddo DIRECTION
```

initialize

update

reuse

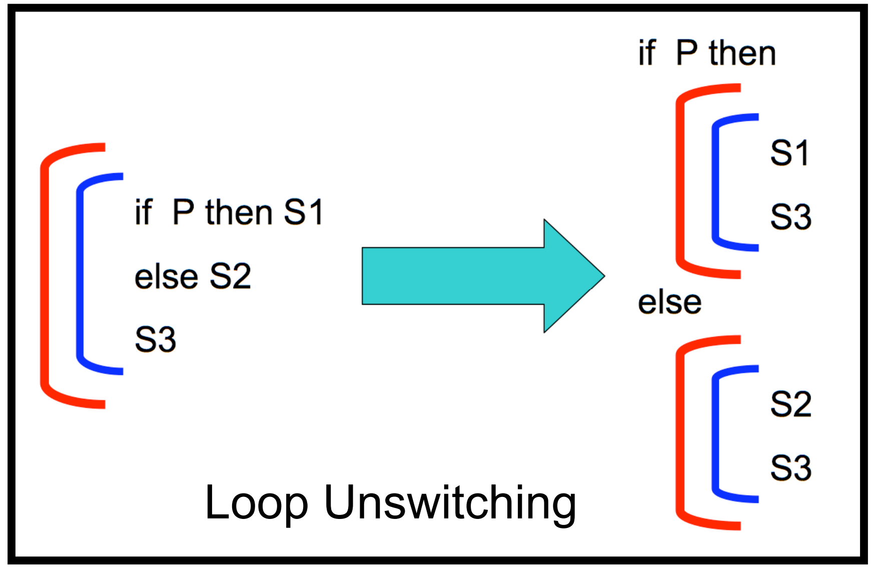
reuse

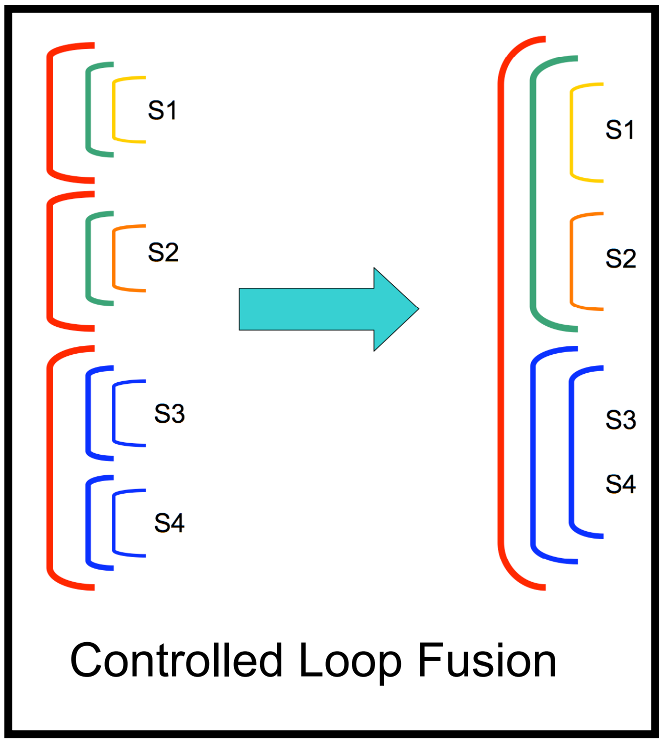
reuse

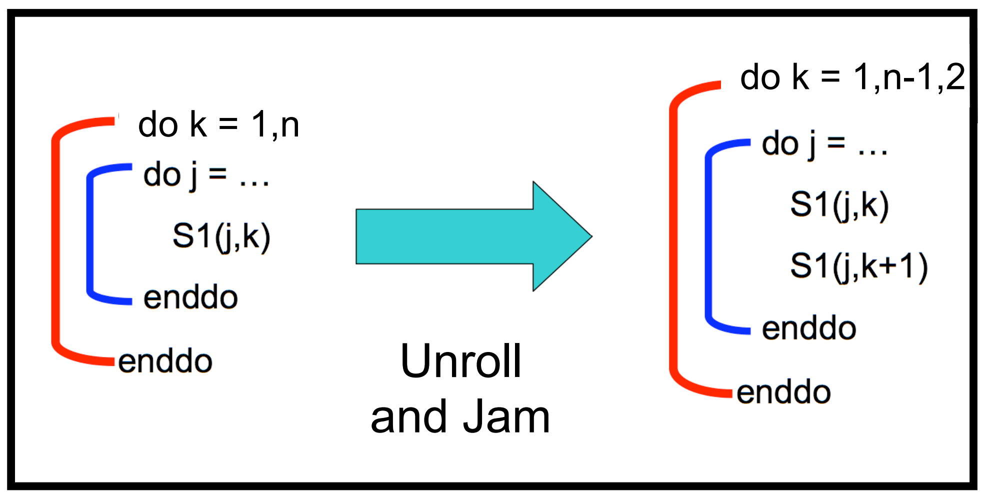
performance problem
data streams in/out of memory

LoopTool: Loop Optimization of Fortran

Rice University's tool for source-to-source transformation of Fortran
(transformation subset shown)







Markup of S3D Diffusive Flux Loop

```
!dir$ uj 3
  do m=1,3 ! DIRECTION
!dir$ uj 2
    do n=1,n_spec-1 ! SPECIES

!dir$ unswitch 2
      if (baro_switch) then
        ! driving force includes gradient in mole fraction and baro-diffusion:
!dir$   fuse 1 1 1
        diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                              + Ys(:,:,:,n) * ( grad_mixMW(:,:,:,m)    &
                              + (1 - molwt(n)*avmolwt) * grad_P(:,:,:,m)/Press))
      else
        ! driving force is just the gradient in mole fraction:
!dir$   fuse 1 1 1
        diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * ( grad_Ys(:,:,:,n,m)  &
                             + Ys(:,:,:,n) * grad_mixMW(:,:,:,m) )
      endif

      ! Add thermal diffusion:
!dir$ unswitch 2
      if (thermDiff_switch) then
!dir$   fuse 1 1 1
        diffFlux(:,:,:,n,m) = diffFlux(:,:,:,n,m) - Ds_mixavg(:,:,:,n) *
          Rs_therm_diff(:,:,:,n) * molwt(n) * avmolwt * grad_T(:,:,:,m) / Temp
      endif

          ! compute contribution to nth species diffusive flux
          ! this will ensure that the sum of the diffusive fluxes is zero.
!dir$     fuse 1 1 1
      diffFlux(:,:,:,n_spec,m) = diffFlux(:,:,:,n_spec,m) - diffFlux(:,:,:,n,m)

    enddo ! SPECIES
  enddo ! DIRECTION
```

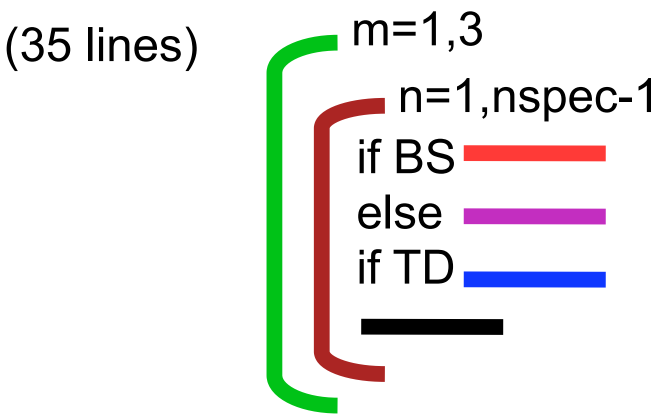
unroll and jam directives

unswitching directives

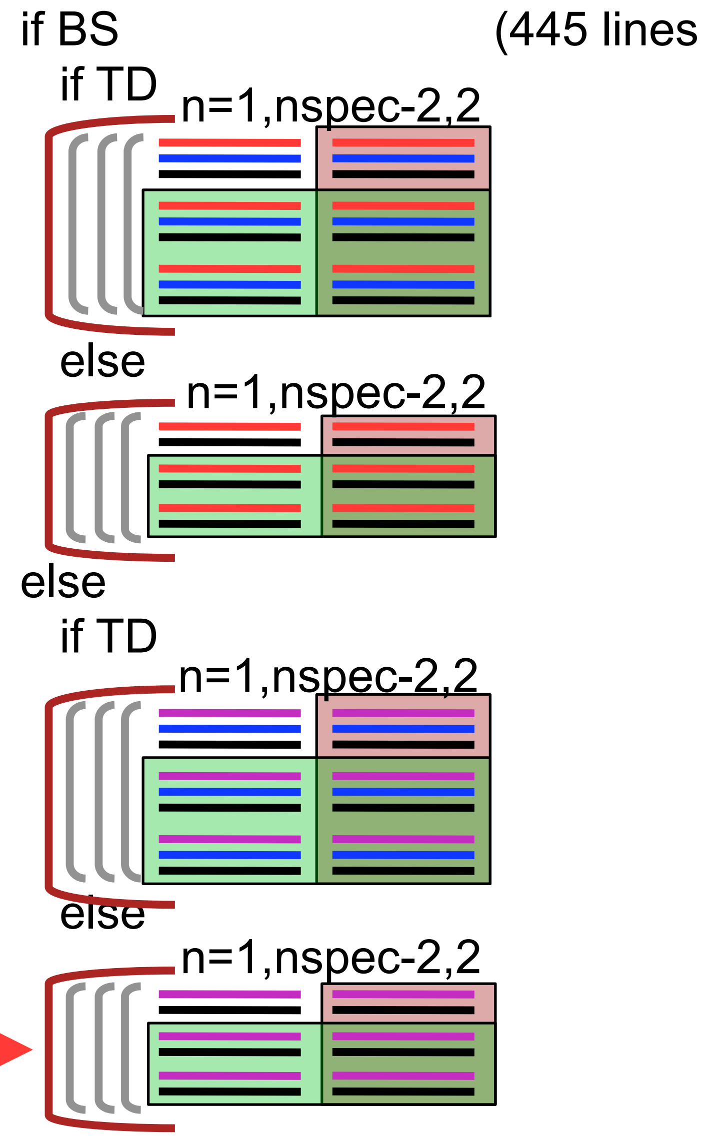
controlled fusion directives

Add LoopTool directives to source program

Optimization of S3D Diffusive Flux Loop



LoopTool



Transformation Log:

- scalarization (4 stmts)
- loop unswitching (2 conditions)
- fusion (loops within 4 outer nests)
- unroll-and-jam (2 loops)
- peeling excess iterations (4 nests)

2.94x faster than original
(6.7% total savings)

Engagement: Other

- Enabling technologies engagement
  - APDEC: Chombo (structured AMR)
  - ITAPS: Moab/iMESH (meshing)
- Application engagement using HPCToolkit
  - UNEDF: MFDn (many Fermion dynamics - nuclear)
  - USQCD: Chroma (quantum chromodynamics)
  - Center for Turbulence Research: Hybrid (shock + turbulence)
  - NETL: MFiX (multiphase flow with interface exchanges)
  - Iowa State: CAM-EULAG (atmospheric modeling)
  - Gromacs (cellulosic ethanol)
- Working with Fortran 2008 J3 standards committee on parallelism via coarrays

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FY09 Plans

- ANL
  - continue to replace components in BG/P s/w stack with open source
- Berkeley
  - release UPC and GASNet with improved support for BG/P, XT, and IB
  - optimize sparse linear algebra libraries for multicore (with UTK)
- Rice
  - performance tools
    - deploy HPCToolkit on the leadership computing platforms
    - devise support for working with data from a huge # of cores
  - compilers
    - continue work on dynamic optimization, ROSE, scripting languages
    - release a version of LoopTool for use by application teams
- Tennessee
  - explore dynamic and adaptive out-of-order execution patterns for linear algebra on multicore and heterogeneous nodes
- Wisconsin
  - continue development of InstructionAPI and ControlFlowAPI