Center for Scalable Application Development Software - Overview

John Mellor-Crummey, Keith Cooper (Rice)
Peter Beckman, Ewing Lusk (ANL)
Jack Dongarra (UTK)
Bart Miller (Wisconsin)
Katherine Yelick (UCB/LBNL)

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

Scope of Activities

- Community engagement
- Research and development
  - system software
  - communication for partitioned global address space languages
  - math libraries for multicore
  - performance tools
  - compilers
- Open source software infrastructure
  - performance tool components
  - compilers
- Application outreach

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

R&D: System Software

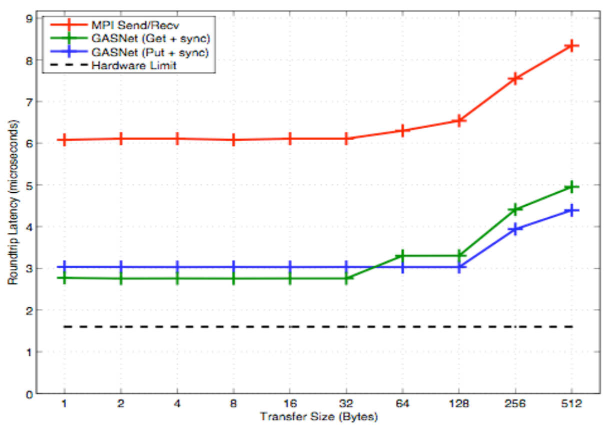
Developing open software stack for leadership computing platforms

- Focus
  - compute node operating system
  - I/O communication layer
- Benefits
  - facilitates infusion of software research into production systems
  - rapid (local) resolution of problems that might arise
- Results
  - Blue Gene/P compute node OS and I/O layer operational
  - supports BG/P for high throughput computing (HTC) as well as HPC
  - negligible performance penalty compared to IBM's s/w stack

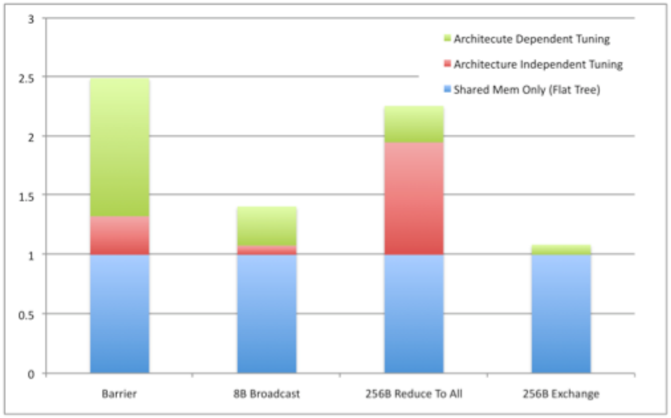
R&D: PGAS Communication Layer

Goals: low latency; high bandwidth; efficient collectives

- Planned SC08 release of GASNet and Berkeley UPC
  - updated Portals conduit for Cray XT3/4/5 platforms with “firehose”
  - 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 supported by PModels and others
- Optimization of UPC collectives for multicore



BG/P: GASNet vs. MPI latency
(lower is better)



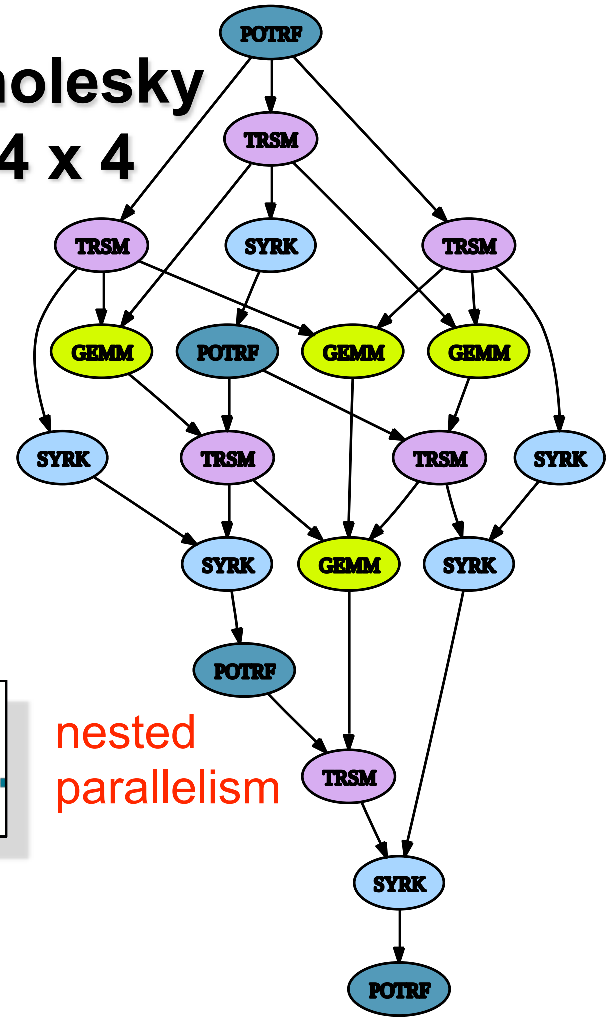
Autotuning collectives for Niagara2
(higher is better)

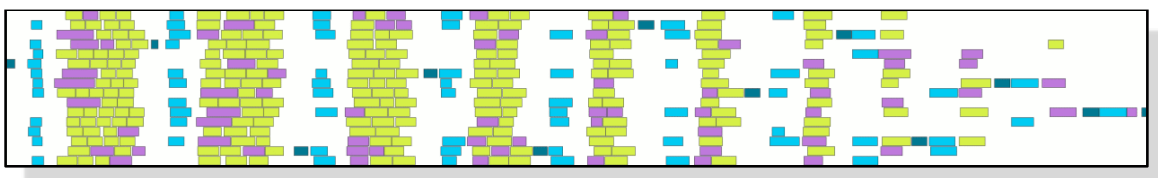
R&D: Parallel Linear Algebra

PLASMA: Parallel Linear Algebra s/w for Multicore Architectures

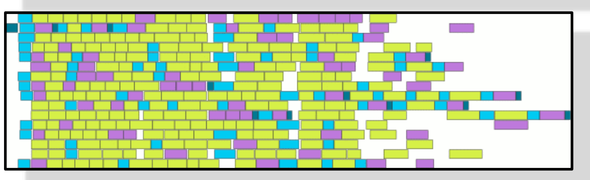
- Objectives
  - high utilization of each core
  - scaling to large number of cores
  - shared or distributed memory
- Methodology
  - DAG scheduling
  - explicit parallelism
  - implicit communication
- Arbitrary DAG with fully dynamic scheduling

Cholesky 4 x 4





nested parallelism



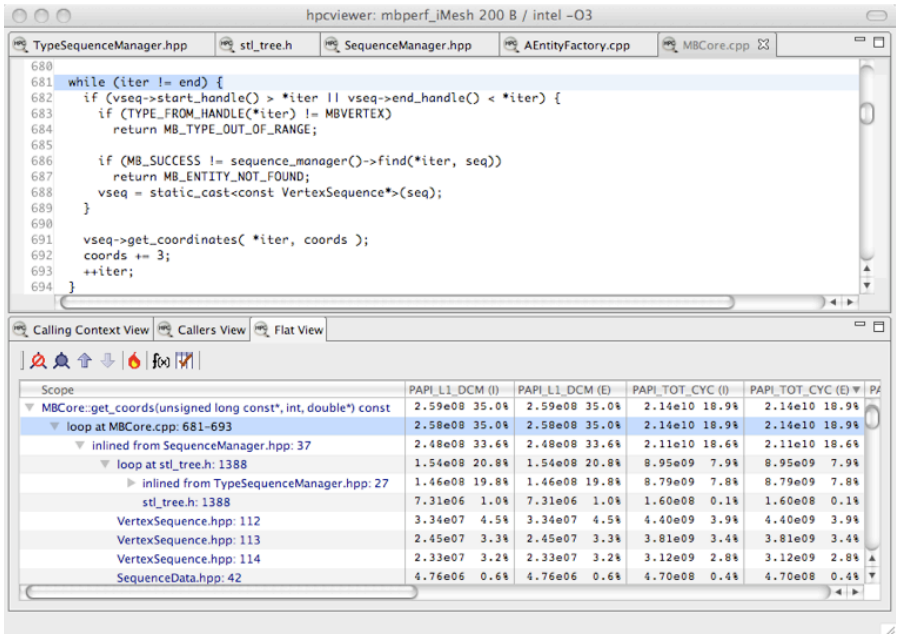
PLASMA

R&D: HPCToolkit Performance Tools

Support measurement, analysis, and attribution of performance problems on petascale systems

- Partnership between
  - Performance Engineering Research Institute
  - Center for Scalable Application Development Software
- New capabilities
  - sampling-based measurement of fully-optimized parallel codes on both Cray XT and Blue Gene systems
    - uses on-the-fly binary analysis for stack unwinding of fully-optimized code
    - supports different kinds of executables
      - statically-linked: Blue Gene, Cray XT
      - dynamically-linked: Linux
  - strategies for pinpointing bottlenecks and quantifying inefficiencies
    - across scalable parallel systems
    - within multicore nodes

R&D: Performance Tool User Interfaces



hpcviewer

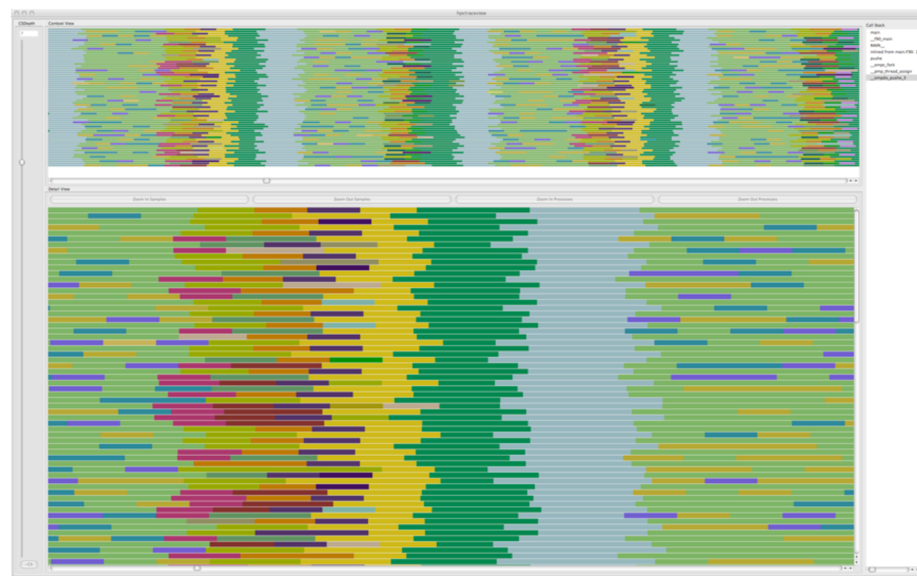
- correlates measurements with source
- provides actionable feedback
- supports scalability analysis on and between nodes with derived metrics

(status: deployment fall 2008)

hpctraceviewer

- displays temporal behavior of parallel applications
- provides hierarchical view call stack sample traces from HPCToolkit

(status: prototype summer 2008)



R&D: Compilers for 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
- Classic compilers cannot improve this kind of code
  - compiler never sees all the pieces; can’t optimize them together
  - good application for runtime re-optimization
- Opportunities in large-scale applications
  - improve procedure calls & chains of calls (libraries, CCA)
    - runtime inlining and specialization of calls
  - runtime selection of library components
- Ongoing work
  - experimentation to quantify opportunities and estimate benefits
  - compiler analysis for runtime estimation of benefits
  - compiler analysis to support runtime optimization

Open Source: Performance Tools

Performance Tool Components

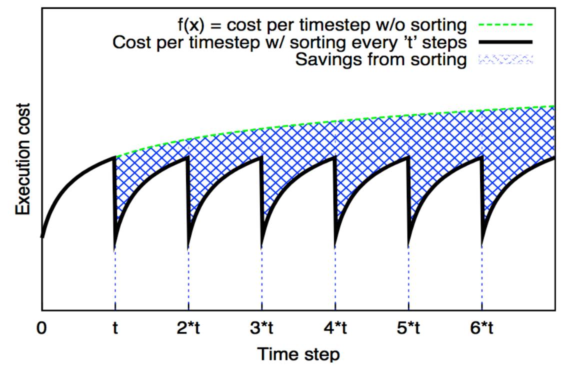
- libmonitor: first-party interface between performance tools and OS
  - manages process init/fork/exec/exit, thread create/init/join, signal delivery etc.
  - clients: HPCToolkit, Open|Speedshop, SciCortex
- InstructionAPI
  - abstract representation of instruction decode and address modes.
- ControlFlowAPI
  - platform independent representation of CFG, associated query routines, and extensible data structures

Open Source: Compiler Technology

- LLNL's ROSE compiler: working with LLNL and LANL
  - adding full-featured Fortran support
  - adding support for Coarray Fortran 2.0
- LoopTool: memory hierarchy optimization of Fortran programs
  - source-to-source transformation of Fortran
  - capabilities include scalarization, loop fusion, blocking, unswitching
  - refined to ameliorate bottlenecks in S3D

Application Engagement: GTC

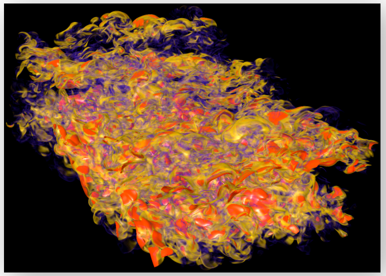
- GTC: simulates turbulent plasma in tokamak reactors
  - 3D particle-in-cell code; 1D decomposition along toroidal direction
    - charge: deposit charge from particles to grid points
    - solve: compute the electrostatic potential and field on grid points
    - push: compute the force on each particle from nearby grid points
- Grand challenge simulations require petascale systems
    - microprocessor-based petascale systems are scarce resources
    - efficient use requires effective use of multi-level memory hierarchies
- Data locality optimization of GTC by CScADS & PERI @ Rice
  - restructured program data and loops
  - adaptively reorder ions at run time
    - at run time, locality degrades gradually as ions in the plasma become disordered
    - periodic particle reordering restores locality and performance



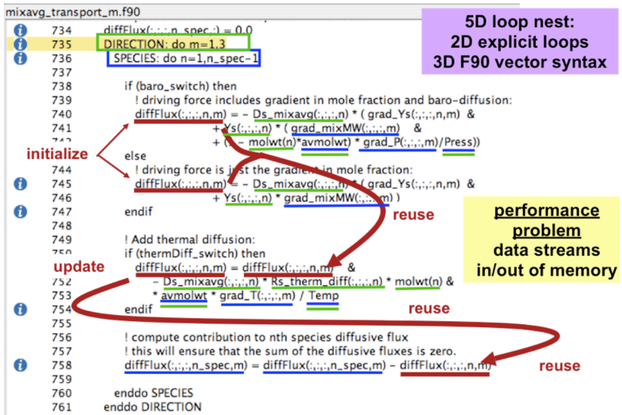
- Reduces GTC shaped plasma simulation time by 21% on Cray XT

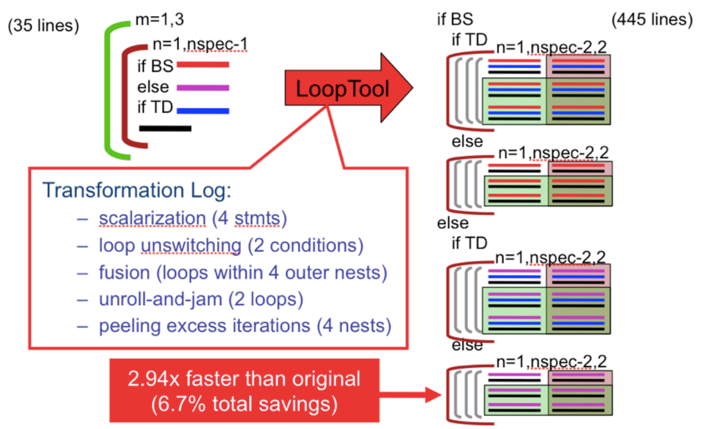
Application Engagement: S3D

- 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



- Identified node performance bottlenecks with HPCToolkit
  - low temporal reuse in diffusive flux calculation among others
  - unnecessary array copying at subroutine interfaces
- Improved loop nests with LoopTool's semi-automatic transforms





Engagement: Other

- Enabling technologies engagement
  - APDEC: Chombo (structured AMR)
  - ITAPS/TASCS: Moab/iMESH (meshing)
  - PERI: performance tools development; Tiger teams
- 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