

HPCToolkit: Sampling-based Performance Tools for Leadership Computing

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http://hpctoolkit.org



Acknowledgments

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Challenges

- Gap between typical and peak performance is huge
- Complex architectures are harder to program effectively
 - processors that are pipelined, out of order, superscalar
 - multi-level memory hierarchy
 - multi-level parallelism: multi-core, SIMD instructions
- Complex applications pose challenges
 - for measurement and analysis
 - for understanding and tuning
- Leadership computing platforms: additional complexity
 - more than just computation: communication, I/O
 - immense scale
 - unique microkernel-based operating systems

Performance Analysis Principles

- Without accurate measurement, analysis is irrelevant
 - avoid systematic measurement error
 - instrumentation-based measurement is often problematic
 - measure actual system, not a mock up
 - fully optimized production code on the platform of interest
- Without effective analysis, measurement is irrelevant
 - pinpoint and explain problems in terms of source code
 - binary-level measurements, source-level insight
 - compute insightful metrics
 - "unused bandwidth" or "unused flops" rather than "cycles"
- Without scalability, a tool is irrelevant
 - large codes
 - large-scale node parallelism + multithreading

Performance Analysis Goals

- Accurate measurement of complex parallel codes
 - large, multi-lingual programs
 - fully optimized code: loop optimization, templates, inlining
 - binary-only libraries, sometimes partially stripped
 - complex execution environments
 - dynamic loading (e.g. Linux clusters) vs. static linking (Cray XT, BG/P)
 - SPMD parallel codes with threaded node programs
 - batch jobs
- Effective performance analysis
 - insightful analysis that pinpoints and explains problems
 - correlate measurements with code (yield actionable results)
 - intuitive enough for scientists and engineers
 - detailed enough for compiler writers
- Scalable to leadership computing systems

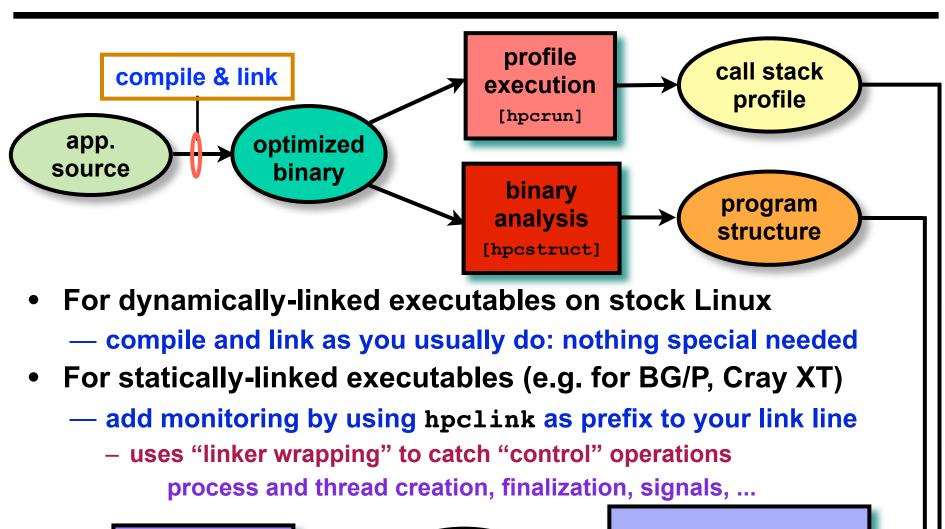
HPCToolkit Design Principles

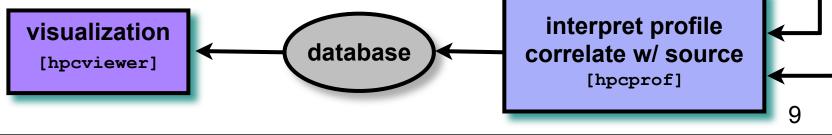
- Binary-level measurement and analysis
 - observe fully optimized, dynamically linked executions
 - support multi-lingual codes with external binary-only libraries
- Sampling-based measurement (avoid instrumentation)
 - minimize systematic error and avoid blind spots
 - enable data collection for large-scale parallelism
- Collect and correlate multiple derived performance metrics
 - diagnosis requires more than one species of metric
 - derived metrics: "unused bandwidth" rather than "cycles"
- Associate metrics with both static and dynamic context loop nests, procedures, inlined code, calling context
- Support top-down performance analysis
 - intuitive enough for scientists and engineers to use
 - detailed enough to meet the needs of compiler writers

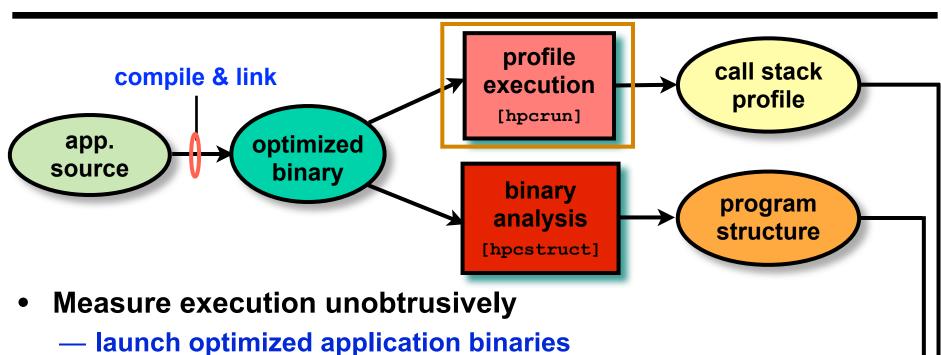
Outline

- Overview of Rice's HPCToolkit
- Accurate measurement
- Useful source-level feedback
- Effective performance analysis
 - derived metrics for understanding performance
 - pinpointing scalability bottlenecks [SC09]
 - analyzing lock contention in threaded codes [PPoPP10]
 - pinpointing load imbalance [SC10]
 - understanding temporal dynamics of parallel codes
- Using HPCToolkit
- Coming attractions

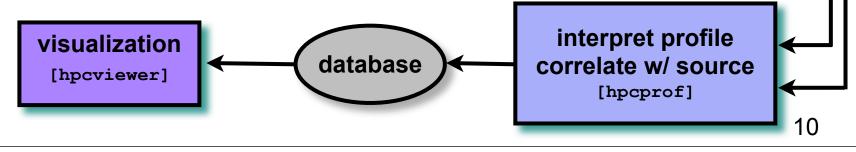
HPCToolkit Workflow profile call stack compile & link execution profile [hpcrun] app. optimized source binary binary program analysis structure [hpcstruct] interpret profile visualization database correlate w/ source [hpcviewer] [hpcprof] 8

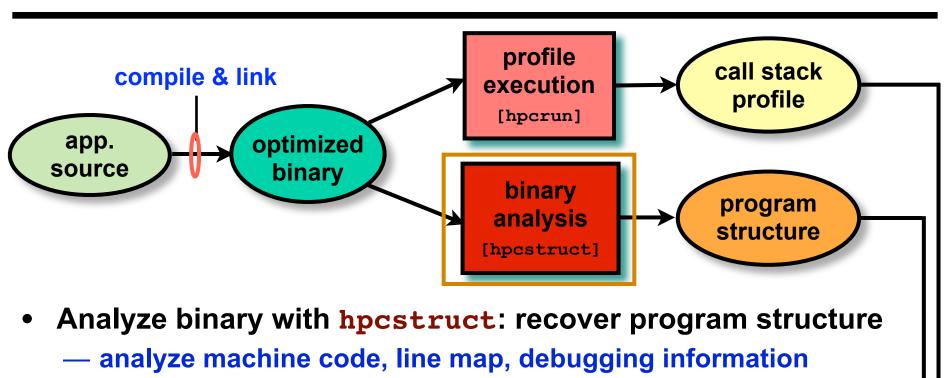




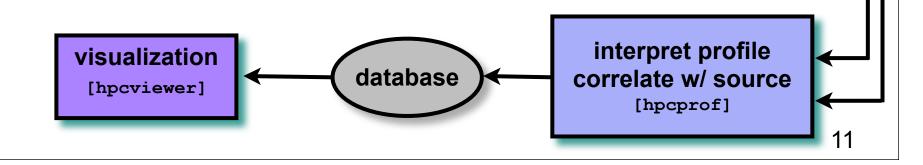


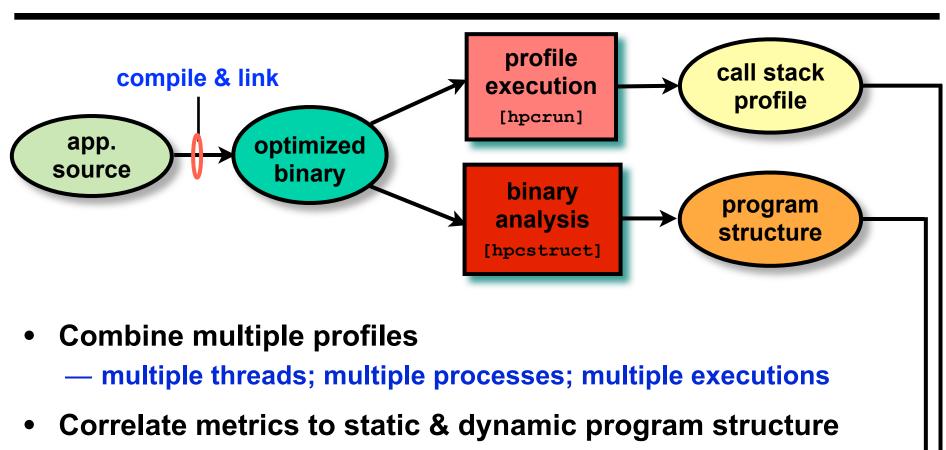
- dynamically-linked applications: launch with hpcrun to measure
- statically-linked applications: measurement library added at link time control with environment variable settings
- collect statistical call path profiles of events of interest

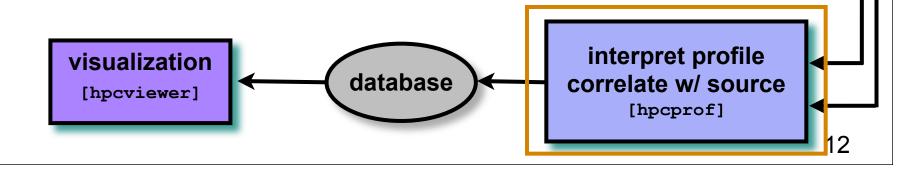


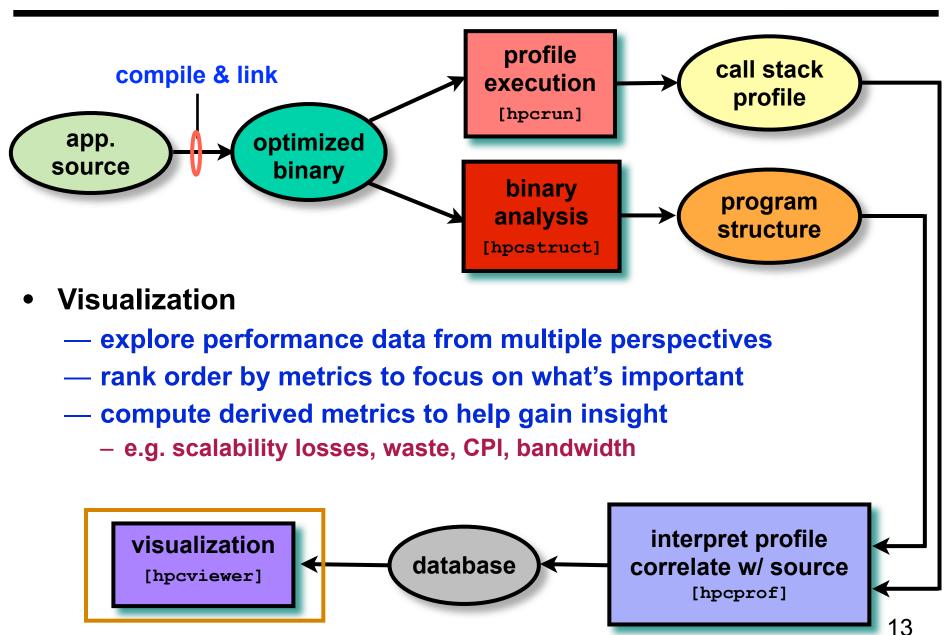


- extract loop nesting & identify inlined procedures
- map transformed loops and procedures to source



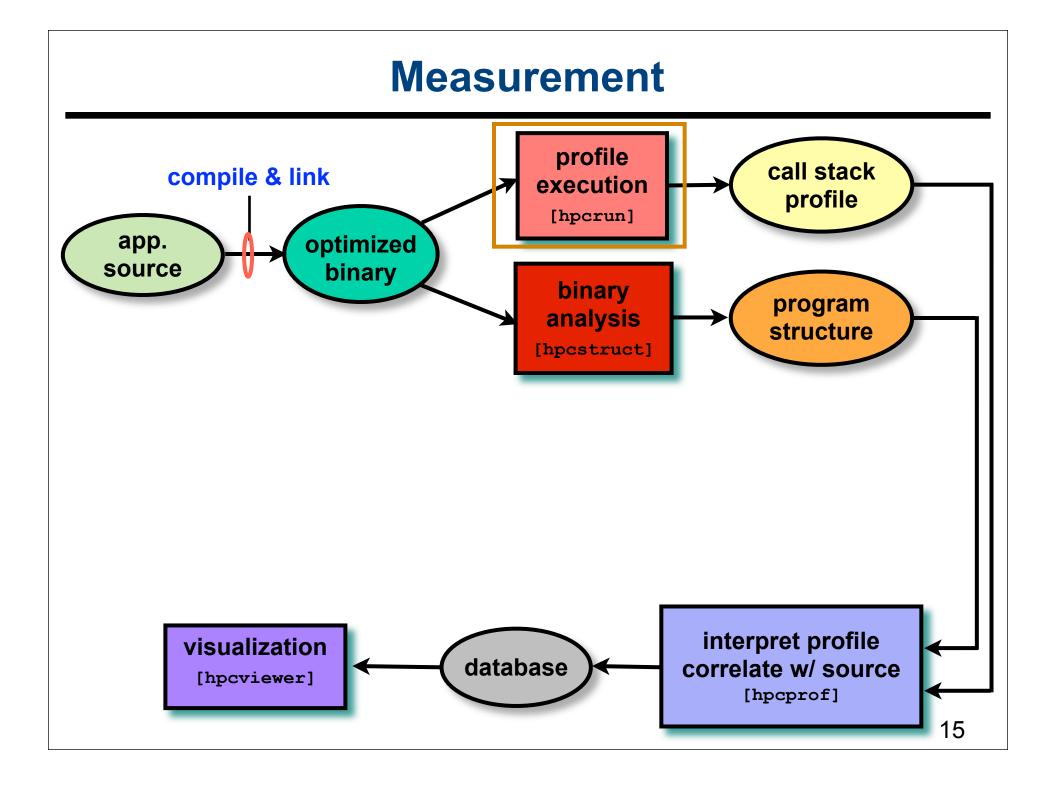






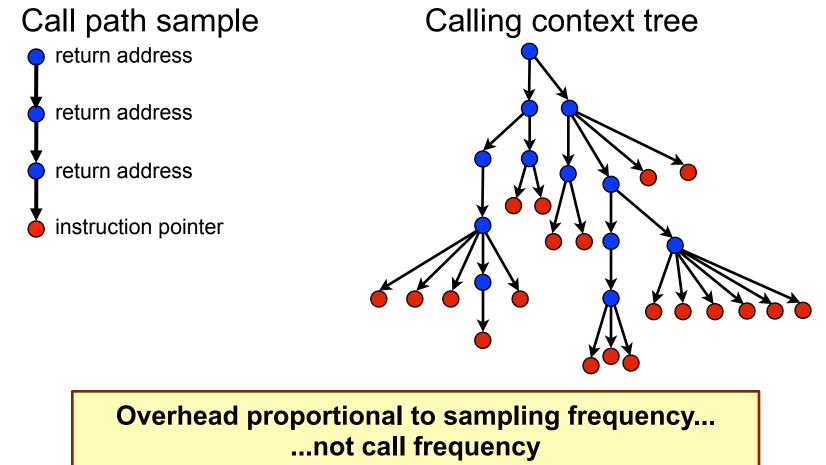
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Call Path Profiling

- Measure and attribute costs in context
 - sample timer or hardware counter overflows
 - gather calling context using stack unwinding



Unwinding Optimized Code

- Optimized code presents challenges for unwinding
 - -optimized code often lacks frame pointers
 - -no compiler information about epilogues
 - -routines may have multiple epilogues, multiple frame sizes
 - -code may be partially stripped: no info about function bounds
- What we need
 - —where is the return address of the current frame?
 - a register, relative to SP, relative to BP
 - —where is the FP for the caller's frame?
 - a register, relative to SP, relative to BP
- Approach: use binary analysis to support unwinding

Dynamically Loaded Code (Linux)

New code may be loaded/unloaded at any time

• When a new module is loaded

—note new code segment mappings—build table of new procedure bounds

• When a module is unloaded

-mark end of profiler epoch: code addresses no longer apply

-flush stale cached information

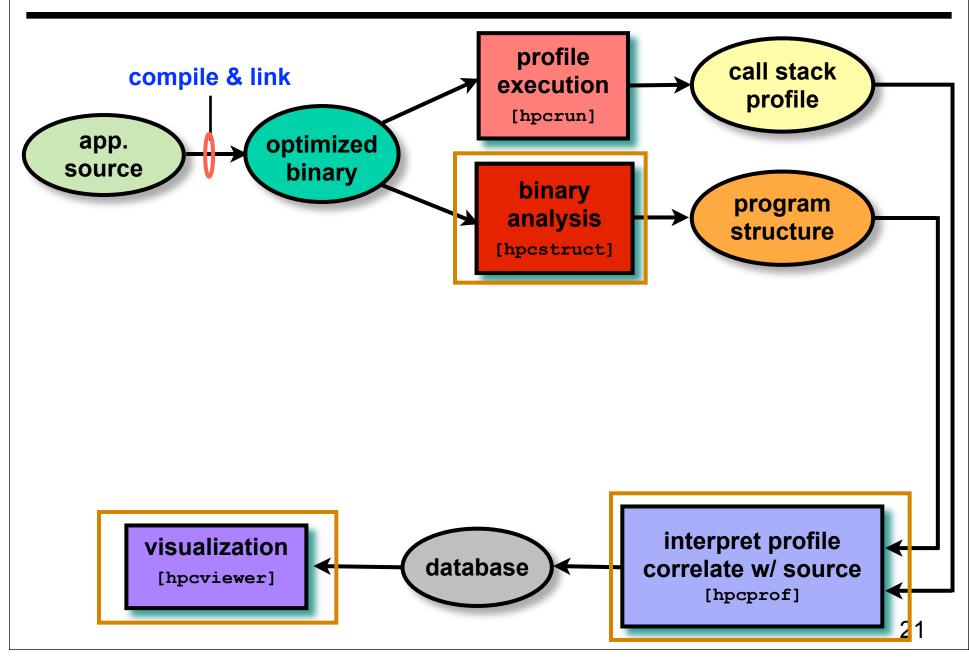
Measurement Effectiveness

- Accurate
 - PFLOTRAN on Cray XT @ 8192 cores
 - 148 unwind failures out of 289M unwinds
 - 5e-5% errors
 - Flash on Blue Gene/P @ 8192 cores
 - 212K unwind failures out of 1.1B unwinds
 - 2e-2% errors
 - SPEC2006 benchmark test suite (sequential codes)
 - fully-optimized executables: Intel, PGI, and Pathscale compilers
 - 292 unwind failures out of 18M unwinds (Intel Harpertown)
 - 1e-3% error
- Low overhead
 - e.g. PFLOTRAN scaling study on Cray XT @ 512 cores
 - measured cycles, L2 miss, FLOPs, & TLB @ 1.5% overhead
 - suitable for use on production runs

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Useful Source-level Feedback



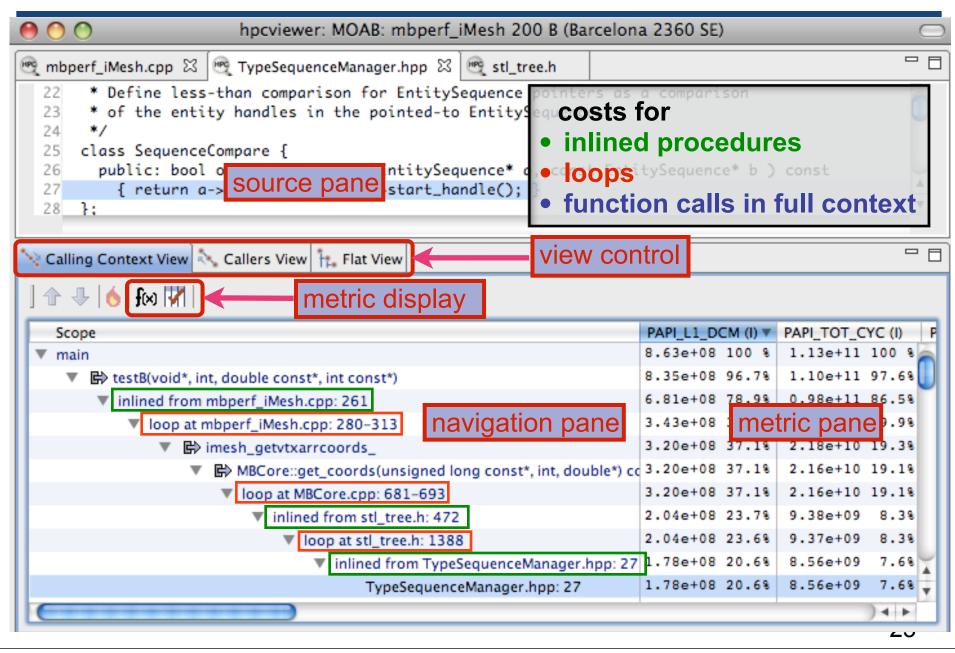
Recovering Program Structure

- Analyze an application binary
 - identify object code procedures and loops
 - decode machine instructions
 - construct control flow graph from branches
 - identify natural loop nests using interval analysis
 - map object code procedures/loops to source code
 - leverage line map + debugging information
 - discover inlined code
 - account for many loop and procedure transformations

Unique benefit of our binary analysis

- Bridges the gap between
 - lightweight measurement of fully optimized binaries
 - desire to correlate low-level metrics to source level abstractions

Analyzing Results with hpcviewer



Principal Views

- Calling context tree view
 - "top-down" (down the call chain)
 - associate metrics with each dynamic calling context
 - high-level, hierarchical view of distribution of costs
- Caller's view
 - "bottom-up" (up the call chain)
 - apportion a procedure's metrics to its dynamic calling contexts
 - understand costs of a procedure called in many places
- Flat view
 - "flatten" the calling context of each sample point
 - aggregate all metrics for a procedure, from any context
 - attribute costs to loop nests and lines within a procedure

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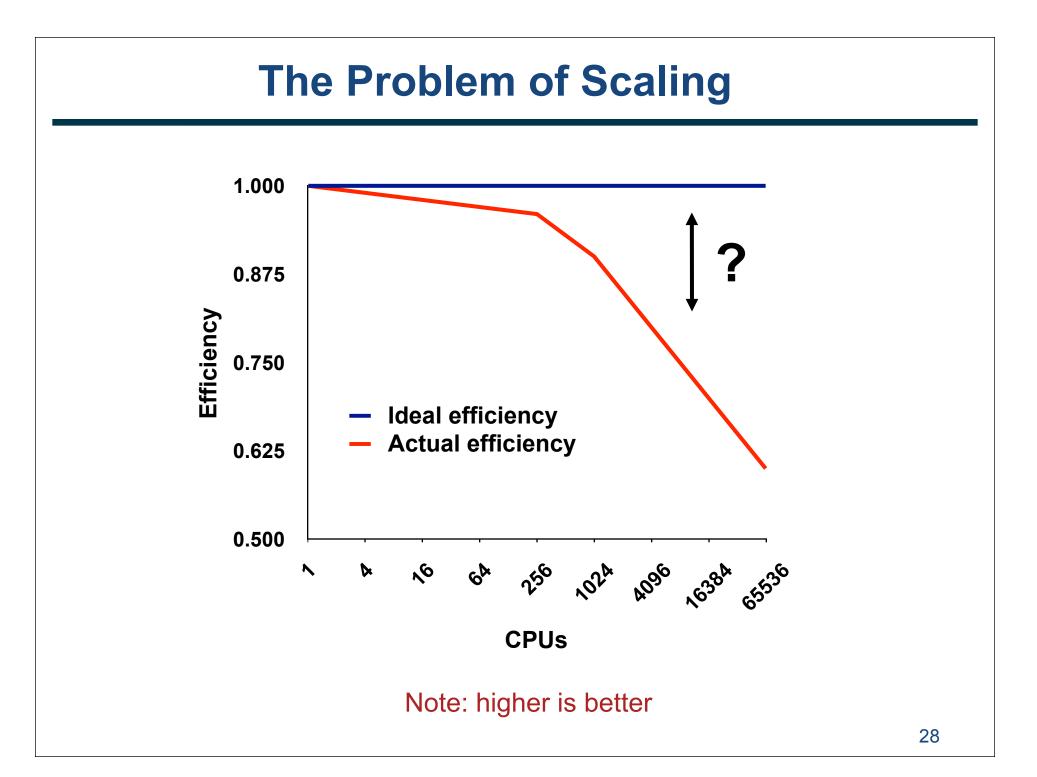
S3D Solver for Turbulent, Reacting Flows

Users/johnmc/Documents/Admin/Grants/Active/DOE/PERI/Tiger Teams/S3D/s3d-opteron-1cpu-20iterations-hpctoolkit-db. mixavg_transport_m.f90 **Overall performance** (15% of peak) $diffFlux(:,:,:,n_spec,:) = 0.0$ 734 735 DIRECTION: do m=1.3 2.05 x 10¹¹ FLOPs / 6.73 x 10¹¹ cycles= .305 FLOPs/cycle 736 SPECIES: do n=1,n_spec-1 737 738 if (baro_switch) then 739 ! driving force includes gradient in mole fraction and baro-diffusion: 740 $diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * (grad_Ys(:,:,:,n,m) \&$ + Ys(:,:,:,n) * (grad_mixMW(:,:,:,m) & 741 742 + (1 - molwt(n)*avmolwt) * grad_P(:,:,:,m)/Press)) 743 else ! driving force is just the gradient in mole fraction: 744 $diffFlux(:,:,:,n,m) = - Ds_mixavg(:,:,:,n) * (grad_Ys(:,:,:,n,m) \&$ 745 + Ys(:,:,:,n) * grad_mixMW(:,:,:,m)) 746 747 endif 748 ! Add thermal diffusion: 749 750 if (thermDiff_switch) then diffFlux(:,:,:,n,m) = diffFlux(:,:,:,n,m) &751 752 - Ds_mixavg(:,:,:,n) * Rs_therm_diff(:,:,:,n) * molwt(n) & 753 * avmolwt * grad_T(:,:,:,m) / Temp highlighted loop accounts for 754 endif 755 11.4% of total program waste ! compute contribution to nth species diffusive flux 756 ! this will ensure that the sum of the diffusive fluxes is zero. 757 758 diffFlux(:,:,:,n_spec,m) = diffFlux(:,:,:,n_spec,m) - diffFlux(:,:,:,n_spec,m) - diffFlux(:,:,:,n_spec,m) = diffFlux(:,:,:,n_spec 759 enddo SPECIES 760 761 enddo DIRECTION $) \rightarrow \rightarrow$ Flat View D.A. 41 CD. 1810 PAPI_STL_ICY Scopes PAPI_TOT_INS WASTE V Wasted Opportunity 6.73e11 100.0 2.05e11 100.0 4.56e11 100.0 1.59e10 100 1.14e12 100 Experiment Aggregate Metrics (Maximum FLOP rate 1.32e09 8. 1.30e11 11.4% 0.90010 10.35 3.00003 4.06e10 8.9% loop at mixavg_transport_m.f90: 735-760 6.96e10 10.3% 9.00e09 4.4% 4.06e10 8.9% 1.32e09 8. 1.30e11 11.4% loop at mixavg_transport_m.f90: 736-7 * cycles -1.00e06 0.0% 2.00e06 0.0% mixavg_transport_m.f90: 735 7.58e10 11.3% 4.23e10 20.6% 8.29e10 18.2% 1.07e09 6. 1.09e11 9.6% ~~~s3d_f90.x:<unknown-file>~~~: 0 (actual FLOPs)) 3.88e10 5.8% 1.79e10 3.9% 4.24e08 2. 7.75e10 6.8% loop at rhsf.f90: 209-210 1.46e10 3.2% 4.80e08 3. 5.95e10 5.2% 3.19e10 4.7% 4.41e09 2.1% loop at mixavg_transport_m.f90: 908-914 0 - - F

26

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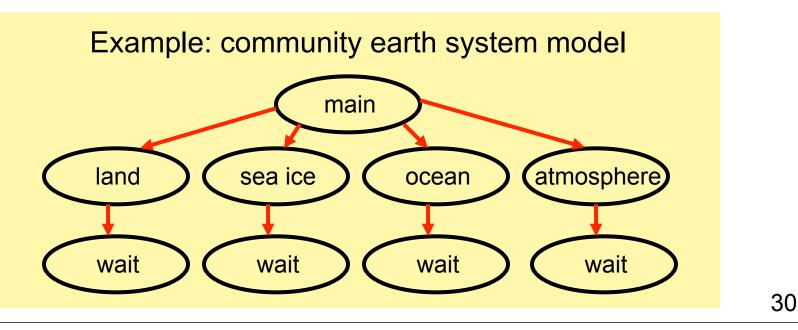


Goal: Automatic Scaling Analysis

- Pinpoint scalability bottlenecks
- Guide user to problems
- Quantify the magnitude of each problem
- Diagnose the nature of the problem

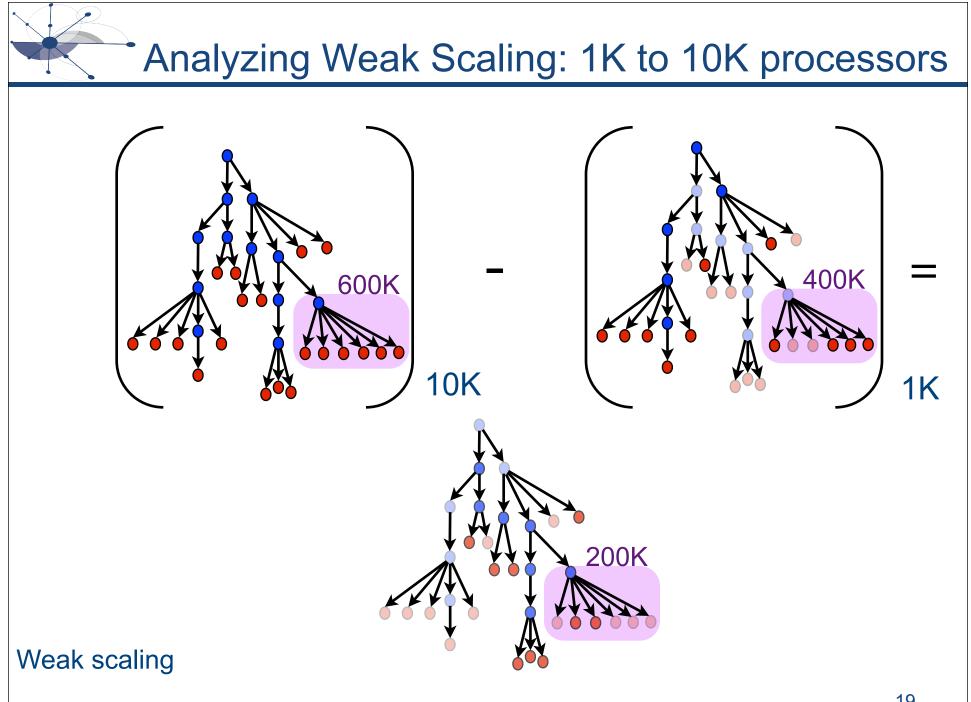
Challenges for Pinpointing Scalability Bottlenecks

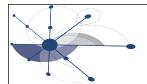
- Parallel applications
 - modern software uses layers of libraries
 - performance is often context dependent
- Monitoring
 - bottleneck nature: computation, data movement, synchronization?
 - 2 pragmatic constraints
 - acceptable data volume
 - low perturbation for use in production runs



Performance Analysis with Expectations

- Users have performance expectations for parallel codes
 - strong scaling: linear speedup
 - weak scaling: constant execution time
- Putting expectations to work
 - measure performance under different conditions
 - e.g. different levels of parallelism or different inputs
 - express your expectations as an equation
 - compute the deviation from expectations for each calling context
 - for both inclusive and exclusive costs
 - correlate the metrics with the source code
 - explore the annotated call tree interactively

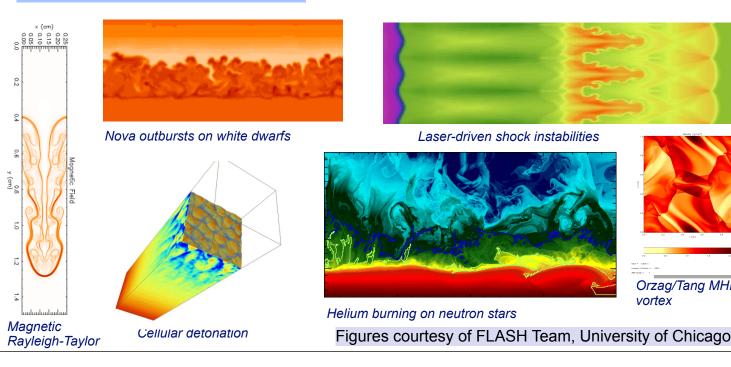


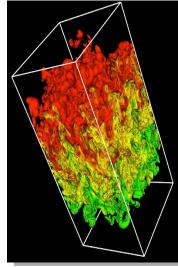


Scalability Analysis Demo: FLASH

Code: Simulation: **Platform**: **Experiment**: Scaling type:

University of Chicago FLASH white dwarf detonation Blue Gene/P 8192 vs. 256 processors weak





Rayleigh-Taylor instability

Orzag/Tang MHD

vortex

33

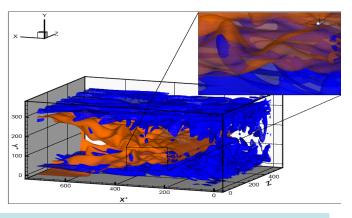
Scaling on Multicore Processors

- Compare performance
 - single vs. multiple processes on a multicore system
- Strategy
 - differential performance analysis
 - subtract the calling context trees as before, unit coefficient for each

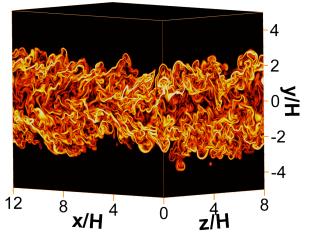


S3D - DNS Solver

- Solves compressible reacting Navier-Stokes equations
- High fidelity numerical methods
 - 8th order finite-difference
 - 4th order explicit RK integrator
- Hierarchy of molecular transport models
- Detailed chemistry
- Multi-physics (sprays, radiation and soot)
 - from SciDAC-TSTC (Terascale Simulation of Turbulent Combustion)



Text and figures courtesy of Jacqueline H. Chen, SNL



- S3D: Multicore Losses at the Loop Level

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- Overview of Rice's HPCToolkit
- Accurate measurement
- Useful source-level feedback
- Effective performance analysis
 - derived metrics for understanding performance
 - pinpointing scalability bottlenecks [SC09]
 - analyzing lock contention in threaded codes [PPoPP10]
 - pinpointing load imbalance [SC10]
 - understanding temporal dynamics of parallel codes
- Using HPCToolkit
- Coming attractions

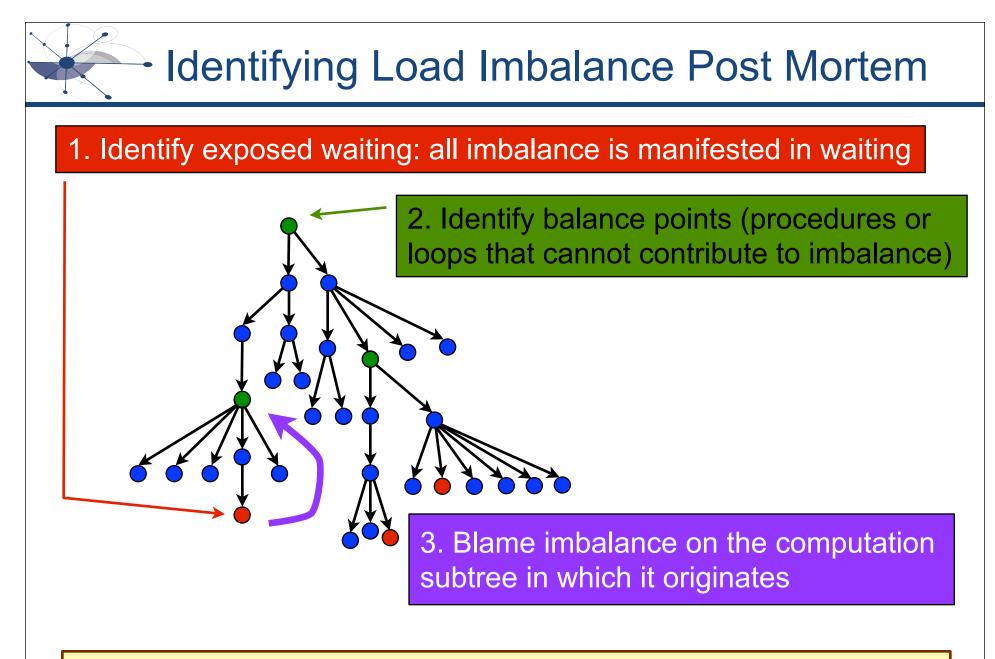
Understanding Lock Contention in Threaded Code

- Lock contention => idleness
 - explicitly threaded programs (Pthreads, etc)
 - implicitly threaded programs (critical sections in OpenMP, ...)
- Strategy: "blame-shifting" of contention from victim to perpetrator
 - use shared state (locks) to communicate blame
- How it works
 - consider spin-waiting
 - sample a working thread:
 - charge to 'work' metric
 - sample an idle thread
 - accumulate in idleness counter associated with a lock (atomic add)
 - working thread releases a lock
 - atomically swap 0 with lock's idleness counter
 - exactly represents contention while that thread held the lock
 - unwind the call stack to attribute lock contention to a calling context

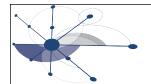
Lock Contention in MADNESS		
580const arg1T& arg1, const arg2T& arg2, const a581Future <remfuture(memfun_returnt(memfunt))> re582add(new TaskMemfun<memfunt>(result,obj,memfun583return result;</memfunt></remfuture(memfun_returnt(memfunt))>	const arg2T& arg2, const a EMFUN_RETURNT(memfunT))> re • max. of 340K live locks	
584 }	*******	1-5% overhead
🔧 Calling Context View 🔧 Callers View 🕴 Flat View		
] 🛧 🕹 🔥 🌆 🕅 📰 🖈 🖛 🛛 16 cores; 1 thread/core (4 x	Barcelona)	μs
Scope % idleness (all/E) idleness (all/E)		
Experiment Aggregate Metrics		.57e+09 100 %
▼ pthread_spin_unlock	2.35e+01 100.0	lock contention
madness::Spinlock:unlock() const	2.35e+01 100.0	accounts for 23.5%
▼ 🗇 inlined from worldmutex.h: 142	1.788401 75.88	of execution time.
madness::ThreadPool::add(madness::PoolTaskInterface*)	1.788401 75.86	.92e+08 31.2%
Inlined from worldtask.h: 581		
 madness::Future<> madness::WorldObject<>::task<: inlined from worldtask.h: 569 	4.56e+00 19.4% 3	Adding futuros
Maintee Hon Wondtaskin, 505 Maintee Hon Wondtaskin, 505 Maintee Hon Wondtaskin, 505		to charad alabal
Inlined from worlddep.h: 68	1.53e+00 6.5% 1	
v 🔁 inlined from worldtask.h: 570	1.49e+00 6.3% 9	.97e+07 6.3%
## madness::Future<> madness::WorldObject<>::task<:	> 1.49e+00 6.3% 9	.97e+07 6.3%
Inlined from worldtask.h: 558		.26e+07 5.9%
Madness::Future<> madness::WorldTaskQueue::add<>(madness::WorldTaskQueue::add<>)	na 6.72e-01 2.9% 4	.49e+07 2.9%
		39

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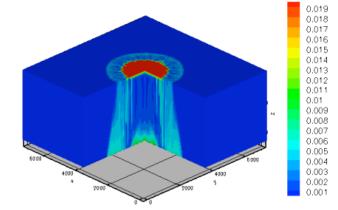
4. Associate each (summary) node with thread-level metric values

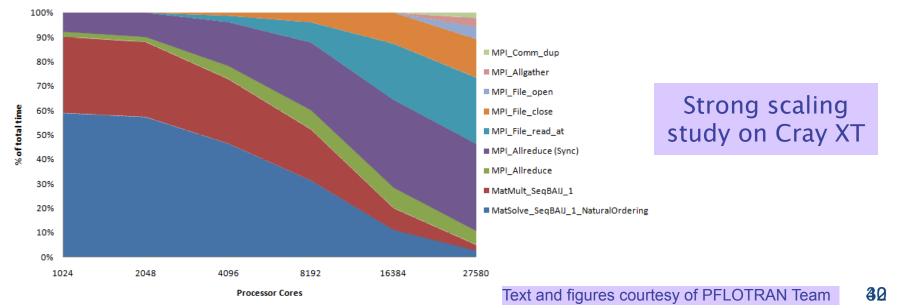


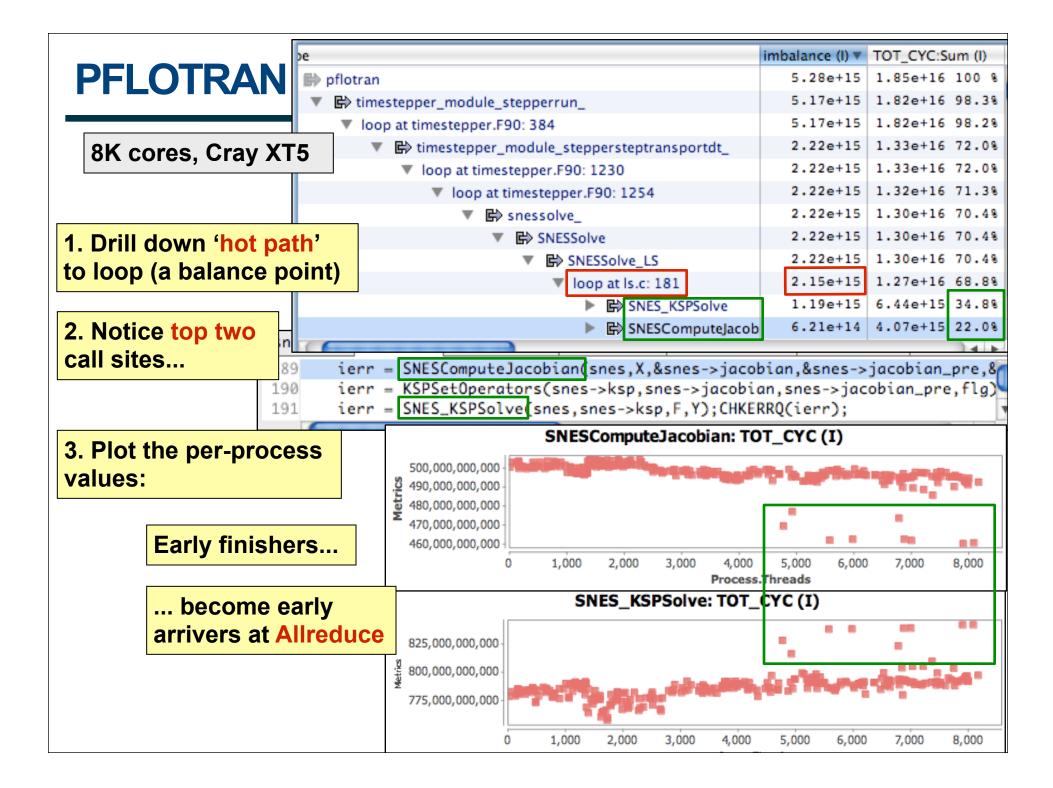
Load Imbalance Analysis Example

PFLOTRAN: modeling multi-scale, multiphase, multi-component subsurface reactive flows

Example use: modeling sequestration of CO₂ in deep geologic formations, where resolving density-driven fingering patterns is necessary to accurately describe the rate of dissipation of the CO₂ plume





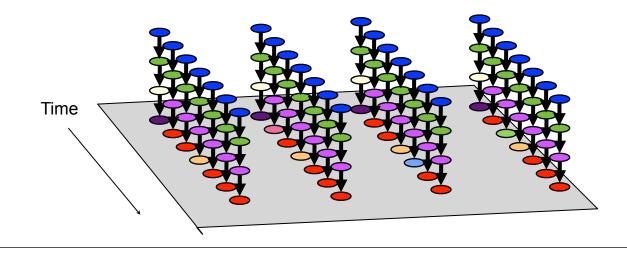


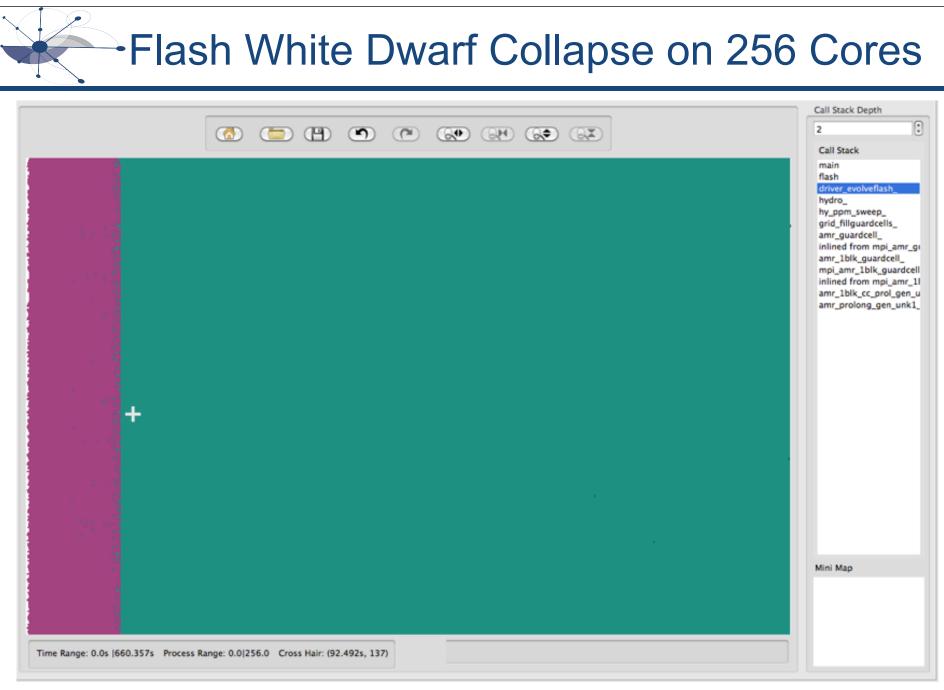
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Understanding Temporal Behavior

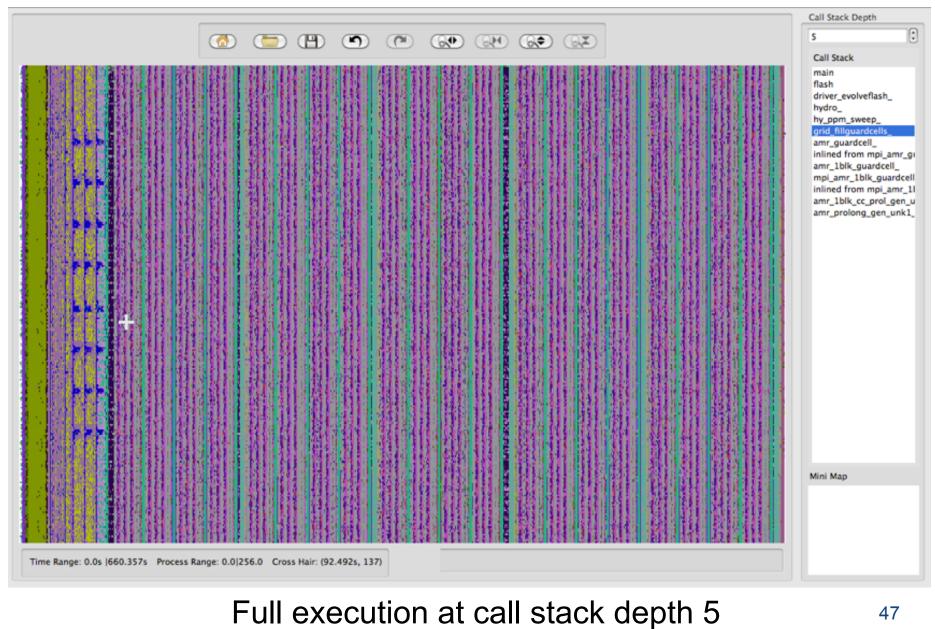
- Profiling compresses out the temporal dimension
 - that's why serialization is invisible in profiles
- What can we do? Trace call path samples
 - sketch:
 - N times per second, take a call path sample of each thread
 - organize the samples for each thread along a time line
 - · view how the execution evolves left to right
 - what do we view?
 - assign each procedure a color; view execution with a depth slice



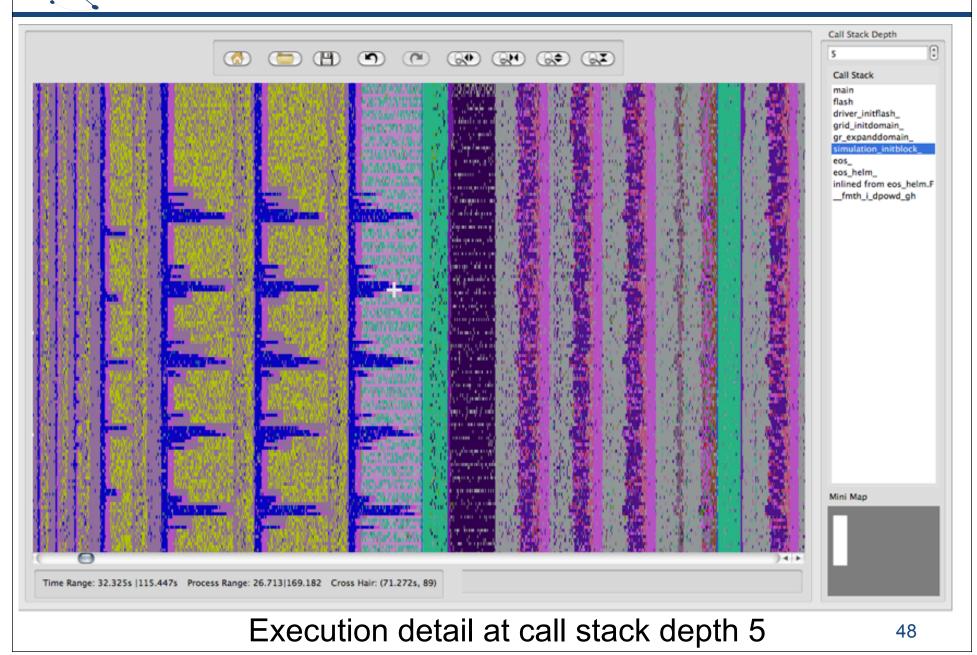


Full execution at call stack depth 2





-Flash White Dwarf Collapse on 256 Cores



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Where to Find HPCToolkit

- DOE Systems
 - jaguar: /ccs/proj/hpctoolkit/pkgs/hpctoolkit
 - intrepid: /home/projects/hpctoolkit/pkgs/hpctoolkit
 - franklin: /project/projectdirs/hpctk/pkgs/hpctoolkit
- NSF Systems
 - ranger: /scratch/projects/hpctoolkit/pkgs/hpctoolkit

• For your local Linux systems, you can download and install it

- documentation, build instructions, link to our svn repository
 - svn repository: https://outreach.scidac.gov/svn/hpctoolkit
- we recommend downloading and building from svn
- important notes:
 - obtaining information from hardware counters requires downloading and installing PAPI
 - installing PAPI

on Linux 2.6.32 or better: built-in kernel support for counters earlier Linux needs a kernel patch (perfmon2 or perfctr)

Available Guides

http://hpctoolkit.org/documentation.html

- Using HPCToolkit with statically linked programs [pdf]
 a guide for using hpctoolkit on BG/P and Cray XT
- Quick start guide [pdf]

— essential overview that almost fits on one page

- The hpcviewer user interface [pdf]
- Effective strategies for analyzing program performance with HPCToolkit [pdf]

— analyzing scalability, waste, multicore performance ...

- HPCToolkit and MPI [pdf]
- HPCToolkit Troubleshooting [pdf]
 - why don't I have any source code in the viewer?
 - hpcviewer isn't working well over the network ... what can I do?

Setup

- Add hpctoolkit's bin directory to your path

 see earlier slide for HPCToolkit's HOME directory on your system
- Adjust your compiler flags (if you want <u>full</u> attribution to src)
 add -g flag after any optimization flags
- Add hpclink as a prefix to your Makefile's link line
 e.g. hpclink mpixlf -o myapp foo.o ... lib.a -lm ...
- Decide what hardware counters to monitor
 - dynamically-linked executables (e.g., Linux)
 - use hpcrun -L to learn about counters available for profiling
 - use papi_avail
 - you can sample any event listed as "profilable"
 - statically-linked executables (e.g., Cray XT, BG/P)
 - use hpclink to link your executable
 - launch executable with environment var HPCRUN_EVENT_LIST=LIST (currently BG/P hardware counters unsupported)

Launching your Job

- Modify your run script to enable monitoring
 - Cray XT: set environment variable in your PBS script
 - e.g. setenv HPCRUN_EVENT_LIST "PAPI_TOT_CYC@3000000
 PAPI_L2_DCM@400000 PAPI_TLB_DM@400000
 PAPI_FP_OPS@400000"
 - to collect a trace of WALLCLOCK samples

setenv HPCRUN_OPT_TRACE=1

- Blue Gene/P: pass environment settings to qsub
 - qsub -A YourAllocation -q prod -t 30 -n 2048 \setminus
 - --proccount 8192 --mode vn --env \
 - HPCRUN_EVENT_LIST=WALLCLOCK@1000 flash3.hpc
 - to collect a trace of WALLCLOCK samples use

HPCRUN_EVENT_LIST=WALLCLOCK:HPCRUN_OPT_TRACE=1

Binary Analysis and Data Assessment

- Use hpcstruct to reconstruct program structure
 - e.g. hpcstruct myapp
 - creates myapp.hpcstruct

• Use hpcsummary script to summarize measurement data

- e.g. hpcsummary hpctoolkit-myapp-measurements-5912

Analyzing Data with hpcprof-mpi

- Analyze call graph profiles from <u>all cores</u> together
 perform analysis in parallel for acceptable analysis time
- Purpose:
 - compute summary statistics across nodes
 - enables top-down investigation of node differences
 - provide access to thread-level data for detailed comparisons
- Mechanics
 - hpcprof-mpi is just an MPI program
 - launch it on an appropriate number of nodes to reduce analysis time e.g. analysis of PFLOTRAN on Cray XT: 8K profiles, 48 nodes, 10 min
 - e.g. qsub -A YourAllocation -q prod-devel -t 20 -n 64 hpcprof-mpi -S myapp.hpcstruct -I "path_to_src/*" hpctoolkit-myapp-measurements-5912
 - produces hpctoolkit-myapp-database-5912

Analyzing Data with hpcprof

- This runs on the head node; can't analyze all performance data there for large parallel executions
- Use hpcprof to analyze one (or a few) measurement files
 - select one or a few files from your measurements to analyze
 - e.g. hpcprof -S myapp.hpcstruct -I "path_to_src/*"
 hpctoolkit-myapp-measurements-5912/
 myapp-0000-000-983409-764.hpcrun
 - produces hpctoolkit-myapp-database-5912

Using hpcviewer and hpctraceview

- Notes
 - if you collected traces or used hpcprof-mpi, your performance database will be large
 - best approach: analyze it on the leadership computing platform
 - you can tar up a database for analysis on your laptop
 - with patience: copy whole database to laptop
 - impatient way: tar up database without thread or trace data
- Use hpcviewer to open a performance database
 - if using hpcviewer on a the leadership computing platform, add recent Java implementation to your path (for hpcviewer)
 - Cray XT: module load java
 - Blue Gene/P: add /opt/soft/.../java/bin to your path
 - on a front-end node, run hpcviewer with the performance database as an argument
 - ALCF: can also run hpcviewer on gadzooks or eureka
- Use hpctraceview to open call stack traces of core activity
 run hpctraceview and open performance database

hpcviewer and hpctraceview tip

- When running interactive viewers on leadership platforms
 - create a virtual desktop with vncserver
 - view the virtual desktop with vncviewer
 - run hpcviewer or hpctraceview inside your virtual desktop

A Note About hpcstruct and Fortran

- Fortran compilers emit machine code that have an unusual mapping back to source
- To compensate, hpcstruct needs a special option
 - --loop-fwd-subst=no
 - without this option, many nested loops will be missing in hpcstruct's output and (as a result) hpcviewer
- Useful for IBM's xlf, PGI's pgf90 and others

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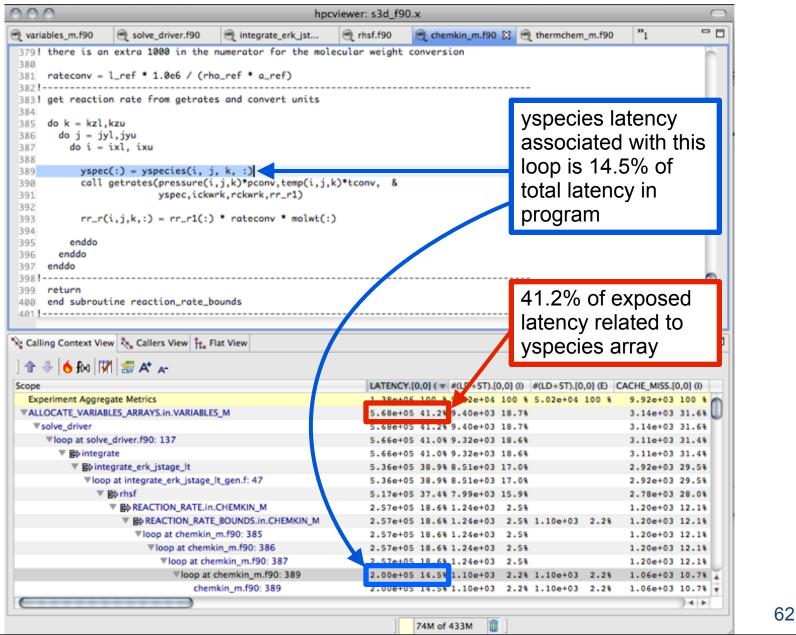
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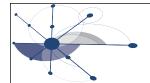
Coming Attraction: Data Centric Analysis

- Goal: associate memory hierarchy locality problems with particular data structures
- Approach
 - intercept memory allocations to associate data range with allocation
 - associate latency with data structures using "instruction based sampling" capability of AMD Opteron CPUs
 - identify instances of loads and store instructions
 - identify the data structure an access touches based on L/S address
 - measure the total latency associated with each L/S
 - present results in hpcviewer



Data Centric Analysis of S3D





HPCToolkit Summary

- Obtain insight, accuracy & precision by combining call path profiling, binary analysis, and blame shifting
- Show surprisingly effective measurement and source-level attribution for fully optimized code (1-3% overhead)
 - statements in their full static and dynamic context
 - project low-level measurements to much higher levels
- Sampling-based measurements can deliver insight into a range of phenomena
 - scalability bottlenecks
 - sources of lock contention
 - load imbalance
 - temporal dynamics
 - problematic data structures



Some Challenges Ahead

- Data management for scalable measurement and analysis
- Moving from descriptive to prescriptive feedback
- Increasing importance of threading as core counts increase
- Heterogeneous architectures, e.g. GPU accelerators