

# Gaining Insight into Parallel Program Performance Using Sampling

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Collaborators: Nathan Tallent, Michael Fagan, Mark Krentel, Laksono Adhianto, Xu Liu, Reed Landrum, Michael Franco



#### hpctoolkit.org

### **Motivation**

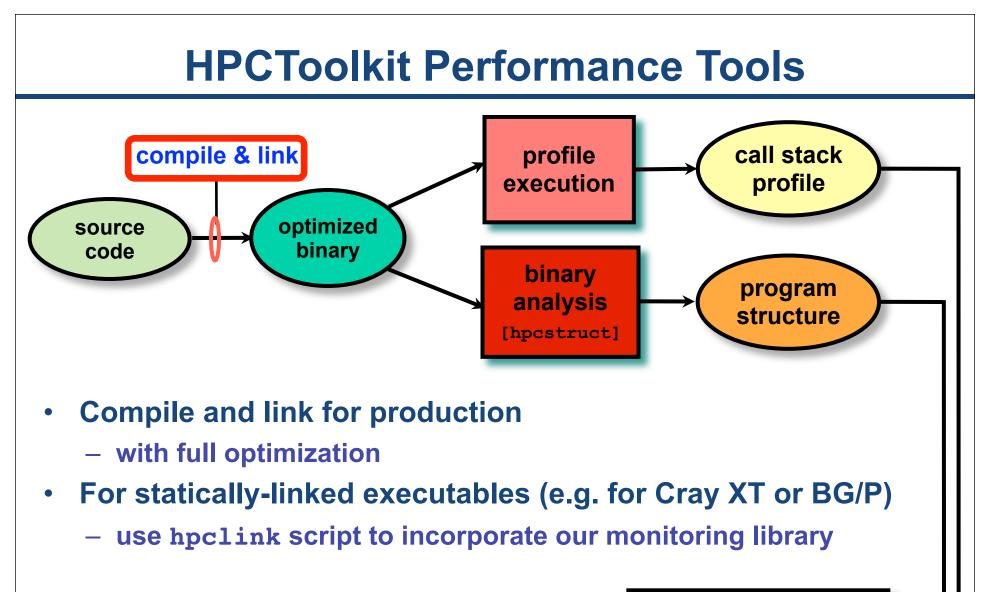
- Complex hardware
  - multi-level parallelism
    - ILP, short vectors, multiple cores, multiple sockets, multiple nodes
  - large-scale parallelism
- Sophisticated software
  - multiphysics, multiscale, adaptive
- Wide gap between peak and typical performance

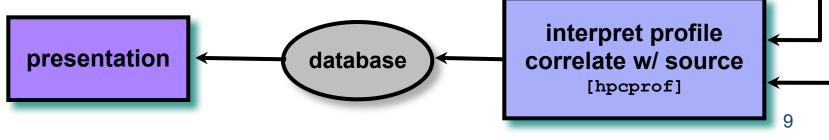
#### Challenges

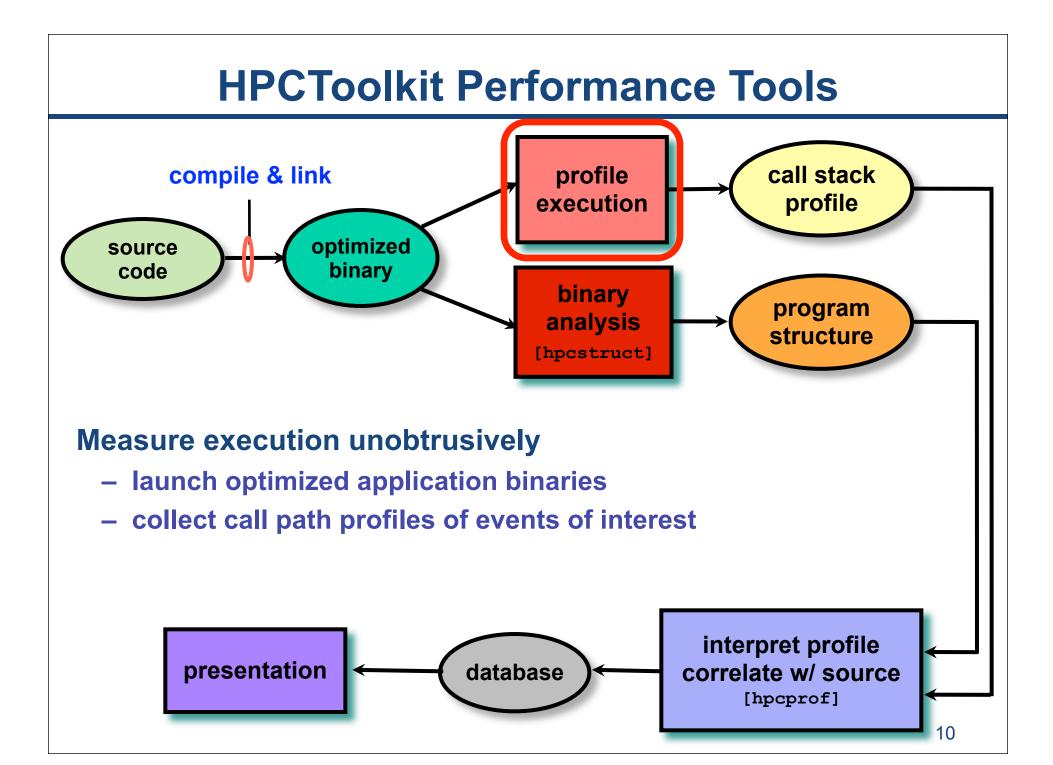
- Understand where and why performance losses occur in sophisticated parallel codes on complex parallel hardware
- Identify opportunities for improvement
- Quantify potential benefits

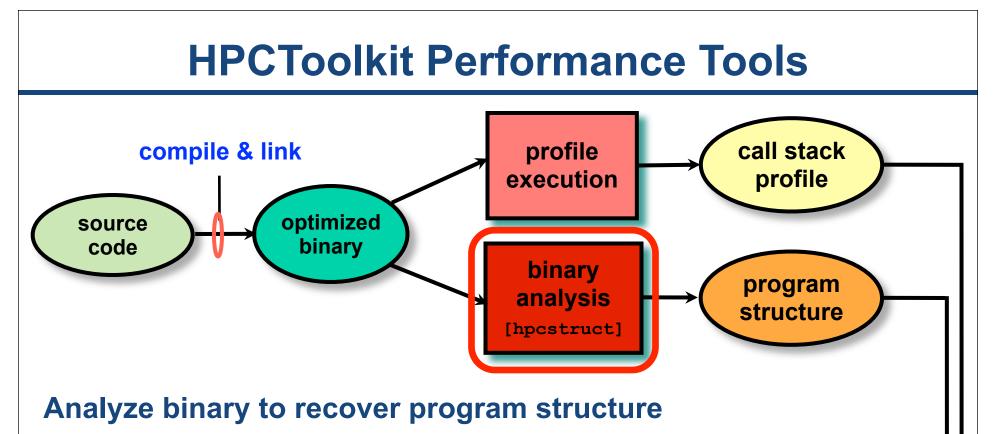
### **Performance Analysis Goals**

- Accurate measurement of parallel scientific codes
  - large, multi-lingual programs
  - fully optimized code: loop optimization, templates, inlining
  - binary-only libraries, sometimes partially stripped
  - complex execution environments
    - dynamic loading or static binaries
    - SPMD parallel codes with threaded node programs
    - batch jobs
  - production executions
- Effective performance analysis
  - pinpoint and explain problems
    - intuitive enough for scientists and engineers
    - detailed enough for compiler writers
  - yield actionable results
- Scalable to petascale systems

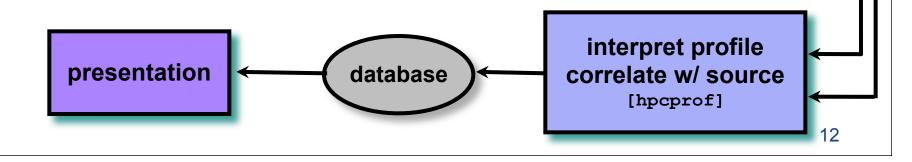


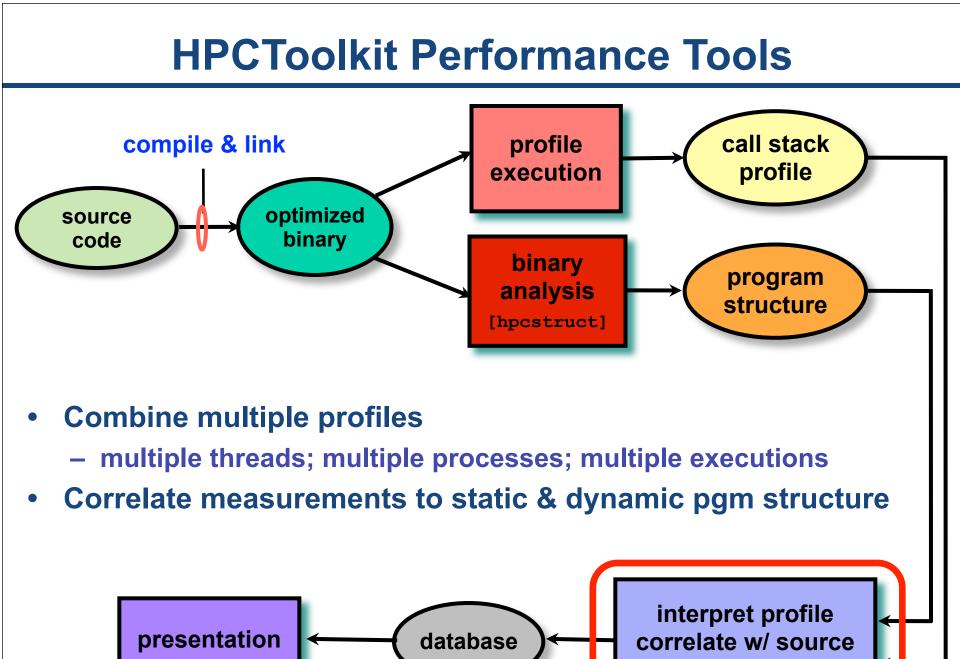


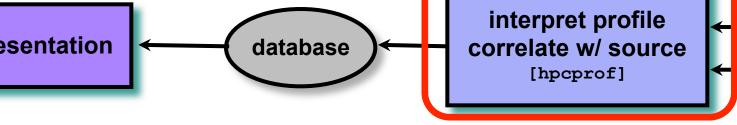


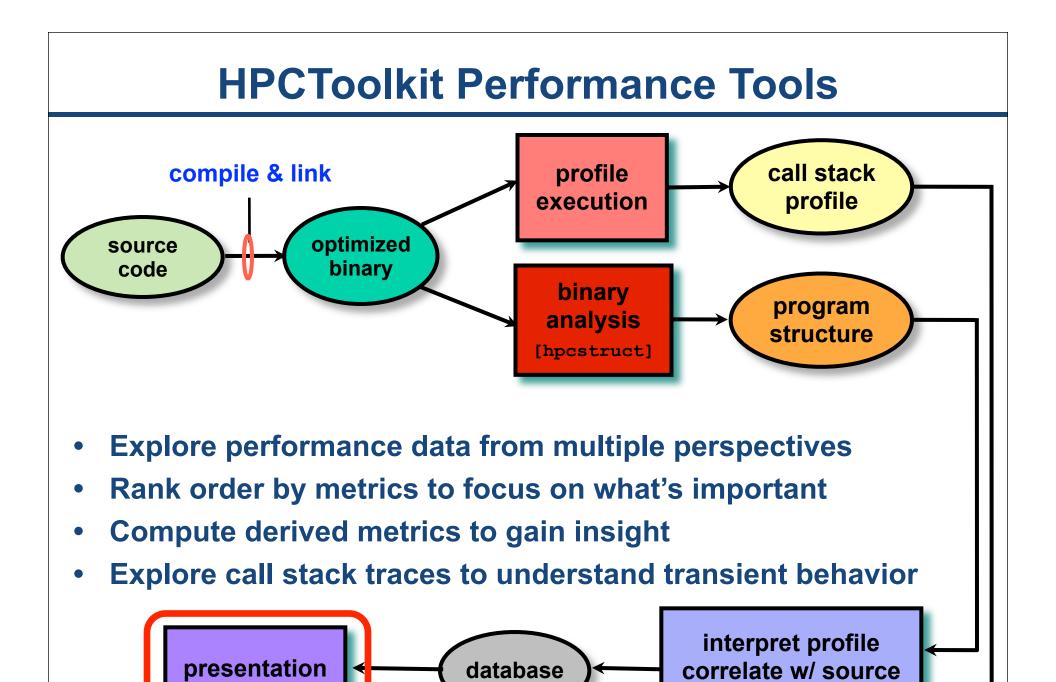


- analyze machine code, line map, and debugging information
- extract loop nesting information and identify inlined procedures
- map transformed loops and procedures back to source









[hpcprof]

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### **Attribution to Static + Dynamic Context**

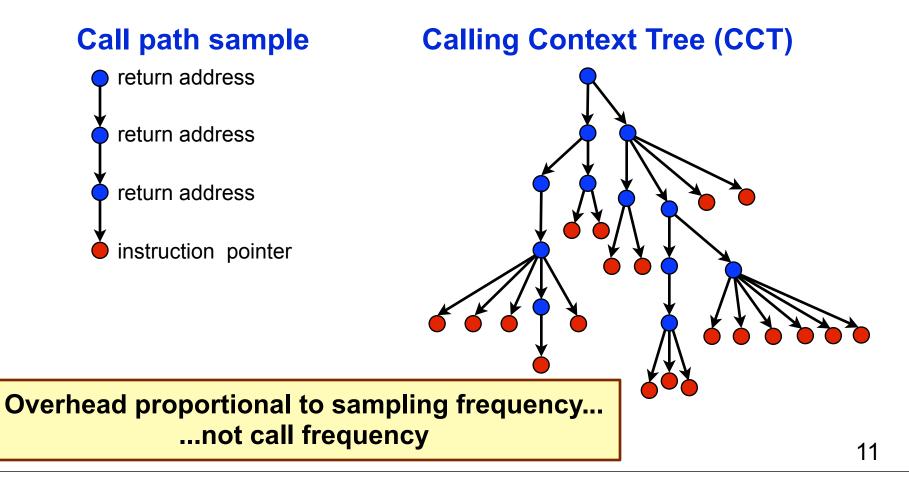
hpcviewer: MOAB: mbperf_iMesh 200	B (Barcelona 2360 SE) calling context
👻 mbperf_iMesh.cpp 🖾 🞯 TypeSequenceManager.hpp 🖾 🞯 stl_tree.	
22 * Define less-than comparison for EntitySequence po 23 * of the entity handles in the pointed-to EntitySeq 24 */	
<pre>25 class SequenceCompare { 26   public: bool operator()( const EntitySequence* a, 27       { return a-&gt;end_handle() &lt; b-&gt;start_handle(); } 28 };</pre>	<ul> <li>costs for</li> <li>inlined procedures</li> </ul>
Calling Context View Callers View 👫 Flat View	<ul> <li>loops</li> <li>function calls in full context</li> </ul>
] 🕆 🐣   🌜   f 🐼 📝	
Scope	PAPI_L1_DCM (I) V PAPI_TOT_CYC (I) P
▼ main	8.63e+08 100 % 1.13e+11 100 %
testB(void*, int, double const*, int const*)	8.35e+08 96.7% 1.10e+11 97.6%
inlined from mbperf_iMesh.cpp: 261	6.81e+08 78.9% 0.98e+11 86.5%
loop at mbperf_iMesh.cpp: 280-313	3.43e+08 39.8% 3.37e+10 29.9%
Imesh_getvtxarrcoords_	3.20e+08 37.1% 2.18e+10 19.3%
MBCore::get_coords(unsigned long const*, in	t, double*) cc 3.20e+08 37.1% 2.16e+10 19.1%
Ioop at MBCore.cpp: 681–693	3.20e+08 37.1% 2.16e+10 19.1%
inlined from stl_tree.h: 472	2.04e+08 23.7% 9.38e+09 8.3%
V loop at stl_tree.h: 1388	2.04e+08 23.6% 9.37e+09 8.3%
inlined from TypeSequenceMan	ager.hpp: 27 1.78e+08 20.6% 8.56e+09 7.6%
TypeSequenceManager.hp	-
	)4 ►(

- Call path profiling in HPCToolkit
- Pinpointing and quantifying scalability bottlenecks
- Blame shifting
  - analyzing multithreaded computations based on work stealing
  - quantifying the impact of lock contention on threaded code
  - pinpointing load imbalance in parallel codes
- Understanding execution behavior over time
- Associating memory hierarchy inefficiency with data
- Conclusions
- Challenges ahead
- Related work

### **Call Path Profiling**

Measure and attribute costs in their calling context

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



### **Unwinding Fully-optimized Parallel Code**

#### Unwinding using demand-driven binary analysis

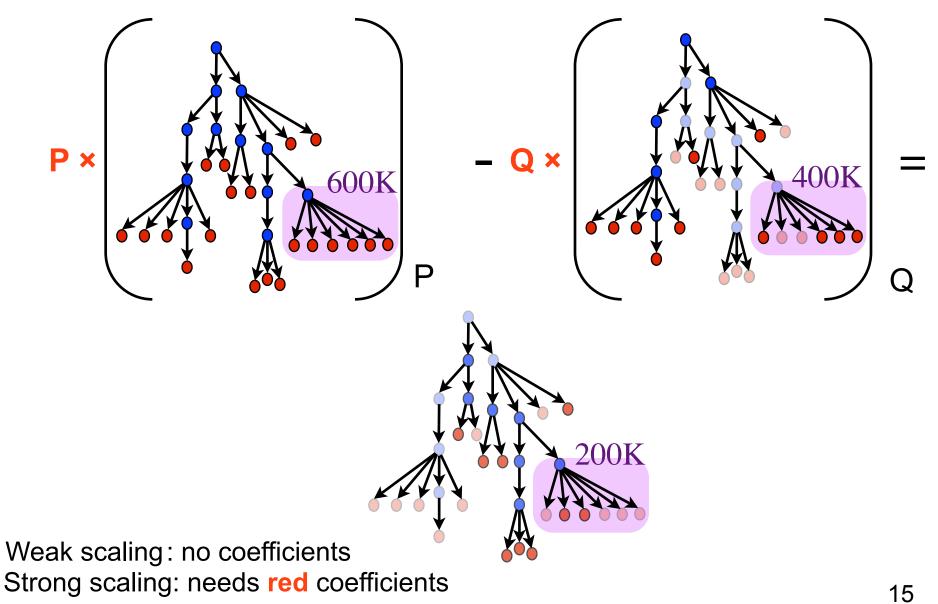
- Identify procedure bounds
  - for dynamically-linked code, do this at runtime
  - for statically-linked code, do this at compile time
- Compute unwind recipes for a procedure on the fly
  - scan the procedure's object code, tracking the locations of
    - caller's program counter
    - caller's frame and stack pointer
  - create unwind recipes between pairs of frame-relevant instructions
- Processors: x86-64, PowerPC (BG/P), MIPS (SiCortex)
- Results
  - accurate call path profiles
  - overheads of < 2% for sampling frequencies of 200/s</p>

Nathan Tallent, John Mellor-Crummey, and Michael Fagan. Binary analysis for measurement and attribution of program performance. PLDI 2009, Dublin, Ireland, **Distinguished Paper Award.** 

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#### **The Problem of Scaling Losses** 1.00 .75 Efficiency .50 **Ideal efficiency Actual efficiency** .25 .00 4096 1638A ~6 0 64 250 N 1024 65536 **CPUs** Note: higher is better 14

#### **Pinpointing and Quantifying Scalability Bottlenecks**



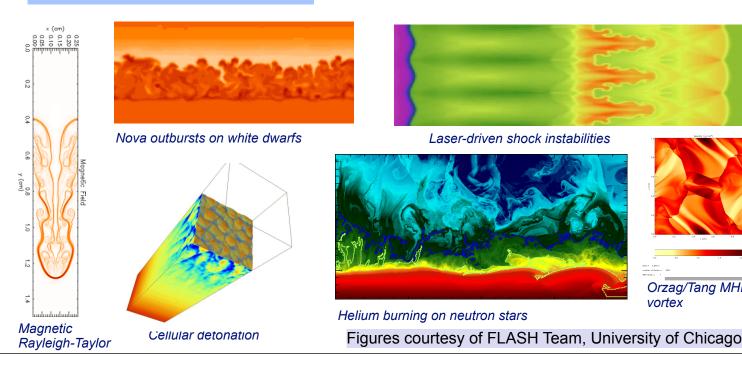
### Scalability Analysis of Flash

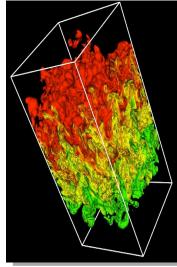
Code: Simulation: **Platform: Experiment: Scaling type:** 

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

Orzag/Tang MHD

vortex



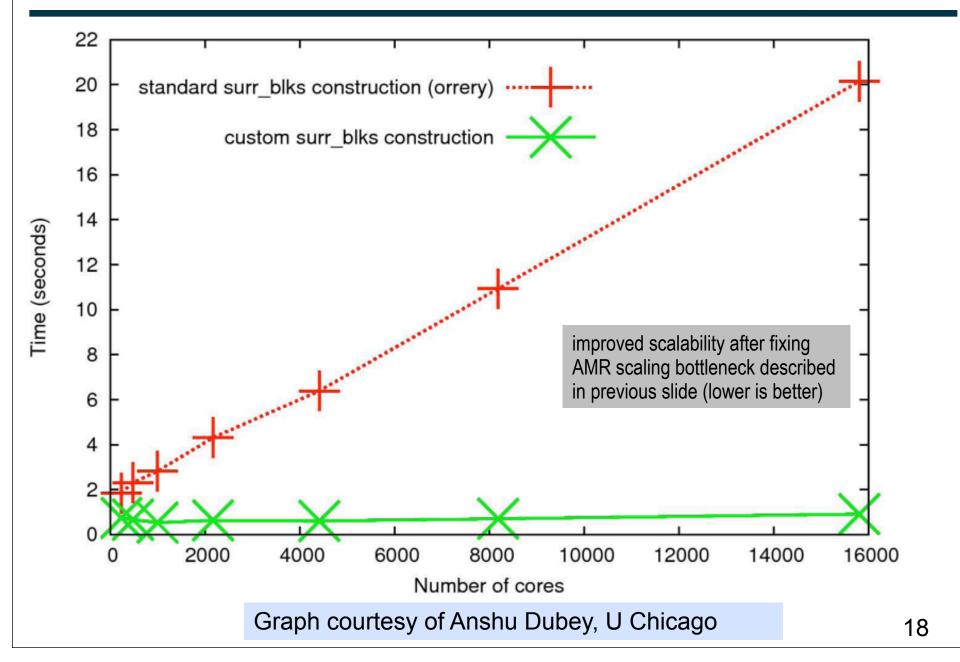


Rayleigh-Taylor instability

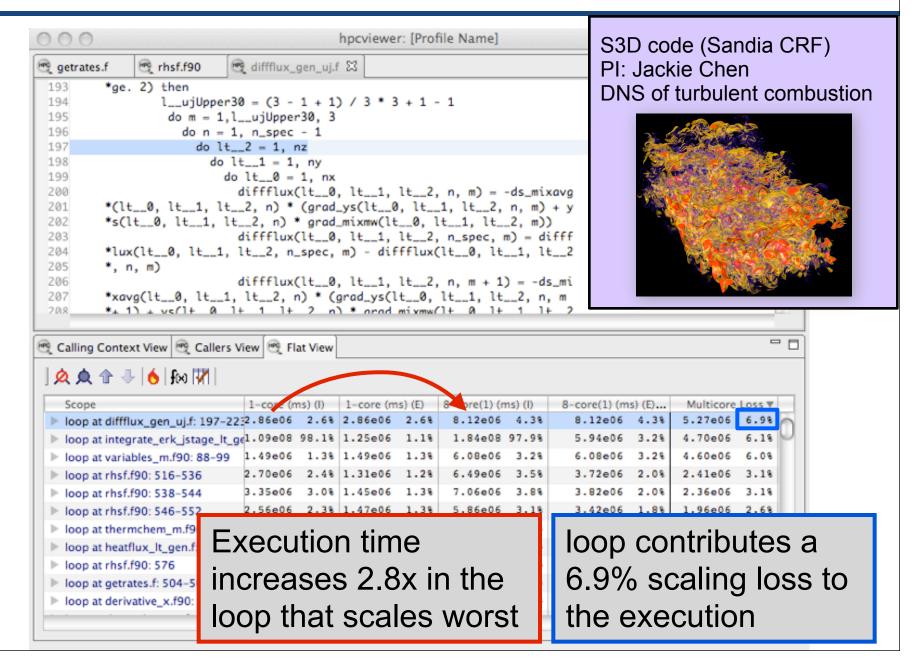
### System-wide Scaling Losses in Flash

niver_initFlash.F90 🛛 🞯 local_tree_build.F90 🔀 🞯 Driver_evolveFl	ash.F90						-	
207!Second pass add the rest of the blocks.	^	13.4% of	the scalin	ig losse	es in F	Flash execution	on are	; d
208 Do ipass = 1,2		to the use of a "digital orrery" all-to-all communication						
209			•		•			
210 lnblocks_old = lnblocks		battern as	s part of a	laptive	mes	h refinement.	INIS	
211 proc = mype 212!Loop through all processors		shows up in the code as a loop over all processors						
212 Do iproc = 0, nprocs-1		containing pairwise communication. This single						
214			• •			•	•	
215 If (iproc -= 0) Then	ŗ	oroblem a	accounts f	for almo	ost 1/-	4 of the scala	bility l	0
216 off_proc = .False. 217 Else		during Ela	ash's evol	ution pł	าลรค		•	
217 Else 218 off_proc = .True.		auning i ie			1000.			
210 End TF								
		This prob	lem cause	ed a 21	% sc	alability loss i	n the	
Calling Context View 🔨 Callers View 📊 Flat View		This problem caused a 21% scalability loss in the initialization phase as well						
😪 Calling Context View 💦 Callers View 📊 Flat View		•						
		•						
Calling Context View 🔧 Callers View 👫 Flat View	i	nitializati	on phase	as well				
] 1 4 5 foo foo foo foo foo	i %	nitializati	on phase	as well	us) (l)	8192/WALLCLOCK (	(us) (l)	
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### Improved Flash Scaling of AMR Setup



#### **Scalability Losses at the Loop Level**

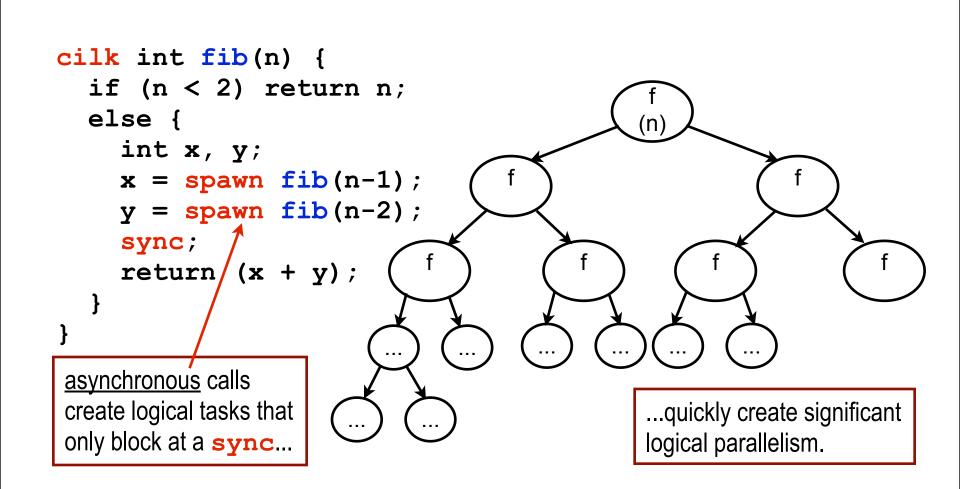


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### **Blame Shifting**

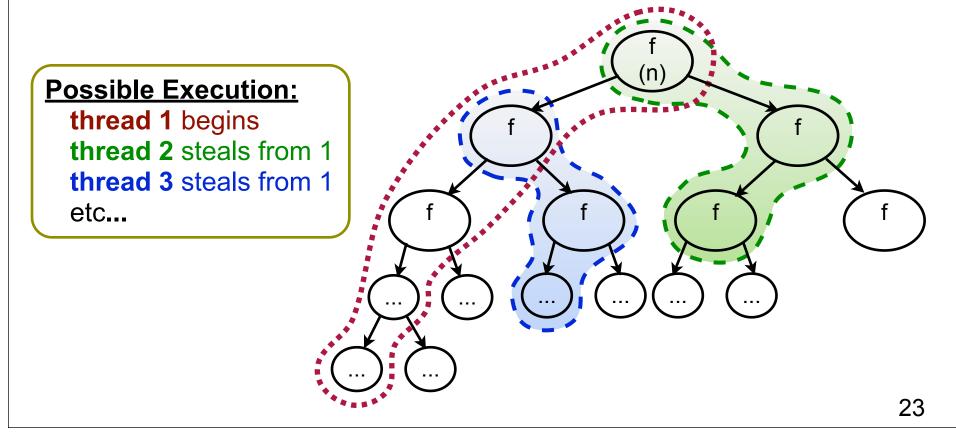
- Problem: in many circumstances sampling measures symptoms of performance losses rather than causes
  - worker threads waiting for work
  - threads waiting for a lock
  - MPI process waiting for peers in a collective communication
- Approach: shift blame for losses from victims to perpetrators
- Flavors
  - active measurement
  - analysis only

### **Cilk: A Multithreaded Language**

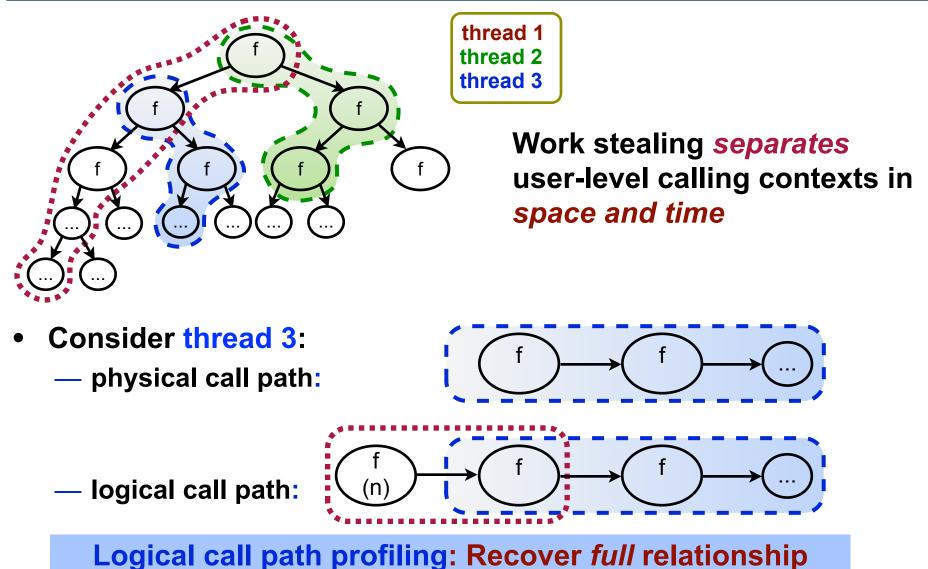


### **Cilk Program Execution using Work Stealing**

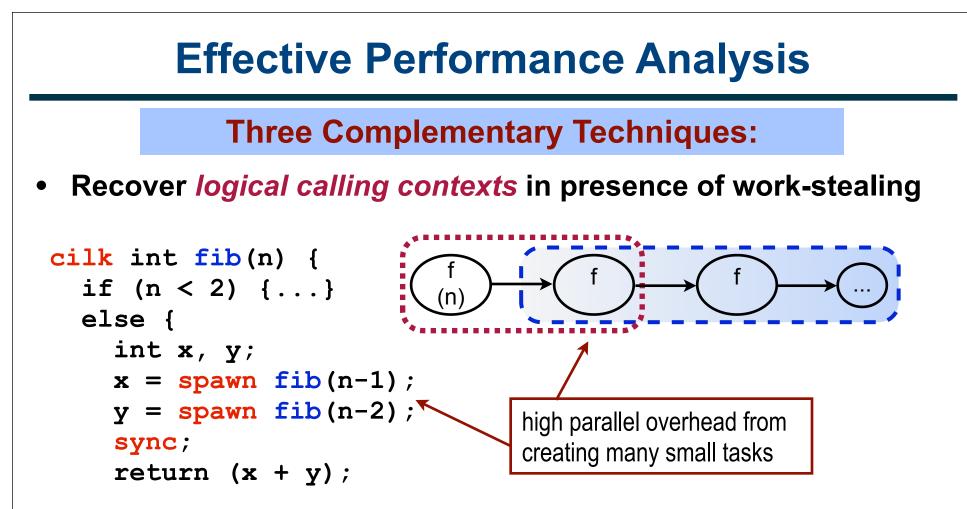
- Challenge: Mapping logical tasks to compute cores
- Cilk approach:
  - lazy thread creation plus work-stealing scheduler
    - spawn: a potentially parallel task is available
    - an idle thread steals tasks from a random working thread



### Wanted: Call Path Profiles of Cilk



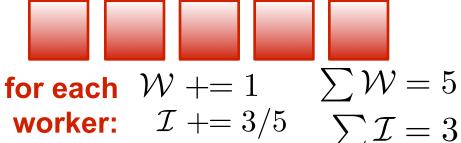
between physical and user-level execution



- Quantify *parallel idleness* (insufficient parallelism)
- Quantify parallel overhead
- Attribute *idleness* and *overhead* to *logical contexts* — at the source level

### **Measuring & Attributing Parallel Idleness**

- Metrics: Effort = "work" + "idleness"
  - associate metrics with user-level calling contexts
    - insight: attribute idleness to its cause: context of working thread
      - a thread looks past itself when 'bad things' happen to <u>others</u>
- Work stealing-scheduler: one thread per core
  - maintain W (# working threads) and I (# idling threads)
    - slight modifications to work-stealing run time
      - atomically incr/decr W when thread exits/enters scheduler
    - when a sample event interrupts a working thread
      - -I = #cores W
      - apportion <u>others</u>' idleness to <u>me</u>: I / W
- Example: Dual quad-cores; on a sample, 5 are working:



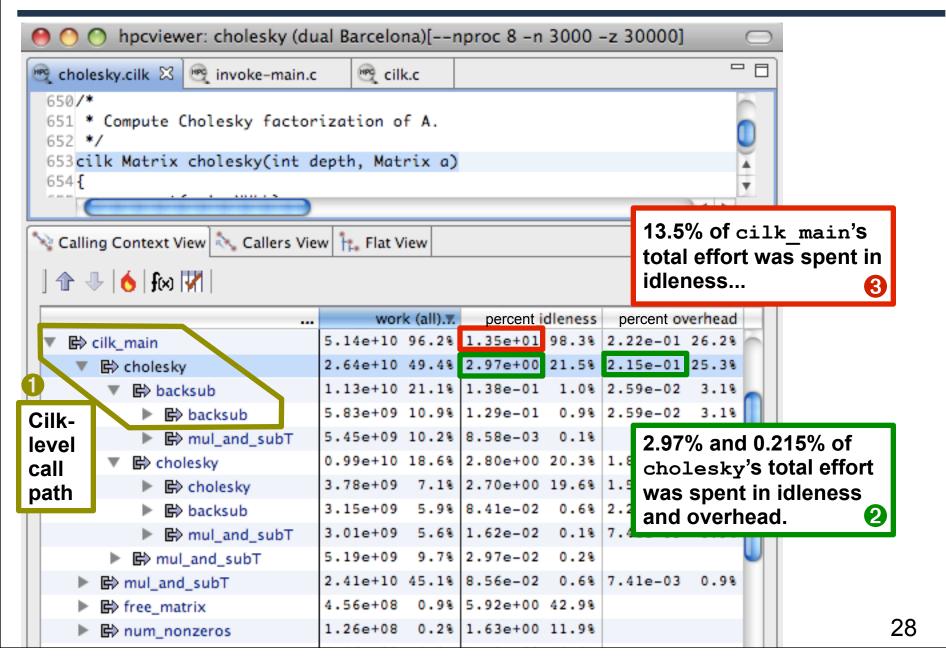
idle: drop sample (it's in the scheduler!)

26

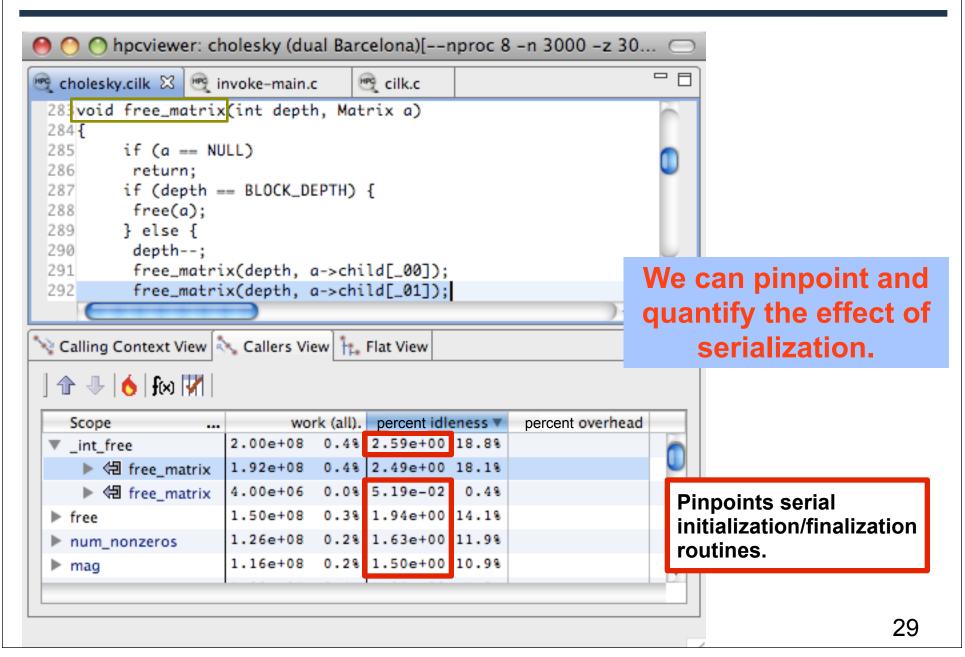
### **Parallel Overhead**

- Parallel overhead
  - when a thread works on something other than user code
    - (we classify waiting for work as idleness)
- Pinpointing overhead with call path profiling
  - impossible, without prior arrangement
    - work and overhead are both machine instructions
  - insight: have compiler tag instructions as overhead
  - quantify samples attributed to instructions that represent ovhd
    - use post-mortem analysis

### **Top-down Work for Cilk 'Cholesky'**



### **Bottom-up Idleness for Cilk 'Cholesky'**



### **Using Parallel Idleness & Overhead**

- Total effort = useful work + idleness + overhead
- Enables powerful and precise interpretations

idleness	overhead	interpretation
low	low	effectively parallel
low	high	coarsen concurrency granularity
high	low	refine concurrency granularity
high	high	switch parallelization strategies

- Normalize w.r.t. total effort to create
  - percent idleness or percent overhead

Nathan Tallent, John Mellor-Crummey. Effective performance measurement and analysis of multithreaded applications. PPoPP 2009, Raleigh, NC.

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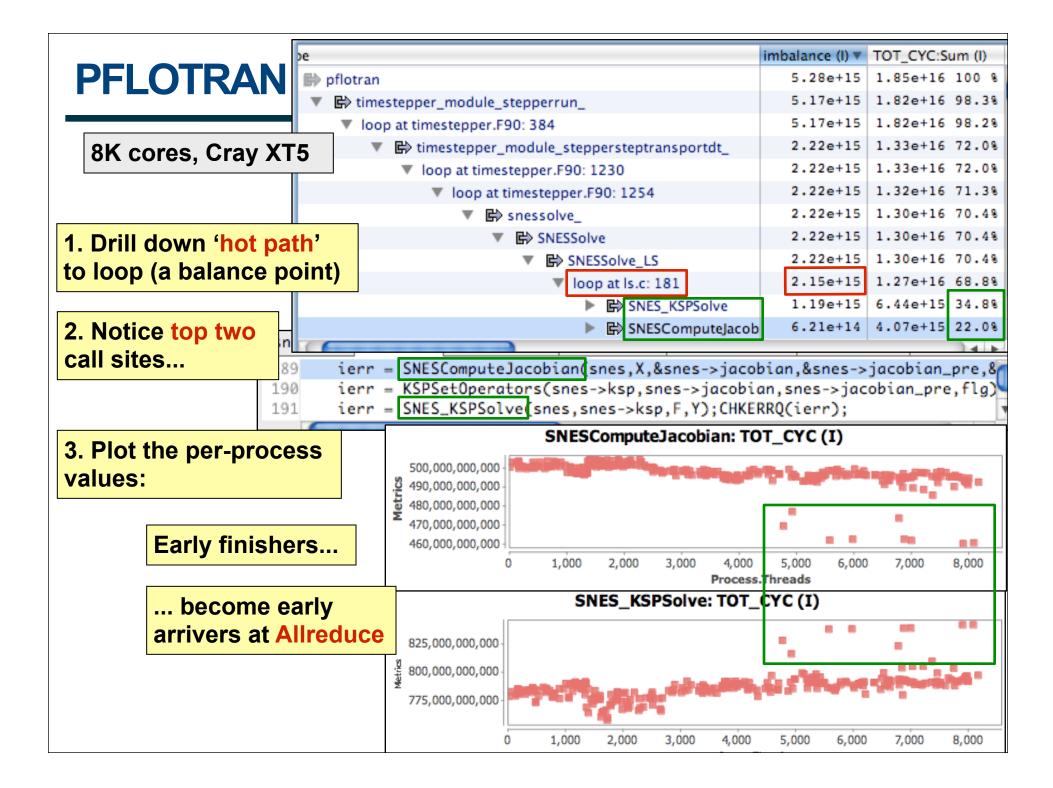
### **Understanding Lock Contention**

- Lock contention causes idleness
  - explicitly threaded programs (Pthreads, etc)
  - implicitly threaded programs (critical sections in OpenMP, Cilk...)
- Use "blame-shifting" to shift blame 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 assoc. with 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

578 add(MEMFUN_OBJT(memfunT)& obj,						
579 memfunT memfun,						
580 const arg1T& arg1, const arg2T& arg2, const arg3T& arg3, const TaskAttributes&						
581 Future <remfuture(memfun_returnt(memfunt))> result;</remfuture(memfun_returnt(memfunt))>						
582 add(new TaskMemfun <memfunt>(result,obj,memfun,arg1,arg2,arg3,attr)); 583 return result;</memfunt>						
auontum obomiotav: MDL $\pm$ atbroad						
584   }						
Calling Context View 💫 Callers View 🚏 Flat View						
] 16 cores; 1 thread/core (4 x E	Barcelona)	μs				
Scope	% idleness (all/E).	idleness (all/E)				
Experiment Aggregate Metrics	2.35e+01 100 %	1.57e+09 100 %				
▼ pthread_spin_unlock	2.35e+01 100.0	look contentio	~			
🔻 🖽 madness::Spinlock::unlock() const	2.35e+01 100.0	lock contention				
Inlined from worldmutex.h: 142	1.78e+01 75.6%	accounts for 2				
Madness::ThreadPool::add(madness::PoolTaskInterface*)	1.78e+01 75.6%	of execution ti	me.			
🔻 🖽 inlined from worldtask.h: 581	7.35e+00 31.2%	4.92e+08 31.2%				
madness::Future<> madness::WorldObject<>::task<>	7.35e+00 31.2%	4.92 A dalla a fact				
🔻 ا inlined from worldtask.h: 569	4.56e+00 19.4%	3.05 Adding fut				
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🔻 🖏 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		9.26e+07 5.9%				
Madness::Future<> madness::WorldTaskQueue::add<>(mathematical add)	a 6.72e-01 2.9%	4.49e+07 2.9%				
			<b>^</b>			
			33			

- Call path profiling in HPCToolkit
- Pinpointing and quantifying scalability bottlenecks
- Blame shifting
  - analyzing multithreaded computations based on work stealing
  - quantifying the impact of lock contention on threaded code
  - pinpointing load imbalance in parallel codes
- Understanding execution behavior over time
- Associating memory hierarchy inefficiency with data
- Conclusions
- Challenges ahead
- Related work



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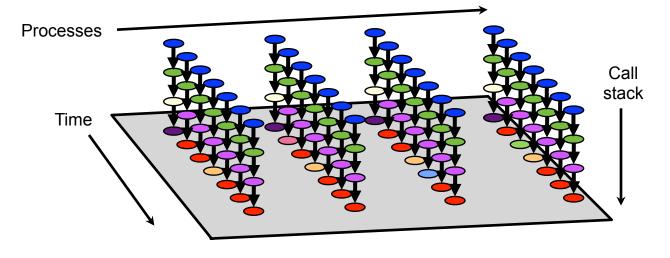
### **Understanding Temporal Behavior**

- Profiling compresses out the temporal dimension
   —temporal patterns, e.g. serialization, are invisible in profiles
- What can we do? Trace call path samples

-sketch:

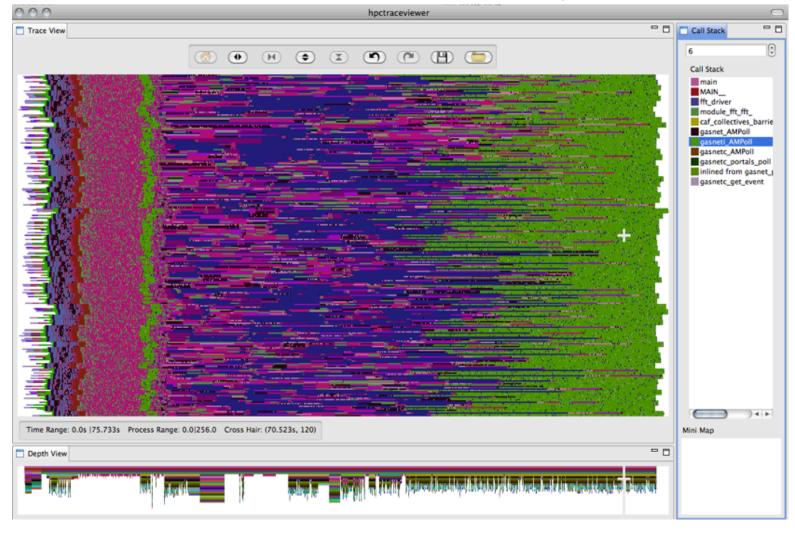
- N times per second, take a call path sample of each thread
- organize the samples for each thread along a time line
- view how the execution evolves left to right
- what do we view?

assign each procedure a color; view a depth slice of an execution



### **Call Path Tracing for Parallel Programs**

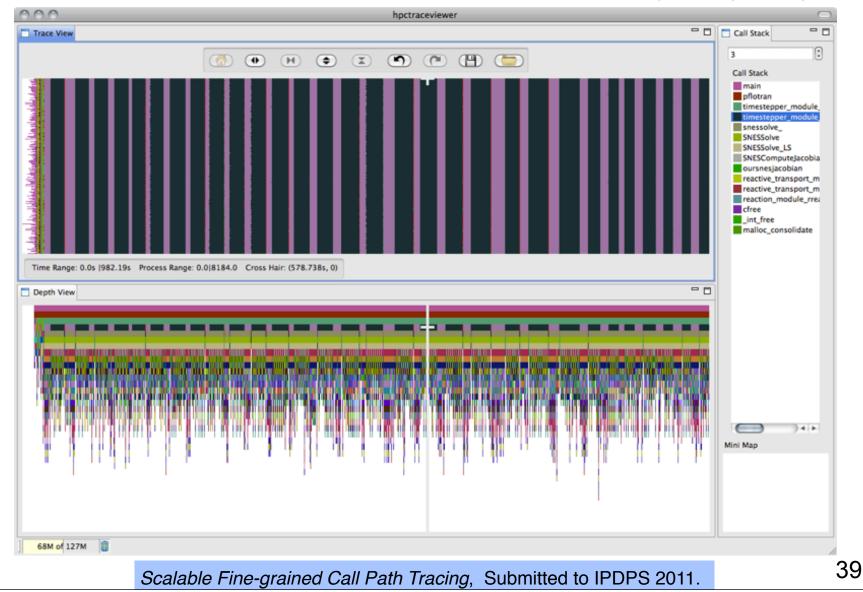
### 1D FFT, CAF 2.0, 256 processes, Cray XT, 128M/core



Scalable Fine-grained Call Path Tracing, Submitted to IPDPS 2011.

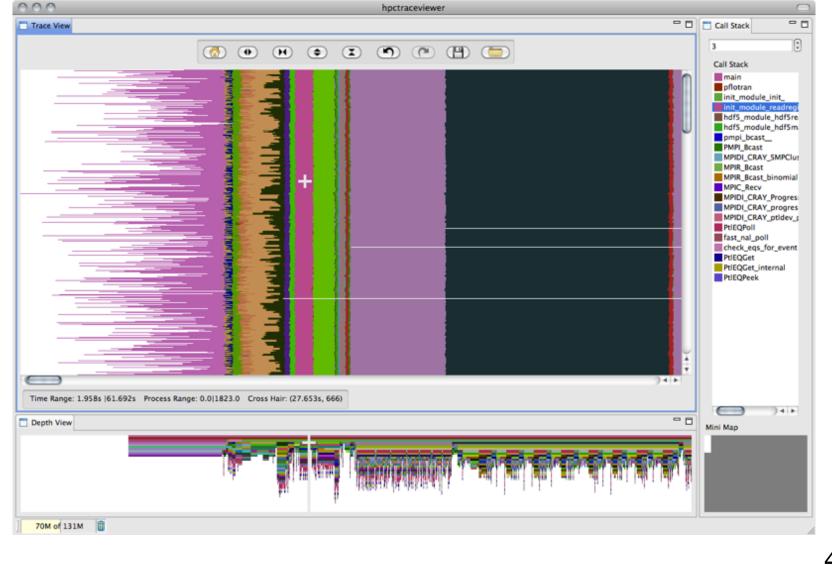
## **Call Path Tracing for Parallel Programs**

### PFLOTRAN: Fortran+MPI, 8184 cores, Cray XT (982s)



# **Call Path Tracing for Parallel Programs**

### **PFLOTRAN:** Fortran+MPI, 8184 cores, Cray XT (1st minute)



# Outline

- Call path profiling in HPCToolkit
- Pinpointing and quantifying scalability bottlenecks
- Blame shifting
  - analyzing multithreaded computations based on work stealing
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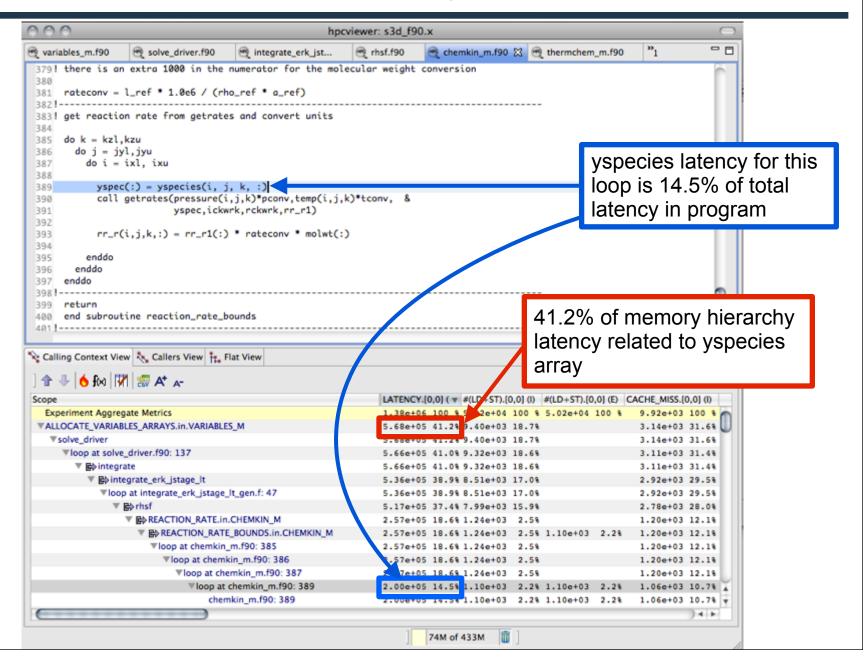
# **Data Centric Analysis**

• Goal: associate memory hierarchy performance losses with data

### • Approach

- intercept allocations to associate with their data ranges
- associate latency with data using "instruction-based sampling" on 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 quantitative results using hpcviewer

### **Data Centric Analysis of S3D**



# Conclusions

- 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
  - where insufficient parallelism lurks
  - sources of lock contention
  - load imbalance
  - temporal dynamics
  - problematic data structures

# **Some Challenges Ahead**

- Support characteristics of emerging hardware and software
  - heterogeneous hardware
    - manycore, CPU+GPU
    - dynamic power and frequency scaling
  - software
    - one-sided communication
    - asynchronous operations
    - dynamic parallelism
    - adaptation
    - failure recovery
- Augment monitoring capabilities throughout the stack — hardware, OS, runtime, language-level API
- Improve data management for extreme scale parallelism
- Transition from descriptive to prescriptive feedback
- Guide online adaptation and tuning

# **Some Related Work**

• Sampling

- e.g., gprof, Speedshop, Shark, PTU, DCPI, Oprofile, CrayPat

• Instrumentation

- e.g., Tau, Vtune, IBM HPC Toolkit, Dyninst, CrayPat, Pin

• Tracing

- e.g., vt, Tau, CEBPA,

- Call stack profiling — e.g., mpiP, Tau, PTU, Shark
- Visualization

- e.g., Paraver, Projections, Vampir, Jumpshot, EXPERT

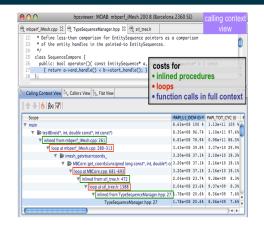
Parallel Analysis

— e.g., Scalasca

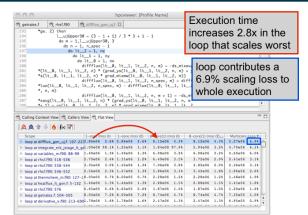
• Analysis

- e.g., IBM HPCS Toolkit, Cray Apprentice, EXPERT, PerfExpert 46

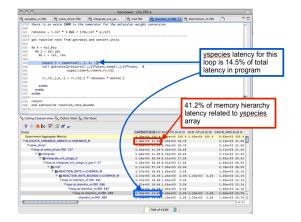
# **HPCToolkit Capabilities at a Glance**



### Attribute Costs to Code



#### Pinpoint & Quantify **Scaling Bottlenecks**

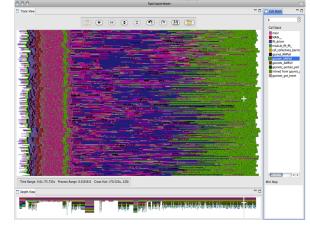


### Associate Costs with Data

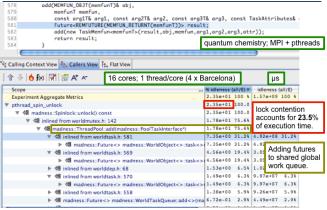
B pflotran

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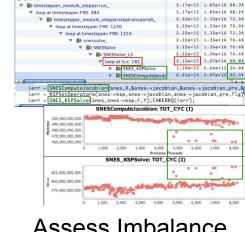
5,17e+15 1,82e+16 98,38



Analyze Behavior over Time



#### Shift Blame from Symptoms to Causes



Assess Imbalance and Variability

hpctoolkit.org

# **HPCToolkit Publications**

#### Measurement

- Binary analysis for (1) recovering functions in partially stripped code, (2) unwinding fully-optimized code, (3) recovering program structure
- Nearly perfect call stack sampling of fully optimized code with low overhead

Binary Analysis for Measurement and Attribution of Program Performance, PLDI, June 2009. Distinguished Paper Award.

> Pinpointing Locality Problems Using Data-centric Analysis, Submitted to CGO 2011, April 2011

#### **Pinpoint Scalability Bottlenecks using Differential Profiling**

Scalability Analysis of SPMD Codes using Expectations, ICS, June 2007

#### **Pinpoint Performance Losses in Multithreaded Executions**

Effective Performance Measurement and Analysis of Multithreaded Applications, PPoPP, February 2009.

Analyzing Lock Contention in Multithreaded Applications,

PPoPP, January 2010

### Novel Capabilities of HPCToolkit - II

#### Performance Analysis using Sampling on Leadership Platforms

Diagnosing Performance Bottlenecks in Emerging Petascale Applications, SC09, November 2009

Scalable Identification of Load Imbalance using Call Path Profiles, SC10, November 2010

#### **User Interfaces**

Effectively Presenting Call Path Profiles of Application Performance, PSTI, September 2010.

Scalable Fine-grained Call Path Tracing, Submitted to IPDPS 2011.

#### **Overview Paper**

HPCToolkit: Tools for performance analysis of optimized parallel programs, Concurrency & Computation: Practice and Experience, January 2010

# **Additional Tool Screenshots**

# **Execution Cost Breakdown (Routine-Level)**

### Flash on Blue Gene/P, 8K cores, white dwarf detonation

		viewer: FLASH/wh				
👰 local_tree_build.F90	👻 Grid_updateRefine	👻 rieman.F90	🤓 states.F90	🞅 Eos.F90	🞅 eos_helm.F90 🔀 🔭	<b>-</b>
80						
81 subroutine eos_	helm(eos_jlo,eos_jhi,ma	isk)				
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	, eos_dpdft, eos_dpdfd,				Note: only the rout	
	ombMult, eos_dLo, eos_t			&	~	
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	× (-	1			Layer costs	
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▶eos_helm					1.54e+08 22.9%	8.26e+07 12.3%
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DMA_RecFifoSimplePo	llNormalFifoById				3.22e+07 4.8%	3.08e+07 4.6%
▶_xlddpow					6.31e+07 9.4%	2.85e+07 4.2%
DCMF::Queueing::GI::	giMessage::advance()				7.15e+07 10.6%	2.52e+07 3.8%
▶expinner2					1.94e+07 2.9%	1.94e+07 2.9%
▶ rieman					2.12e+07 3.2%	1.82e+07 2.7%
▶loginner2					1.56e+07 2.3%	1.56e+07 2.3%
▶ states					1.51e+07 2.2%	1.36e+07 2.0%
▶amr_perm_to_1blk					1.30e+07 1.9%	1.30e+07 1.9%
▶xl_log					1.27e+07 1.9%	1.27e+07 1.9%
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▶amr_restrict_unk_gen						
	idvance()				5.71e+07 8.5%	1.20e+07 1.8% 1.12e+07 1.7%

### **Execution Cost Attribution (Callers View)**

### Flash on Blue Gene/P, 8K cores, white dwarf detonation

00	hpcviewer: FLASH/white dwarf: I	BM BG/P, weak	256->8192				1
mpi_an	mr_comm_setup.F90 🛱						
418	<pre>itemp = max(sum(commatrix_send), sum(commatrix_recv))</pre>						
419	Call MPI_ALLREDUCE (itemp,	&	Looki	ng up the call	chain to see		
420	max_blks_sent,	&		the callers the		+- +-	
21	1,	&	where	the callers that	ii caused cos	sis ic	)
22	MPI_INTEGER,	&	be incl	urred for tree	reductions N	Aost	F
23	MPI_MAX,	&				1000	ľ
24	MPI_COMM_WORLD,	8	of the	cost is incurre	d by guard d	cell	
25	ierror)	_	filling	and flux conse	arvation		
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Calling	Context View 📉 Callers View 👬 Flat View						6
							-
<b>₽</b> - ↓	<mark>6</mark> f∞   177   57 ∧*						
Scope				8192/WALLCLOCK (us) (I)	8192/WALLCLOCK (		-
	ment Aggregate Metrics			6.76e+08 100			
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	I inlined from Device.cc: 432			1.07e+08 15.9			ł
	7 In DCMF::Queueing::Tree::Device::postRecv(DCMF::Queueing::Tree::TreeRecvMessage&)			1.07e+08 15.9 1.07e+08 15.9			1
	▼ 4 inlined from Message.h: 516			1.07e+08 15.9			ł
	▼ ≪ DCMF_GlobalAllreduce			1.05e+08 15.5			1
	MPIDO_Allreduce_global_tree     MPIDO_Allreduce			1.05e+08 15.5			ł
	T I PMPLAllreduce			1.05e+08 15.5			ł
	v ( pmpi_allreduce			1.05e+08 15.5		15.5%	ł
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	► 🖶 amr_flux_conserve_udt			3.45e+05 0.1	3.45e+05	0.1%	ł
				6.50e+04 0.0	6.50e+04	0.0%	1
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	▶ 4 mpi_amr_1blk_restrict ▶ 4 amr_refine_derefine			5.04e+06 0.7	\$ 5.04e+06	0.78	U.
				5.04e+06 0.7 2.08e+06 0.3			ľ
	Amr_refine_derefine				8 2.08e+06	0.3%	

# **Execution Cost Attribution (Top Down)**

### Flash on Blue Gene/P, 8K cores, white dwarf detonation

hpcviewer: FLASH/white dwarf: IBM BG/P, weak 2	56->8192
<pre> mpi_amr_comm_setup.F90</pre>	Looking up down the call chain to see where the most of the time wa spent. 80.5% is spent in the loop that calls the hydrodynamics simulation. 52.4% of the time is spent in the hydro routine (or below). The rest is spent in other
N Calling Context View N Callers View H. Flat View ] ☆ ♣   6 f∞   17   27 A* A-	routines called from the main loop
Scope      8192/V       Experiment Aggregate Metrics        ▼ flash        ▼ loop at Driver_evolveFlash.F90: 92        ▼ loop at hy_ppm_sweep        ▶ loop at hy_ppm_sweep.F90: 222        ▶ loop at hy_ppm_sweep.F90: 520        ▶ loop at hy_ppm_sweep        ▶ loop at hy_ppm_sweep        ▶ loop at hy_ppm_sweep        ▶ loop at hy_ppm_sweep	WALLCLOCK (us) (I) = 8192/WALLCLOCK (us) (E) 6.76e+08 100 % 6.76e+08 100 % 5.44e+08 80.5% 5.44e+08 80.5% 1.78e+08 26.4% 5.99e+07 8.9% 2.50e+04 0.0% 2.04e+07 3.0% 5.00e+03 0.0% 1.65e+07 2.4% 1.36e+07 2.0% 9.45e+06 1.4% 5.98e+07 8.8% 1.50e+04 0.0% 5.86e+07 8.7% 1.50e+04 0.0%
	6.07e+07         9.0%         2.00e+04         0.0%           5.91e+07         8.7%         1.50e+04         0.0%           5.58e+07         8.2%         1.50e+04         0.0%

# **Execution Cost Attribution (Top-Down)**

### PFLOTRAN, Cray XT, 8184 cores, Hanford problem

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231					the	e cycles are	spent <sup>2</sup>	in the flow	W
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1234			ne-start_time)						
1235	option%tran_	weight_t1 = (option%		1e)/ &					
1236	L cok donašt		ne-start_time)						
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1 ♣ cope Tmain	of f∞   🕅   📟 .			TOT_C 1.96e	+16 100 %	3.14e+15 100	8	mbalance:Sum (I) 6.29e+15 100	)
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train Train Train Train Train Train Train Train Train Train	f(x) []X   S Z pflotran ⇒ timestepper_mod ▼loop at timesteppe ▶ loop at time ▶ B discretiz ▶ B discretiz ▶ B timesteppe	A <sup>+</sup> A <sup>-</sup> dule_stepperrun_ ber.F90: 384 er_module_steppersteptran: estepper.F90: 1230 zation_module_discretizatio zation_module_discretizatio	ionlocaltolocal_ ionlocaltolocal_ vdt_	TOT_C 1.96e 1.96e 1.94e 1.94e 1.31e 1.31e 8.84e 5.56e 6.05e	+16 100 % +16 100 % +16 98.8% +16 98.7% +16 66.5% +16 66.5% +11 0.0%	3.14e+15 100 3.14e+15 100 3.14e+15 99.9 3.14e+15 99.9 2.94e+15 93.5 2.94e+15 93.5 1.47e+07 0.0 4.90e+06 0.0 1.72e+14 5.5	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	mbalance:Sum (I) 6.29e+15 100 6.29e+15 100 6.21e+15 98.6 6.21e+15 98.6 1.97e+15 31.4 1.97e+15 31.4	9 8 68 68 48 48
train Train Train Train Train Train Train Train Train Train	f(x) []X   S Z pflotran ⇒ timestepper_mod ▼loop at timesteppe ▶ loop at time ▶ B discretiz ▶ B discretiz ▶ B timesteppe	A <sup>+</sup> A <sup>-</sup> dule_stepperrun_ ber.F90: 384 er_module_steppersteptran: estepper.F90: 1230 zation_module_discretizatio zation_module_discretizatio er_module_stepperstepflow er_module_stepperupdateso	ionlocaltolocal_ ionlocaltolocal_ vdt_	TOT_C 1.96e 1.96e 1.94e 1.94e 1.31e 1.31e 8.84e 5.56e 6.05e	+16 100 % +16 100 % +16 98.8% +16 98.7% +16 66.5% +16 66.5% +11 0.0% +11 0.0% +15 30.8% +14 1.1%	3.14e+15 100 3.14e+15 100 3.14e+15 99.9 3.14e+15 99.9 2.94e+15 93.5 2.94e+15 93.5 1.47e+07 0.0 4.90e+06 0.0 1.72e+14 5.5 2.95e+13 0.9	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	mbalance:Sum (I) 6.29e+15 100 6.29e+15 100 6.21e+15 98.6 6.21e+15 98.6 1.97e+15 31.4 1.97e+15 31.4	9 8 68 68 48 48
Tree of the second sec	fix IVI STATES pflotran b timestepper_mod vloop at timesteppe v B timesteppe b b discretiz b B discretiz b B timesteppe b B timesteppe b B timesteppe b B timesteppe b B timesteppe b B timesteppe b B timesteppe	A <sup>+</sup> A <sup>-</sup> dule_stepperrun_ ber.F90: 384 er_module_steppersteptran: estepper.F90: 1230 zation_module_discretizatio zation_module_discretizatio er_module_stepperstepflow er_module_stepperupdateso	ionlocaltolocal_ ionlocaltolocal_ vdt_ olution_	TOT_C 1.96e 1.96e 1.94e 1.94e 1.31e 1.31e 8.84e 5.56e 6.05e 2.24e	+16 100 % +16 100 % +16 98.8% +16 98.7% +16 66.5% +16 66.5% +11 0.0% +11 0.0% +15 30.8% +14 1.1% +13 0.2%	3.14e+15 100 3.14e+15 100 3.14e+15 99.9 3.14e+15 99.9 2.94e+15 93.5 2.94e+15 93.5 1.47e+07 0.0 4.90e+06 0.0 1.72e+14 5.5 2.95e+13 0.9 1.47e+07 0.0	8 8 98 98 98 98 98 98 98 98 98 98 98 98	mbalance:Sum (I) 6.29e+15 100 6.29e+15 100 6.21e+15 98.6 6.21e+15 98.6 1.97e+15 31.4 1.97e+15 31.4	9 8 68 68 48 48
Transformer Contraction Contr	flotran ⇒ timestepper_mod ▼loop at timesteppe ▼loop at timesteppe ► bioop at timesteppe ► biotimesteppe ► bimesteppe ► bimesteppe ► bimesteppe ► bimesteppe ► bimestepper_mod	A <sup>+</sup> A <sup>-</sup> dule_stepperrun_ ber.F90: 384 er_module_steppersteptran: estepper.F90: 1230 zation_module_discretizatio zation_module_discretizatio er_module_stepperstepflow er_module_stepperupdateso idule_output_	ionlocaltolocal_ ionlocaltolocal_ vdt_ olution_ ition_	TOT_C 1.96e 1.96e 1.94e 1.94e 1.31e 1.31e 8.84e 5.56e 6.05e 2.24e 3.45e	+16 100 % +16 100 % +16 98.8% +16 98.7% +16 66.5% +16 66.5% +11 0.0% +11 0.0% +15 30.8% +14 1.1% +13 0.2% +12 0.0%	3.14e+15 100 3.14e+15 100 3.14e+15 99.9 3.14e+15 99.9 2.94e+15 93.5 2.94e+15 93.5 1.47e+07 0.0 4.90e+06 0.0 1.72e+14 5.5 2.95e+13 0.9 1.47e+07 0.0 8.00e+11 0.0	8 8 98 98 98 98 98 98 98 98 98 98 98 98	mbalance:Sum (I) 6.29e+15 100 6.29e+15 100 6.21e+15 98.6 6.21e+15 98.6 1.97e+15 31.4 1.97e+15 31.4	9 8 68 68 48 48

### **Execution Cost Attribution (Top-Down)**

### PFLOTRAN, Cray XT, 8184 cores, Hanford problem

hpcv	iewer: pflotran			
bcgs.c 🔀 👰 zsnesf.c 🛛 👰 timestepper.F90				
<pre>66 ierr = VecSet(V,0.0);CHKERRQ(ierr);</pre>				Ċ.
67 68 i-0:	Л	atailed analy	ysis of the transp	ort
69 do {		•	J 1	
	<- (r,rp) */ Ca	alculation: N	Aost of the time	is
71 beta = (rho/rhoold) * (alpha/omegaold);		ant in the D	ETCo incido tho	
<pre>72 ierr = VecAXPBYPCZ(P,1.0,-omegaold*beta,beta,R,V);CHKER 73 ierr = KSP_PCApplyBAorAB(ksp,P,V,T);CHKERRQ(ierr); /*</pre>		pent in the P	ETSc inside the	
<pre>74 ierr = VecDot(V,RP,&amp;d1);CHKERRQ(ierr); /*</pre>		iconiugate g	gradient solver.	
75 if (d1 -= 0.0) SETERRQ(PETSC_ERR_PLIB, "Divide by zero")		1 J 8 E		
76 alpha = rho / d1; /* a <- rho / (v,rp				÷
77 ionn - VocWAVDV/C alaba V Dl:CUVEDDA/ionnl: /#	• • • • • • /			
			1	
Calling Context View 🥾 Callers View 🙀 Flat View	<b>Overall: 1 FLOP</b>	everv 7.4 c	cycles	
		•	•	
1 🕆 🖖 🧴 fixi 🕎 🐖 🗛 👝		J	·	
	TOT_CYC:Sum (I) =	FP_OPS:Sum (I)		dle
icope		FP_OPS:Sum (I)	imbalance:Sum (I) ic	12
scope ▼ ⊯ pflotran	TOT_CYC:Sum (I) =			.2
icope	TOT_CYC:Sum (I. + 1.96e+16 100 %	FP_OPS:Sum (I) 3.14e+15 100 %	imbalance:Sum (l) ic 6.29e+15 100 % 6.	.2
scope ▼ ■ pflotran ▼ B timestepper_module_stepperrun_	TOT_CYC:Sum (I ¥ 1.96e+16 100 % 1.94e+16 98.8%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9%	imbalance:Sum (l) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6.	. 2 . 2 . 2
icope ▼  pflotran ▼  timestepper_module_stepperrun_ ▼ loop at timestepper.F90: 384	TOT_CYC:Sum (I, ¥ 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9%	imbalance:Sum (l) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6.	. 2 . 2 . 2 . 9
Scope ▼  pflotran ▼  timestepper_module_stepperrun_ ▼ loop at timestepper.F90: 384 ▼  timestepper_module_steppersteptransportdt_	TOT_CYC:Sum (I, ¥ 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1.	. 2 . 2 . 2 . 9
<pre>scope</pre>	TOT_CYC:Sum ([.▼ 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 66.5%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5%	imbalance:Sum (I) id 6.29e+15 100 % 6 6.21e+15 98.6% 6 6.21e+15 98.6% 6 1.97e+15 31.4% 1 1.97e+15 31.4% 1	· 2 . 2 . 2 . 9 . 9 . 9
<pre>scope</pre>	TOT_CYC:Sum ([. v 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 66.5% 1.29e+16 65.9%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 92.9%	imbalance:Sum (I) id 6.29e+15 100 % 6 6.21e+15 98.6% 6 6.21e+15 98.6% 6 1.97e+15 31.4% 1 1.97e+15 31.4% 1 1.97e+15 31.3% 1	. 2 . 2 . 2 . 9 . 9 . 9 . 9 . 9
icope ▼  pflotran ▼  b timestepper_module_stepperrun_ ▼  loop at timestepper.F90: 384 ▼  b timestepper_module_steppersteptransportdt_ ▼  loop at timestepper.F90: 1230 ▼  loop at timestepper.F90: 1254 ▼  b snessolve_	TOT_CYC:Sum ([ ▼ 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 66.5% 1.29e+16 65.9% 1.28e+16 65.1%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 92.9% 2.89e+15 91.9%	imbalance:Sum (l) ic 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1.	.2 .2 .9 .9 .9 .9 .9
icope	TOT_CYC:Sum ([.▼ 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 66.5% 1.29e+16 65.9% 1.28e+16 65.1% 1.28e+16 65.1%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 92.9% 2.69e+15 91.9%	imbalance:Sum (l) ic 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1.	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9
icope	TOT_CYC:Sum (I v 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 66.5% 1.29e+16 65.9% 1.28e+16 65.1% 1.28e+16 65.1%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.92e+15 93.5% 2.92e+15 92.9% 2.69e+15 91.9% 2.69e+15 91.9%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1.	. 2 . 2 . 9 . 9 . 9 . 9 . 9 . 9 . 9 . 9 . 9 . 9
icope	TOT_CYC:Sum (! v 1.96e+16 100 % 1.94e+16 98.8% 1.94e+16 98.7% 1.31e+16 66.5% 1.31e+16 65.5% 1.29e+16 65.9% 1.28e+16 65.1% 1.28e+16 65.1% 1.28e+16 65.1% 1.25e+16 63.6%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 92.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.91e+15 30.3% 1.	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9
scope ▼  pflotran ▼  b timestepper_module_stepperrun_ ▼ loop at timestepper.F90: 384 ▼  b timestepper_module_steppersteptransportdt_ ▼ loop at timestepper.F90: 1230 ▼ loop at timestepper.F90: 1254 ▼  b snessolve_ ▼  b SNESSolve_ ▼  b SNESSolve_LS ▼  loop at ls.c: 181 ▼  b SNES_KSPSolve ▼  b KSPSolve ▼  b KSPSolve_BCGS	TOT_CYC:Sum (! ▼           1.96e+16         100 %           1.94e+16         98.8%           1.94e+16         98.7%           1.31e+16         66.5%           1.31e+16         65.9%           1.28e+16         65.1%           1.28e+16         65.1%           1.28e+16         65.1%           1.25e+16         63.6%           6.37e+15         32.4%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 92.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5% 1.85e+15 58.9%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.91e+15 30.3% 1. 7.23e+14 11.5% 1.	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .1 .1
<pre>scope</pre>	TOT_CYC:Sum (I, ▼           1.96e+16         100 %           1.94e+16         98.8%           1.94e+16         98.7%           1.31e+16         66.5%           1.31e+16         65.9%           1.28e+16         65.1%           1.28e+16         65.1%           1.28e+16         65.1%           1.25e+16         63.6%           6.37e+15         32.4%           6.37e+15         23.5%           3.90e+15         19.9%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5% 1.85e+15 58.9% 1.85e+15 58.9% 5.70e+14 18.1% 5.21e+14 16.6%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 30.3% 1. 7.23e+14 11.5% 1.	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .1 .1
<pre>scope</pre>	TOT_CYC:Sum (() ▼           1.96e+16         100 %           1.94e+16         98.8%           1.94e+16         98.7%           1.31e+16         66.5%           1.31e+16         65.9%           1.28e+16         65.1%           1.28e+16         65.1%           1.28e+16         65.1%           1.25e+16         63.6%           6.37e+15         32.4%           4.62e+15         23.5%           3.90e+15         19.9%           1.58e+15         8.1%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5% 1.85e+15 58.9% 1.85e+15 58.9% 5.70e+14 18.1% 5.21e+14 16.6% 2.54e+14 8.1%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.91e+15 30.3% 1. 7.23e+14 11.5% 1. 7.23e+14 11.5% 1. Overall: 1 FLC	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9
iscope         ▼ ➡ pflotran         ▼ ➡ timestepper_module_stepperrun_         ▼ loop at timestepper_module_steppersteptransportdt_         ▼ loop at timestepper.F90: 1230         ▼ loop at timestepper.F90: 1254         ▼ ➡ snessolve_         ▼ ➡ SNESSolve         ▼ ➡ KSPSolve         ▼ ➡ KSPSolve_BCCS         ▼ loop at bcgs.c: 69         ▶ ➡ PCApplyBAorAB         ➡ ➡ PCApplyBAorAB	TOT_CYC:Sum (() ▼           1.96e+16         100 %           1.94e+16         98.8%           1.94e+16         98.7%           1.31e+16         66.5%           1.31e+16         66.5%           1.29e+16         65.9%           1.28e+16         65.1%           1.28e+16         65.1%           1.28e+16         65.1%           1.25e+16         63.6%           6.37e+15         32.4%           4.62e+15         23.5%           3.90e+15         19.9%           1.58e+15         8.1%           1.58e+15         8.0%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5% 1.85e+15 58.9% 1.85e+15 58.9% 5.70e+14 18.1% 5.21e+14 16.6% 2.54e+14 8.1%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.91e+15 30.3% 1. 7.23e+14 11.5% 1.	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9
<pre>scope</pre>	TOT_CYC:Sum (() ▼           1.96e+16         100 %           1.94e+16         98.8%           1.94e+16         98.7%           1.31e+16         66.5%           1.31e+16         65.9%           1.28e+16         65.1%           1.28e+16         65.1%           1.28e+16         65.1%           1.25e+16         63.6%           6.37e+15         32.4%           4.62e+15         23.5%           3.90e+15         19.9%           1.58e+15         8.1%	FP_OPS:Sum (I) 3.14e+15 100 % 3.14e+15 99.9% 3.14e+15 99.9% 2.94e+15 93.5% 2.94e+15 93.5% 2.92e+15 91.9% 2.89e+15 91.9% 2.89e+15 91.9% 2.84e+15 90.5% 1.85e+15 58.9% 1.85e+15 58.9% 5.70e+14 18.1% 5.21e+14 16.6% 2.54e+14 8.1%	imbalance:Sum (I) id 6.29e+15 100 % 6. 6.21e+15 98.6% 6. 6.21e+15 98.6% 6. 1.97e+15 31.4% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.97e+15 31.3% 1. 1.91e+15 30.3% 1. 7.23e+14 11.5% 1. 7.23e+14 11.5% 1. Overall: 1 FLC	.2 .2 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9 .9