

Virtual Institute –

9-10 August 2012

Brian Wylie Jülich Supercomputing Centre b.wylie@fz-juelich.de







awrence Livermore

lational Laboratory

CSCS

















Outline



Thursday 9 August

- 09:00 (start)
- Performance analysis and tools overview (Geimer, JSC)
- Accessing & using CSCS resources
- 10:30-10:45 (break)
- Profile & automatic trace analysis with Scalasca (Wylie/Geimer, JSC)
- 12:30-13:30 (lunch)
- Trace analysis with Vampir (Knüpfer, TU Dresden)
- 15:00-15:15 (break)
- Assisted analysis & tuning of participants' codes
- 17:30 (adjourn)

- We'd like to know a little about you, your application(s), and your expectations and desires from this tutorial
- What programming paradigms do you use in your app(s)?
 - only MPI, only OpenMP, mixed-mode/hybrid OpenMP/MPI, ...
 - Fortran, C, C++, multi-language, …
- What platforms/systems *must* your app(s) run well on?
 - Cray XT/XE/XK, IBM BlueGene, SGI Altix, Linux cluster™, ...
- Who's already familiar with *serial* performance analysis?
 - Which tools have you used?
 - ► time, print/printf, prof/gprof, ...
- Who's already familiar with *parallel* performance analysis?
 - Which tools have you used?
 - ▶ time, print/printf, prof/gprof, Periscope, Scalasca, TAU, Vampir, ...

• Ensure your application codes build and run to completion with appropriate datasets

- initial configuration should ideally run in less than 15 minutes with 1-4 compute nodes (up to 64 processes/threads)
 - ► to facilitate rapid turnaround and quick experimentation
- Iarger/longer scalability configurations are also interesting
 - turnaround may be limited due to busyness of batch queues
- Compare your application performance on other systems
 - VI-HPS tools already installed on a number of HPC systems
 - if not, ask your system administrator to install them (or install a personal copy yourself)

- **Goal**: Improve the quality and accelerate the development process of complex simulation codes running on highly-parallel computer systems
- Start-up funding (2006-2011) by Helmholtz Association of German Research Centres
- Activities
 - Development and integration of HPC programming tools
 - Correctness checking & performance analysis
 - Training workshops
 - Service
 - Support email lists
 - Application engagement
 - Academic workshops

www.vi-hps.org





VI-HPS partners (founders)





- Forschungszentrum Jülich
 - Jülich Supercomputing Centre
- **RWTH Aachen University**
 - Centre for Computing & Communication
- Technical University of Dresden
 - Centre for Information Services & HPC
- University of Tennessee (Knoxville)
 - Innovative Computing Laboratory









VI-HPS partners (cont.)

















Centro Nacional de Supercomputación

German Research School

- Laboratory of Parallel Programming
- Lawrence Livermore National Lab.
 - Centre for Applied Scientific Computing
- **Technical University of Munich**
 - Chair for Computer Architecture
- University of Oregon
 - Performance Research Laboratory
- University of Stuttgart
 - HPC Centre



- University of Versailles St-Quentin
 - LRC ITACA









UNIVERSITY OF OREGON









Marmot/MUST

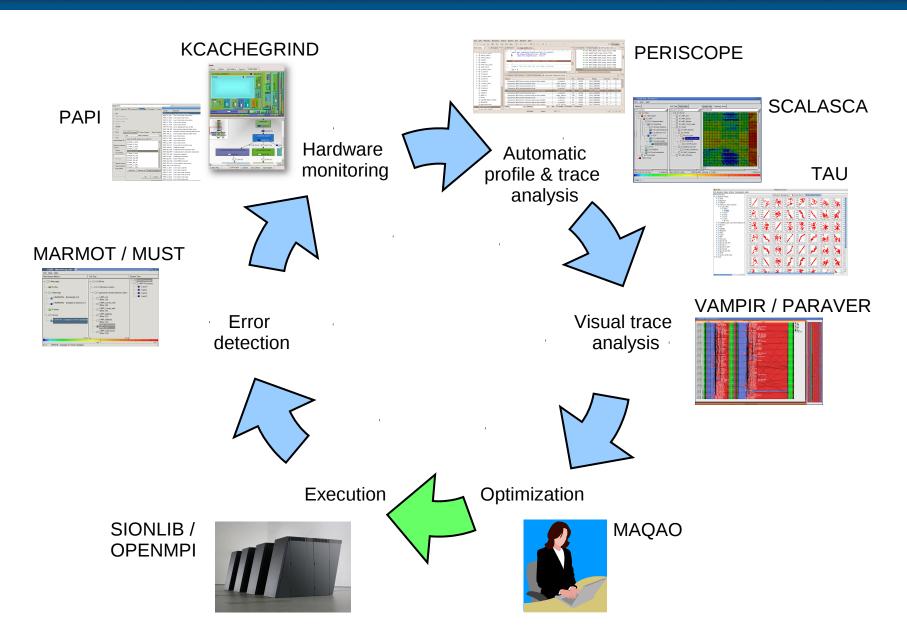
- MPI correctness checking
- PAPI
 - Interfacing to hardware performance counters
- Periscope
 - Automatic analysis driven by on-line distributed search
- Scalasca
 - Large-scale parallel performance analysis
- TAU
 - Integrated parallel performance system
- Vampir/VampirTrace
 - Event tracing and graphical trace visualization & analysis
- Score-P
 - Common instrumentation & measurement infrastructure

- KCachegrind
 - Callgraph-based cache analysis [x86 only]
- MAQAO
 - Assembly instrumentation & optimization [x86 only]

- mpiP/mpiPview
 - MPI profiling tool and analysis viewer
- ompP
 - OpenMP profiling tool
- OpenMPI
 - Memory checking
- Open|SpeedShop
 - Integrated parallel performance analysis environment
- Paraver/Extrae
 - Event tracing and graphical trace visualization & analysis

Technologies and their integration







Tools will *not* automatically make you, your applications or computer systems more *productive*.

However, they can help you understand **how** your parallel code executes and **when / where** it's necessary to work on *correctness* and *performance* issues.

- Goals
 - Give an overview of the programming tools suite
 - Explain the functionality of individual tools
 - Teach how to use the tools effectively
 - Offer hands-on experience and expert assistance using tools
 - Receive feedback from users to guide future development
- For best results, bring & analyse/tune your own code(s)!
- VI-HPS Tutorial series
 - SC'08, ICCS'09, SC'09, Cluster'10, SC'10, SC'11, EuroMPI'12
- VI-HPS Tuning Workshop series
 - 2008 (Aachen & Dresden), 2009 (Jülich & Bremen), 2010 (Garching & Amsterdam), 2011 (Stuttgart & Aachen)
 - 2012/04/23-27 (St-Quentin), 2012/10/15-19 (Garching)

• EuroMPI hands-on tutorial (23 Sep 2012, Vienna, Austria)

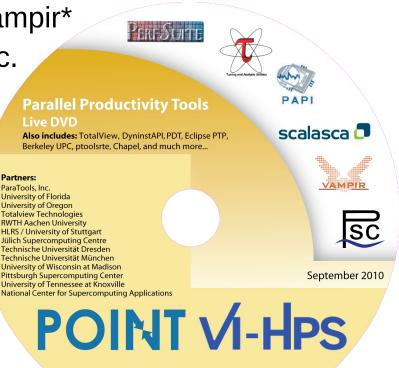
VI-HPS

- Periscope, Scalasca, TAU, Vampir (using Score-P)
- 10th VI-HPS Tuning Workshop (15-19 Oct 2012)
 - hosted by LRZ, Garching-bei-München, Germany
 - using PRACE Tier-0 SuperMUC iDataPlex system
 - Scalasca, Vampir, TAU, Periscope, KCachegrind, MAQAO, ...
- Further events to be determined
 - (one-day) tutorials
 - with guided exercises usually using Live DVD
 - (multi-day) training workshops
 - ► with your own applications on real HPC systems

Check www.vi-hps.org/training for announced events

• Contact us if you might be interested in hosting an event

- Bootable Linux installation ISO (on DVD or USB drive)
- Includes everything needed to try out our parallel tools on an x86-architecture notebook computer
 - VI-HPS tools: KCachegrind, Marmot, PAPI, Periscope, Scalasca, TAU, VT/Vampir*
 - Also: Eclipse/PTP, TotalView*, etc.
 - * time/capability-limited evaluation licences provided for commercial products
 - GCC (w/ OpenMP), OpenMPI
 - Manuals/User Guides
 - Tutorial exercises & examples
- Produced by U. Oregon PRL
 - Sameer Shende





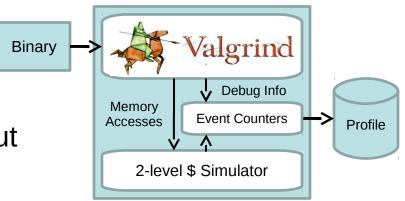
- distributed on DVD or USB drive
- or download from website
- Boot directly from disk
 - enables hardware counter access and offers best performance

- Boot within virtual machine
 - faster boot time and can save/resume state, but no hardware counter access
- Boots into Linux environment
 - supports building and running provided MPI and/or OpenMP parallel application codes
 - and experimentation with VI-HPS (and other) tools

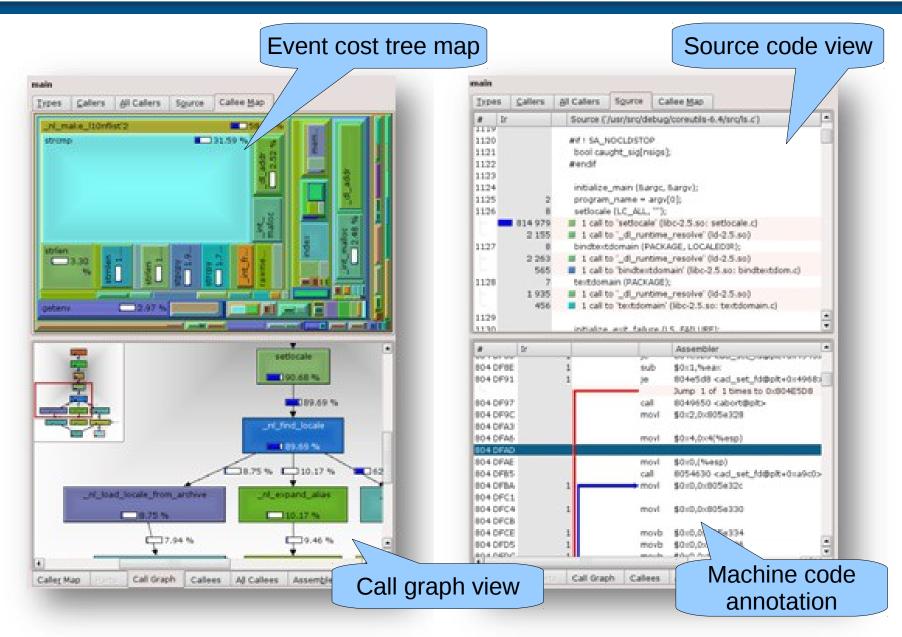
VI-HPS

Cachegrind: cache analysis by simple cache simulation

- Captures dynamic callgraph
- Based on valgrind dynamic binary instrumentation
- Runs on x86/PowerPC/ARM unmodified binaries
 - No root access required
- ASCII reports produced
- [KQ]Cachegrind GUI
 - Visualization of cachegrind output
- Developed by TU Munich
 - Released as GPL open-source
 - http://kcachegrind.sf.net/



KCachegrind GUI



Tool to check for correct MPI usage at runtime

- Checks conformance to MPI standard
 - Supports Fortran & C bindings of MPI-1.2
- Checks parameters passed to MPI
- Monitors MPI resource usage

Implementation

- C++ library gets linked to the application
- Does not require source code modifications
- Additional process used as DebugServer
- Results written in a log file (ASCII/HTML/CUBE)

Developed by HLRS & TU Dresden

- Released as open-source
- http://www.hlrs.de/organization/av/amt/projects/marmot





Marmot logfiles



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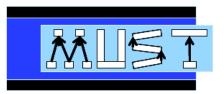


Next generation MPI runtime error detection tool

- Successor of the Marmot and Umpire tools
- Initial merge of Marmot's many local checks with Umpire's non-local checks
- Improved scalability expected in future
- Exploits CMake, GTI & PnMPI infrastructure

Developed by TU Dresden, LLNL & LANL

- BSD license open-source initial release in November 2011
- http://tu-dresden.de/zih/must/







Portable performance counter library & utilities

- Configures and accesses hardware/system counters
- Predefined events derived from available native counters
- Core component for CPU/processor counters
 - instructions, floating point operations, branches predicted/taken, cache accesses/misses, TLB misses, cycles, stall cycles, ...
 - performs transparent multiplexing when required
- Extensible components for off-processor counters
 - ► InfiniBand network, Lustre filesystem, system hardware health, ...
- Used by multi-platform performance measurement tools
 - ► Periscope, Scalasca, TAU, VampirTrace, ...

Developed by UTK-ICL

Available as open-source for most modern processors http://icl.cs.utk.edu/papi/



```
juropa$ papi avail
                                                  juropa$ papi avail -d
Available events and hardware information.
                                                  . . .
                                                  Symbol Event Code Count
                                                                                  |Short Descr.|
                                                   |Long Description|
PAPI Version
                       : 4.1.0.0
Vendor string and code : GenuineIntel (1)
                                                   |Developer's Notes|
Model string and code
                        : Intel(R) Xeon(R) CPU
                                                   |Derived|
                        X5570 @ 2.93GHz (26)
                                                   |PostFix|
                                                   Native Code[n]: <hex> |name|
CPU Revision
                        : 5.000000
CPUID Info
                        : Family: 6 Model: 26
                                                  PAPI L1 DCM
                                                                0x80000000 1 |L1D cache misses|
                          Stepping: 5
                                                   |Level 1 data cache misses|
CPU Megahertz
                        : 1600.000000
CPU Clock Megahertz
                        : 1600
                                                   |NOT DERIVED|
Hdw Threads per core
                        : 2
Cores per Socket
                        : 4
                                                   Native Code[0]: 0x40002028 |L1D:REPL|
NUMA Nodes
                        : 2
                                                  PAPI L1 ICM
                                                                0x80000001 1 |L1I cache misses|
CPU's per Node
                        : 8
                                                   |Level 1 instruction cache misses|
Total CPU's
                        : 16
Number Hardware Counters : 16
                                                   Max Multiplex Counters : 512
                                                   |NOT DERIVED|
                                                   Native Code[0]: 0x40001031 |L1I:MISSES|
        Code Avail Deriv Description
    Name
                                                  PAPI L2 DCM
                                                                0x80000002 2 |L2D cache misses|
PAPI L1 DCM 0x80000000 Yes
                              No
                                                   |Level 2 data cache misses|
                     Level 1 data cache misses
PAPI L1 ICM 0x80000001 Yes
                              No
                                                   |DERIVED SUB|
              Level 1 instruction cache misses
                                                   Native Code[0]: 0x40000437 |L2 RQSTS:MISS|
                                                   Native Code[1]: 0x40002037
Of 107 possible events, 35 are available, of
                                                  L2 RQSTS: IFETCH MISS
which 9 are derived.
                                                  . . .
```

juropa\$ papi native avail Available native events and hardware information. . . . Event Code Symbol | Long Description | 0x40000000 UNHALTED CORE CYCLES | count core clock cycles whenever the cloc | k signal on the specific core is running (not halted). Alias to e | vent CPU CLK UNHALTED:THREAD 0x40000001 **INSTRUCTION RETIRED** | count the number of instructions at retire | ment. Alias to event INST RETIRED: ANY P 0x40000086 UNC SNP RESP TO REMOTE HOME | Remote home snoop response - LLC d | oes not have cache line :I STATE | Remote home snoop response - LLC does not have cache 40000486 | line 40000886 **:S STATE** | Remote home snoop response - LLC has cache line in S l state 40001086 :FWD S STATE | Remote home snoop response - LLC forwarding cache | line in S state. :FWD I STATE | Remote home snoop response - LLC has forwarded a 40002086 | modified cache line :CONFLICT | Remote home conflict snoop response 40004086 :WB | Remote home snoop response - LLC has cache line in the M s 40008086 | tate **:HITM** | Remote home snoop response - LLC HITM 40010086

Total events reported: 135



Automated profile-based performance analysis

- Iterative on-line performance analysis
 - Multiple distributed hierarchical agents
- Automatic search for bottlenecks based on properties formalizing expert knowledge
 - MPI wait states, OpenMP overheads and imbalances
 - Processor utilization hardware counters
- Clustering of processes/threads with similar properties
- Eclipse-based integrated environment

Supports

SGI Altix Itanium2, IBM Power and x86-based architectures

Developed by TU Munich

- Released as open-source
- http://www.lrr.in.tum.de/periscope



MPI

- Excessive MPI communication time
- Excessive MPI time due to many small messages
- Excessive MPI time in receive due to late sender

■ ...

OpenMP

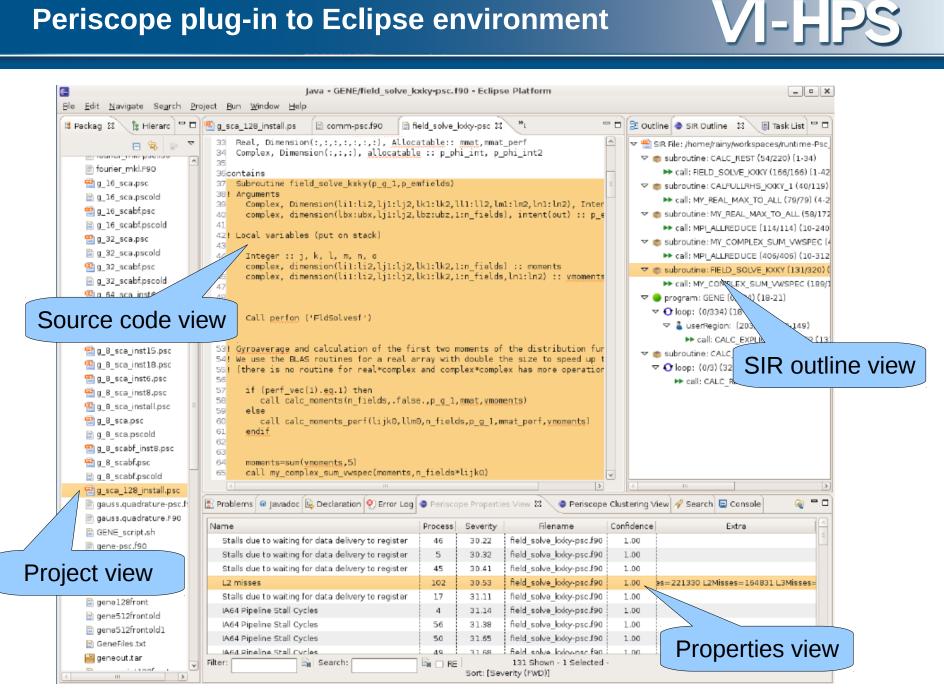
- Load imbalance in parallel region/section
- Sequential computation in master/single/ordered region

■ ...

Hardware performance counters (platform-specific)

- Cycles lost due to cache misses
 - High L1/L2/L3 demand load miss rate
- Cycles lost due to no instruction to dispatch

Periscope plug-in to Eclipse environment



VI-HPS

Automatic performance analysis toolset

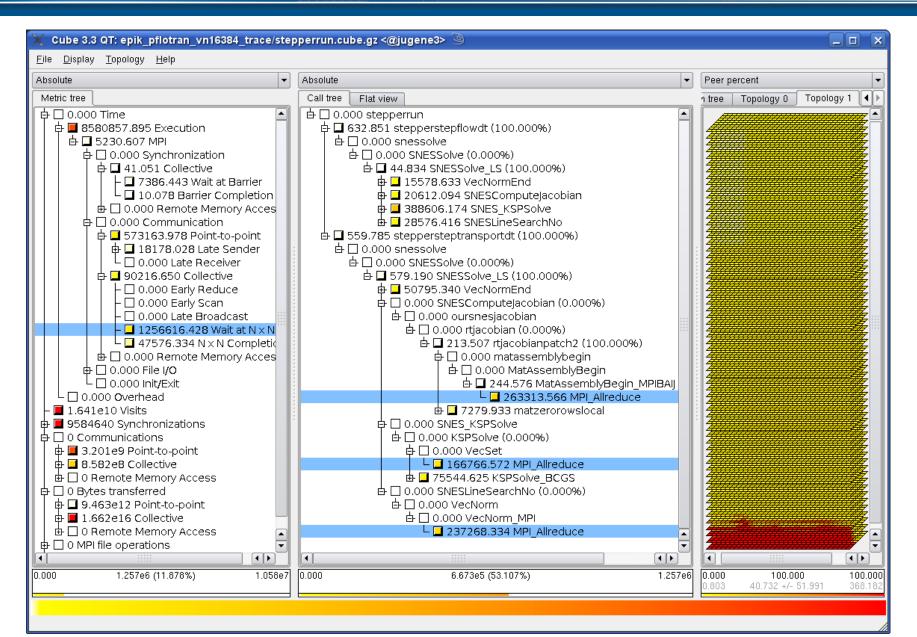
- Scalable performance analysis of large-scale applications
 - particularly focused on MPI & OpenMP paradigms
 - analysis of communication & synchronization overheads
- Automatic and manual instrumentation capabilities
- Runtime summarization and/or event trace analyses
- Automatic search of event traces for patterns of inefficiency
 - Scalable trace analysis based on parallel replay
- Interactive exploration GUI and algebra utilities for XML callpath profile analysis reports

Developed by JSC & GRS

- Released as open-source
- http://www.scalasca.org/



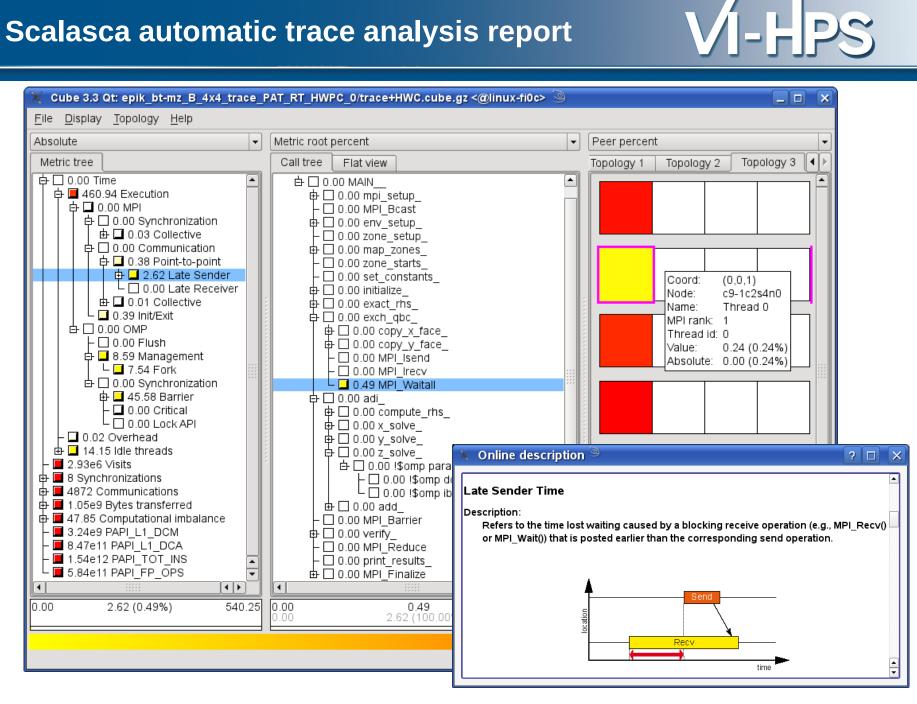
Scalasca automatic trace analysis report



Scalasca hybrid analysis report

Cube 3.3 Ot: epik bt-mz B 4x4 trace PAT RT HWPC 0/trace+HWC.cube.gz <@linux-fi0c> 🥯 _ □ × File Display Topology Help Peer percent Absolute Metric root percent Ŧ • -(Topology 3 Topology 2 Metric tree Call tree Flat view Topology 1 白 🗌 0.00 Time ٠ 占 🗖 0.00 MAIN 占 🔲 460.94 Execution 🖶 🗖 0.00 mpi setup 🕁 🗖 0.00 MPI - 🗌 0.00 MPI Bcast 由口 0.00 Synchronization 🖶 🔲 0.00 envisetup 由 🔲 0.03 Collective 🔲 0.00 zone setup 由 □ 0.00 Communication 🖶 🗖 0.00 map zones 🖨 🔲 0.38 Point-to-point 🔲 0.00 zone starts 由 🗖 2.62 Late Sender 🛛 🔲 0.00 set constants L 0.00 Late Receiver 由 🗖 0.73 initialize 由 🗔 0.10 exact rhs 0.39 Init/Exit 🗗 🗖 0.00 exch qbc 由□0.00 OMP 🖶 🗖 0.43 copy x face - 🗌 0.00 Flush 🖶 🗖 0.37 copy_y_face_ 🖨 🛄 8.59 Management 0.00 MPI Isend L 🗖 7.54 Fork 0.00 MPI Irecv 由 □ 0.00 Synchronization L 🗌 0.00 MPI Waitall 由 🗖 45.58 Barrier 占 🗖 0.00 adi 🗖 0.00 Critical 由 🗖 17.93 compute rhs L 🗆 0.00 Lock API 由 💶 24.87 x solve 0.02 Overhead 🖶 🛄 26.53 y solve 🗄 🔲 14.15 Idle threads 🗗 🔲 0.00 z solve Coord: (3,0,3)2.93e6 Visits 由 □ 0.13 !\$omp parallel @z_solve.f:43 Node: c9-1c2s4n0 🗄 🔳 8 Synchronizations - 27.24 !\$omp do @z solve.f:52 Name: Thread 3 🖶 📕 4872 Communications 0.00 !\$omp ibarrier @z solve.f:428 MPI rank: 3 🖶 📕 1.05e9 Bytes transferred 由 💶 1.51 add Thread id: 3 🖶 📕 47.85 Computational imbalance - 🗌 0.00 MPI Barrier Value: 96.57 (95.79%) – 🔳 3.24e9 PAPI L1 DCM 由 💶 0.15 verify Absolute: 1.78 (95.79%) 🗏 8.47e11 PAPI L1 DCA - 🗌 0.00 MPI Reduce - 🗖 0.00 print results 1.54e12 PAPI TOT INS . ٠ 🗆 🔳 5.84e11 PAPI FP OPS -由 □ 0.00 MPI Finalize • **4** F 4 🕨 • **4** F 0.00 0.00 47.85 (100.00%) 0.00 47.85 27.24 100.00 100.00 100.00 0.81 +/- 0.53 13.03 (27.24%) 47.8

Scalasca automatic trace analysis report



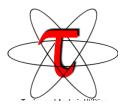


Integrated performance toolkit

- Instrumentation, measurement, analysis & visualization
 - Highly customizable installation, API, envvars & GUI
 - Supports multiple profiling & tracing capabilities
- Performance data management & data mining
- Targets all parallel programming/execution paradigms
 - Ported to a wide range of computer systems
- Performance problem solving framework for HPC
- Extensive bridges to/from other performance tools
 - ► PerfSuite, Scalasca, Vampir, ...

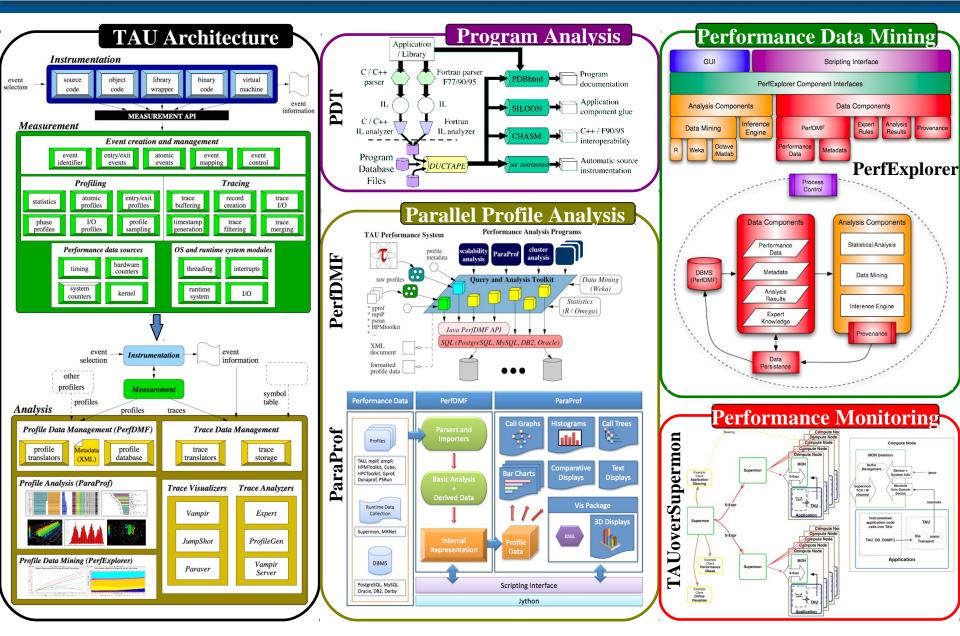
Developed by U. Oregon/PRL

- Broadly deployed open-source software
- http://tau.uoregon.edu/



TAU Performance System components



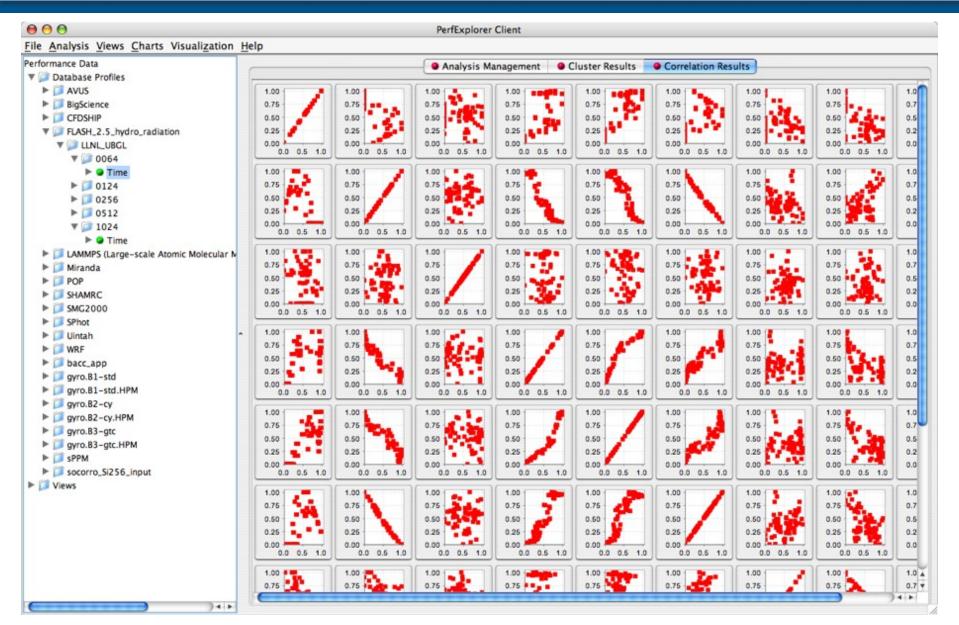


TAU ParaProf GUI displays (selected)



📧 TAU: ParaProf Manager 🥯	TAU: ParaProf: Function Data Window: epik_bt-mz_B_4x4_t	trace 💶 🗙
TAU: ParaProf Manager S File Options Help	File Options Windows Help	
Applications Applications Standard Applications Default App Default Exp Default Exp Default Exp Default Exp TAU: ParaProf: epik_bt-mz_B_4x4_trace_PAT_RT_HWPC_0/tr TAU: ParaProf: epik_bt-mz_B_4x4_trace_PAT_RT_HWPC_0/tr	Name: main => MAIN => adi_ => z_solve_ => !\$omp parallel @z_solv do @z_solve.f:52 Metric Name: Time Value: Exclusive Units: seconds 9.609	e.f:43 => !\$omp node 1, thread 2
	9.547	node 1, thread 0
File Options Windows Help Metric: Time Value: Exclusive Std. Dev. Mean node 0, thread 0 node 0, thread 1 node 0, thread 2 node 0, thread 3 node 1, thread 1 node 1, thread 1 node 1, thread 2 node 2, thread 1	9.54 9.118 9.118 9.104 9.057 9.037 9.025 9.019 8.995 8.995 8.977 8.636 7.477 6.911 6.851 6.788 0.971	node 1, thread 1 node 3, thread 0 node 3, thread 2 node 3, thread 1 node 2, thread 1 node 2, thread 1 node 2, thread 2 node 2, thread 0 node 0, thread 1 node 0, thread 3 node 1, thread 3 node 2, thread 3 node 3, thread 3 std. dev.
node 2, thread 2 node 2, thread 3 node 3, thread 0 node 3, thread 1 node 3, thread 2 node 3, thread 3 main => MAIN => adi_ => z_solve_ => !\$on Exclusive Time: 9.118 seconds Inclusive Time: 9.118 seconds Calls: 3216.0 SubCalls: 0.0	np parallel @z_solve.f:43 => !\$omp do @z_solve.f:52	

TAU PerfExplorer data mining





Interactive event trace analysis

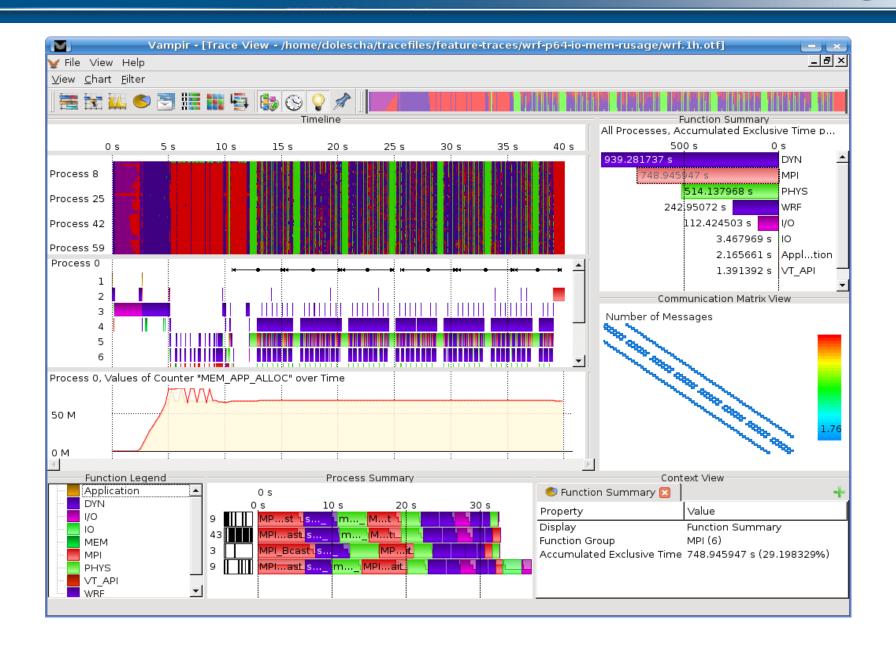
- Alternative & supplement to automatic trace analysis
- Visual presentation of dynamic runtime behaviour
 - event timeline chart for states & interactions of processes/threads
 - communication statistics, summaries & more
- Interactive browsing, zooming, selecting
 - Inked displays & statistics adapt to selected time interval (zoom)
 - scalable server runs in parallel to handle larger traces

Developed by TU Dresden ZIH

- Open-source VampirTrace library bundled with OpenMPI 1.3
- http://www.tu-dresden.de/zih/vampirtrace/
- Vampir Server & GUI have a commercial license
- http://www.vampir.eu/



Vampir interactive trace analysis GUI

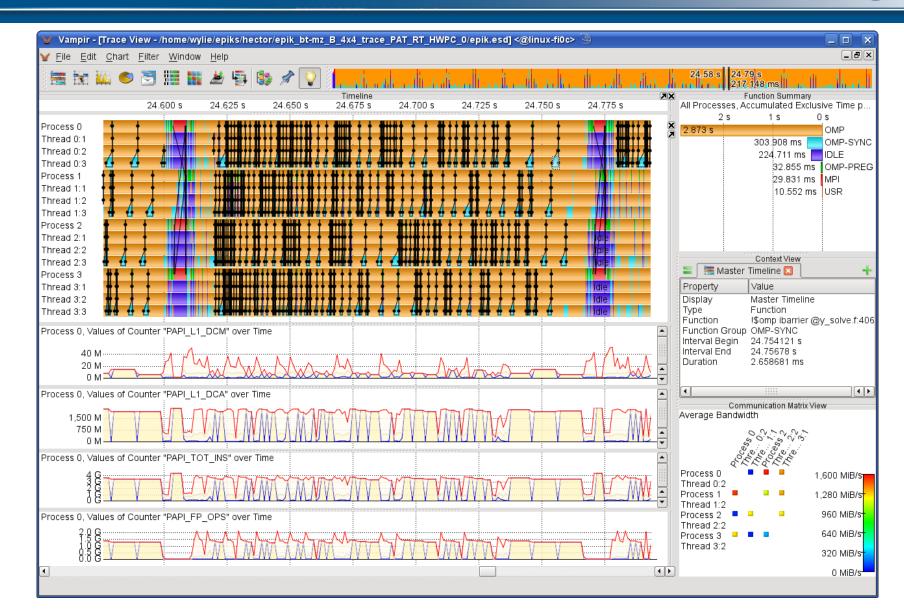


Vampir interactive trace analysis GUI





Vampir interactive trace analysis GUI (zoom)





- Interactive event trace analysis
 - Visual presentation of dynamic runtime behaviour
 - event timeline chart for states & interactions of processes
 - Interactive browsing, zooming, selecting
 - Large variety of highly configurable analyses & displays
- Developed by Barcelona Supercomputing Center
 - Paraver trace analyser and Extrae measurement library
 - Open source available from http://www.bsc.es/paraver/

Paraver interactive trace analysis GUI

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, Window brows		-	thread 0:1		
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process 1	7.33 %	92.67 %	process 2		
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MAQAO



- Modular Assembler Quality Analyzer & Optimizer
 - Framework for binary manipulation
 - using plugins and scripting language
 - Tool exploiting framework to produce reports
 - fast prototyping and batch interface
 - STAN static performance model
 - MIL instrumentation language for dynamic analysis
 - building custom performance evaluation tools using HWCs
 - ► instrumentation of functions, loops, blocks & instructions
- Developed by UVSQ Exascale Computing Research lab
 - Supports Intel x86_64 microarchitecture
 - Available from www.maqao.org



Key tool components also provided as open-source

- Program development environment
 - ► Eclipse PTP ETFw, UNITE
- Program/library instrumentation
 - ► COBI, OPARI, PDToolkit
- Runtime measurement systems
 - ► PⁿMPI, Score-P, UniMCI
- Scalable I/O
 - ► SIONIib
- Libraries & tools for handling (and converting) traces
 - ► EPILOG, OTF, PEARL
- Analysis algebra & hierarchical/topological presentation
 - ► CUBE



Scalable performance measurement infrastructure

- Supports instrumentation, profiling & trace collection, as well as online analysis of HPC parallel applications
- Works with Periscope, Scalasca, TAU & Vampir prototypes
- Based on updated tool components
 - CUBE4 profile data utilities & GUI
 - OA online access interface to performance measurements
 - OPARI2 OpenMP & pragma instrumenter
 - OTF2 open trace format

Created by German BMBF SILC & US DOE PRIMA projects

- JSC, RWTH, TUD, TUM, GNS, GRS, GWT & UO PRL
- Available as BSD open-source from http://www.score-p.org/

VI-HPS

Portable native parallel I/O library & utilities

- Scalable massively-parallel I/O to task-local files
- Manages single or multiple physical files on disk
 - optimizes bandwidth available from I/O servers by matching blocksizes/alignment, reduces metadata-server contention
- POSIX-I/O-compatible sequential & parallel API
 - adoption requires minimal source-code changes
- Tuned for common parallel filesystems
 - ► GPFS (BlueGene), Lustre (Cray), ...
- Convenient for application I/O, checkpointing,
 - Used by Scalasca tracing (when configured)

Developed by JSC

 Available as open-source from http://www.fz-juelich.de/jsc/sionlib/

UNITE



Uniform integrated tool environment

- Manages installation & access to program development tools
 - based on software environment management "modules"
 - commonly used on most cluster and HPC systems
 - configurable for multiple MPI libraries & compiler suites
- Specifies how & where tools packages get installed
 - including integrating tools where possible
- Defines standard module names and different versions
- Supplies pre-defined module files
- Configurable to co-exist with local installations & policies

Developed by JSC, RWTH & TUD

Available as open-source from http://www.vi-hps.org/projects/unite/