

# Virtual Institute – High Productivity Supercomputing



14 March 2012



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Universität Stuttgart











#### Wednesday 14th March

- 09:00 (registration)
- Welcome & Introduction to VI-HPS [Ávila,Gerndt,Wylie]
- Introduction to parallel application engineering [Gerndt]
- Introduction to parallel performance analysis [Oleynik]
- Preparation for hands-on exercises on levque [Wylie]
- 11:45-14:30 (lunch)
- Periscope introduction & overview [Gerndt,Oleynik]
- Periscope hands-on exercise on *levque*
- 15:45-16:00 (break)
- Scalasca introduction & overview [Wylie]
- Scalasca hands-on exercise on *levque*
- 17:15 (adjourn)

## **Outline (cont.)**



#### Thursday 15th March

- **•** 09:00
- Vampir introduction & overview [Petkov]
- (break)
- PAPI introduction & overview [Ávila]
- 12:00-13:30 (lunch)
- Hands-on coaching with participants' codes on levque [all]
- 17:00 (adjourn)

#### Friday 16th March

- **•** 09:00
- Sponsor presentations from IBM, Intel & SGI (OmegaSystem)
- 12:00 (adjourn)



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.

#### **Participant survey**



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, VTune, ...
- Who's already familiar with parallel performance analysis?
  - Which tools have you used?
    - ▶ time, print/printf, prof/gprof, Periscope, Scalasca, TAU, Vampir, ...

## Prepare to analyse your own application codes



- 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 48 processes/threads)
    - ► to facilitate rapid turnaround and quick experimentation
  - larger/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)

## Virtual Institute – High Productivity Supercomputing



- **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.)













#### German Research School

Laboratory of Parallel Programming

#### **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











#### **VI-HPS** productivity tools



- Marmot/MUST
  - MPI correctness checking
- PAPI
  - Interfacing to hardware performance counters
- Periscope
  - Automatic analysis via an on-line distributed search
- Scalasca
  - Large-scale parallel performance analysis
- TAU
  - Integrated parallel performance system
- Vampir/VampirTrace
  - Event tracing and graphical trace visualization & analysis

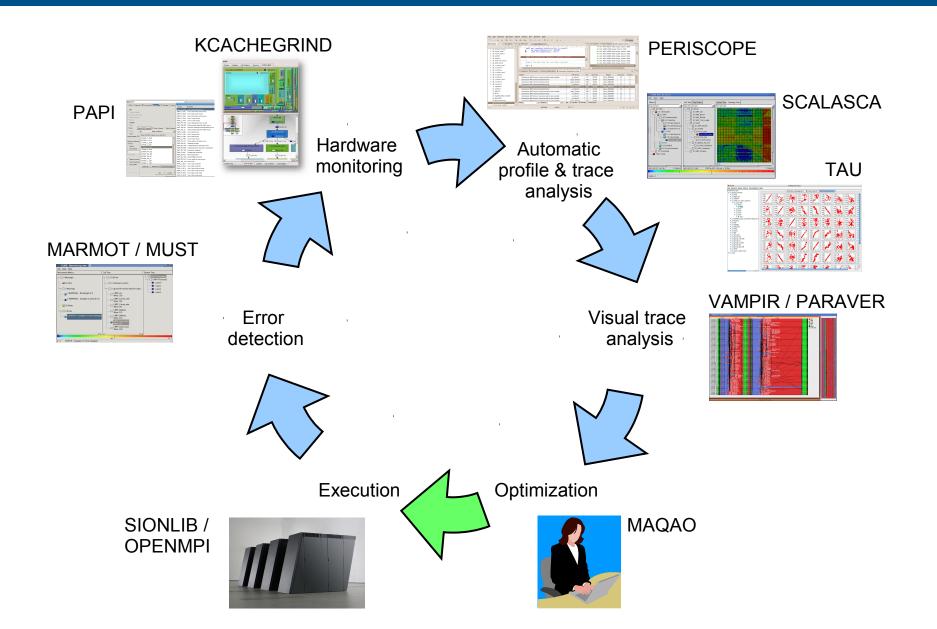
#### VI-HPS productivity tools (cont.)



- KCachegrind
  - Callgraph-based cache analysis [x86 only]
- MAQAO
  - Assembly instrumentation & optimization [x86 only]
- ompP
  - OpenMP profiling tool
- OpenMPI
  - Memory checking
- Paraver/Extrae
  - Event tracing and graphical trace visualization & analysis
- Score-P
  - Common instrumentation & measurement infrastructure
- SIONlib
  - Optimized native parallel file I/O

#### **Technologies and their integration**





#### **VI-HPS Training & Tuning Workshops**



#### 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
- VI-HPS Tuning Workshop series
  - 2008 (Aachen & Dresden), 2009 (Jülich & Bremen),
     2010 (Garching & Amsterdam), 2011 (Stuttgart & Aachen)
  - **2012/04/23-27 (Paris)**, 2012/10/15-19 (Garching)

#### **Upcoming VI-HPS training events**



- 9th VI-HPS Tuning Workshop (23-27 Apr 2012)
  - hosted by UVSQ, St.-Quentin-en-Yvelines, France
  - using PRACE Tier-0 Curie system at CEA / TGCC
  - Scalasca, Vampir, TAU, Periscope, KCachegrind, MAQAO, ...
- Further events to be determined
  - (one-day) tutorials
    - ► with guided exercises 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

#### POINT/VI-HPS Live-ISO/DVD



- Bootable Linux installation ISO (on DVD or USB stick)
- 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

#### **Parallel Productivity Tools** Live DVD

Also includes: TotalView, DyninstAPI, PDT, Eclipse PTP, Berkeley UPC, ptoolsrte, Chapel, and much more...

#### Partners:

ParaTools, Inc. University of Florida University of Oregon **Totalview Technologies RWTH Aachen University** HLRS / University of Stuttgart Jülich Supercomputing Centre Technische Universität Dresden Technische Universität München University of Wisconsin at Madison Pittsburgh Supercomputing Center University of Tennessee at Knoxville National Center for Supercomputing Applications









September 2010



http://nic.uoregon.edu/point http://www.vi-hps.org



#### Cachegrind: cache analysis by simple cache simulation

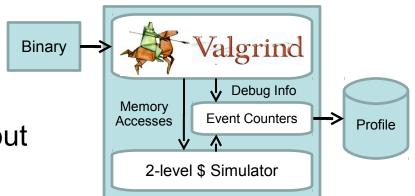
- Captures dynamic callgraph
- Based on valgrind dynamic binary instrumentation
- Runs on x86/PowerPC/ARM unmodified binaries
  - ► No root access required
- ASCII reports produced

## [KQ]Cachegrind GUI

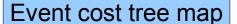
Visualization of cachegrind output

#### Developed by TU Munich

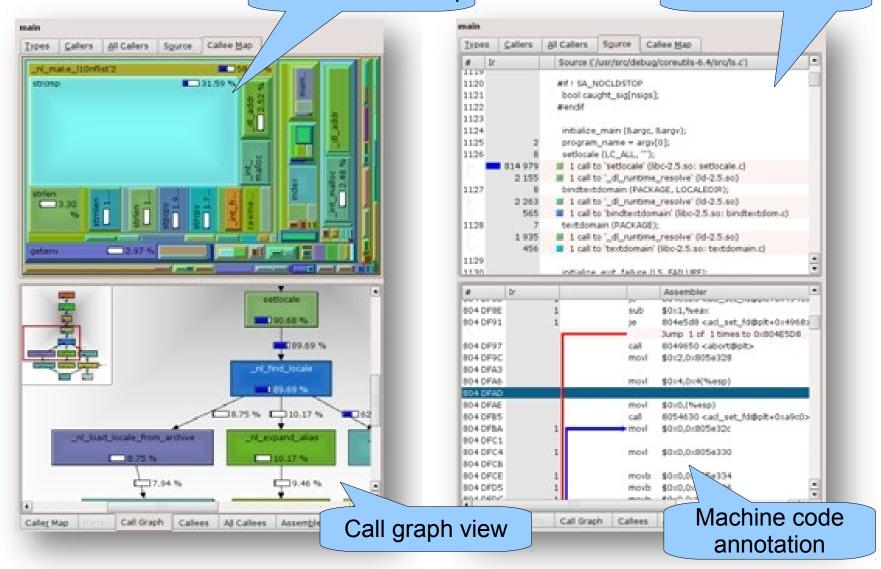
- Released as GPL open-source
- http://kcachegrind.sf.net/







#### Source code view





#### 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)

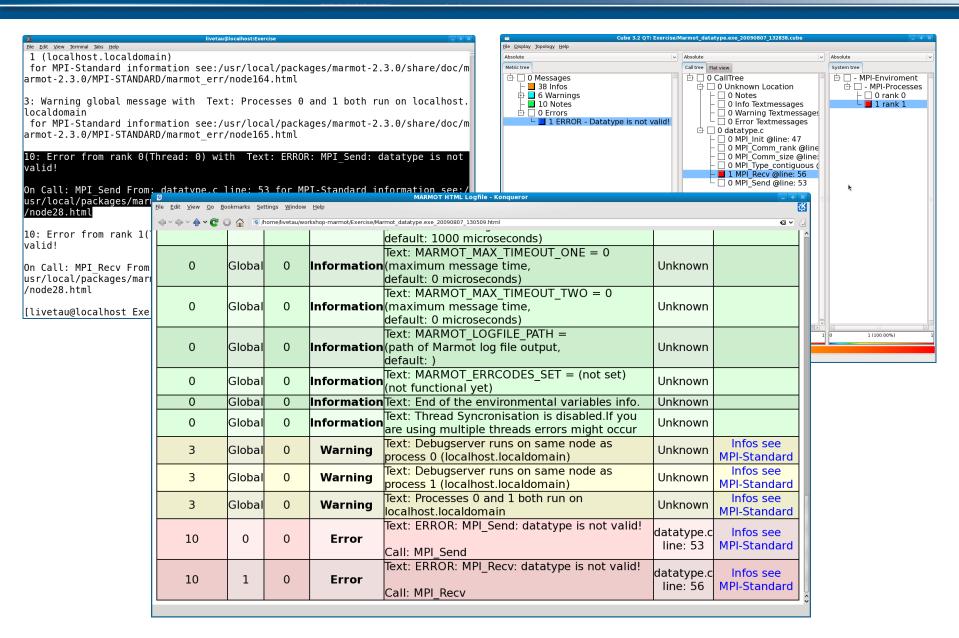
#### Developed by HLRS & TU Dresden

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



#### **Marmot logfiles**







#### 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

## Developed by TU Dresden, LLNL & LANL

- to be released as open-source (BSD license)
- currently in beta-testing for first release in November 2011
- http://tu-dresden.de/.../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/



#### PAPI preset counters (and their definitions)



```
juropa$ papi avail
Available events and hardware information.
PAPI Version
                      : 4.1.0.0
Vendor string and code : GenuineIntel (1)
Model string and code
                        : Intel(R) Xeon(R) CPU
                       X5570 @ 2.93GHz (26)
CPU Revision
                        : 5.000000
CPUID Info
                        : Family: 6 Model: 26
                         Stepping: 5
CPU Megahertz
                        : 1600.000000
CPU Clock Megahertz
                        : 1600
Hdw Threads per core
                        : 2
Cores per Socket
                        : 4
NUMA Nodes
                        : 2
CPU's per Node
                        : 8
Total CPU's
                        : 16
Number Hardware Counters: 16
Max Multiplex Counters : 512
        Code Avail Deriv Description
   Name
PAPI L1 DCM 0x80000000 Yes
                     Level 1 data cache misses
PAPI L1 ICM 0x80000001 Yes
              Level 1 instruction cache misses
Of 107 possible events, 35 are available, of
which 9 are derived.
```

```
juropa$ papi avail -d
Symbol Event Code Count
                                 |Short Descr.|
 |Long Description|
 |Developer's Notes|
 |Derived|
 |PostFix|
 Native Code[n]: <hex> |name|
PAPI L1 DCM
               0 \times 800000000 1 |L1D cache misses|
 |Level 1 data cache misses|
 |NOT DERIVED|
 Native Code[0]: 0x40002028 |L1D:REPL|
PAPI L1 ICM
               0x80000001 1 |L1I cache misses|
 |Level 1 instruction cache misses|
 |NOT DERIVED|
 Native Code[0]: 0x40001031 |L1I:MISSES|
PAPI L2 DCM
               0x80000002 2 |L2D cache misses|
 |Level 2 data cache misses|
 |DERIVED SUB|
 Native Code[0]: 0x40000437 | L2 RQSTS:MISS|
Native Code[1]: 0x40002037
L2 RQSTS: IFETCH MISS
. . .
```

#### PAPI native counters (and qualifiers)



```
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
            INSTRUCTION RETIRED | count the number of instructions at retire
0×40000001
          | ment. Alias to event INST RETIRED: ANY P
0x40000086 UNC SNP RESP TO REMOTE HOME | Remote home snoop response - LLC d
          I oes not have cache line
            :I STATE | Remote home snoop response - LLC does not have cache
 40000486
           I 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
  - 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



## Periscope properties & strategies (examples)



#### MPI

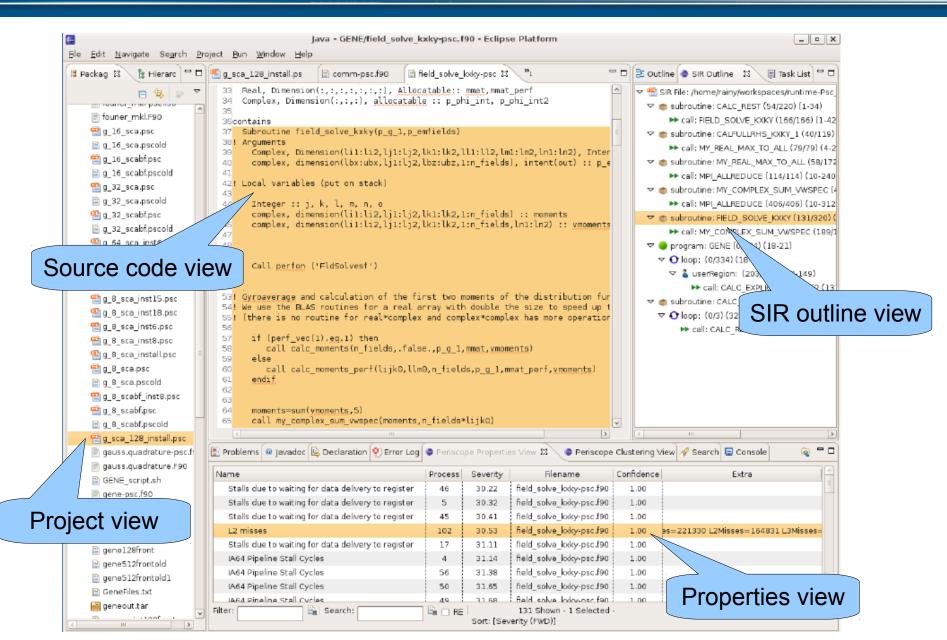
- Excessive MPI communication time
- Excessive MPI time due to many small messages
- Excessive MPI time in receive due to late sender
- **I** ...

Hardware performance counters (platform-specific)

- Cycles lost due to cache misses
  - ► High L1/L2/L3 demand load miss rate
- Cycles lost due to store instructions
- Cycles lost due to address translation misses
- Cycles lost due to no instruction to dispatch
- **...**

#### Periscope plug-in to Eclipse environment







#### 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

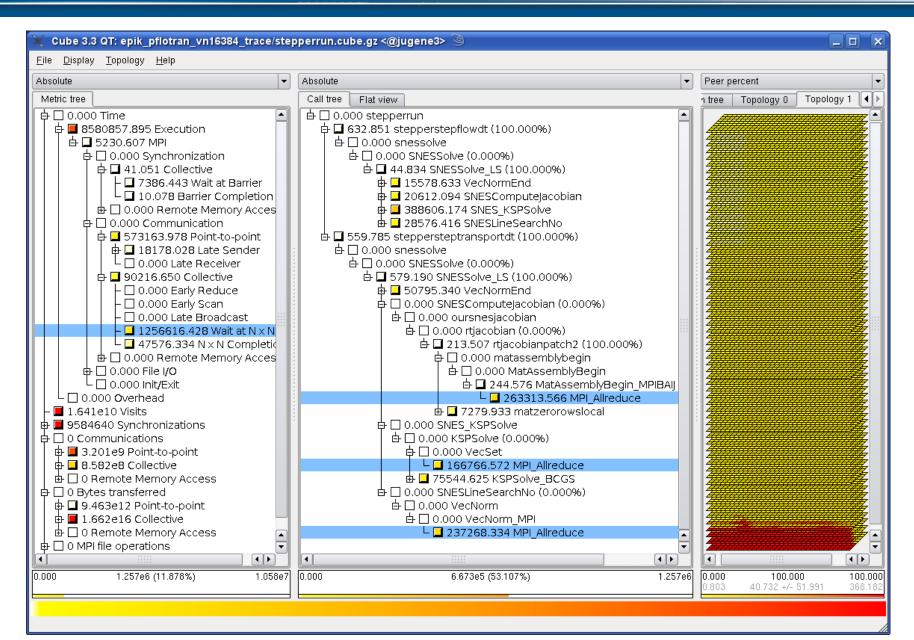
#### Developed by JSC & GRS

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



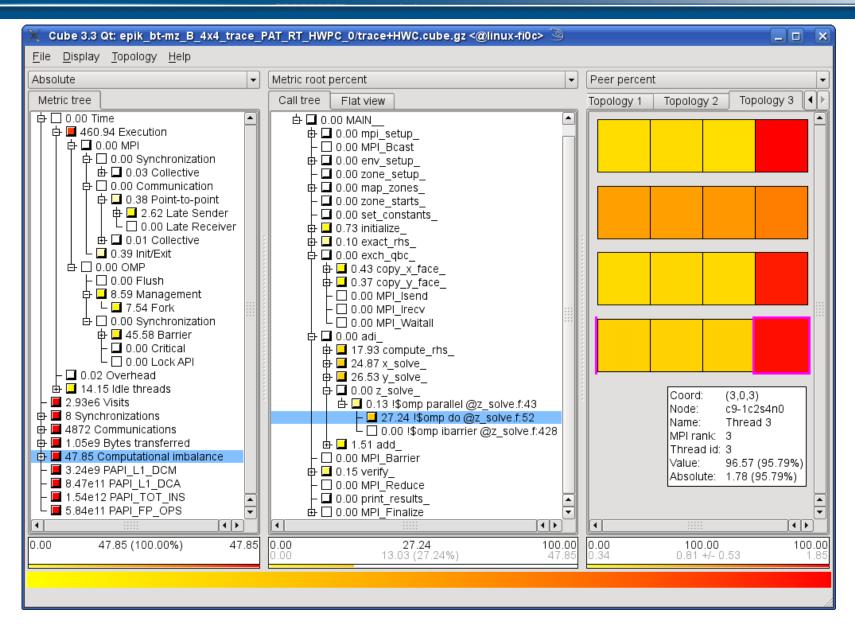
#### Scalasca automatic trace analysis report





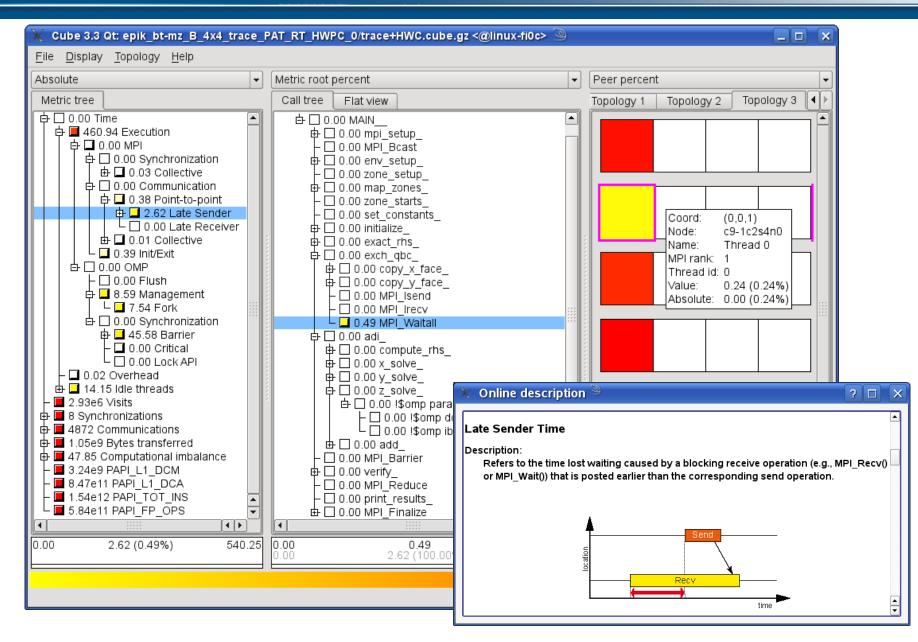
#### Scalasca hybrid analysis report





#### Scalasca automatic trace analysis report





#### **TAU Performance System**

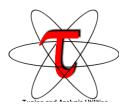


#### Integrated performance toolkit

- 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, ...

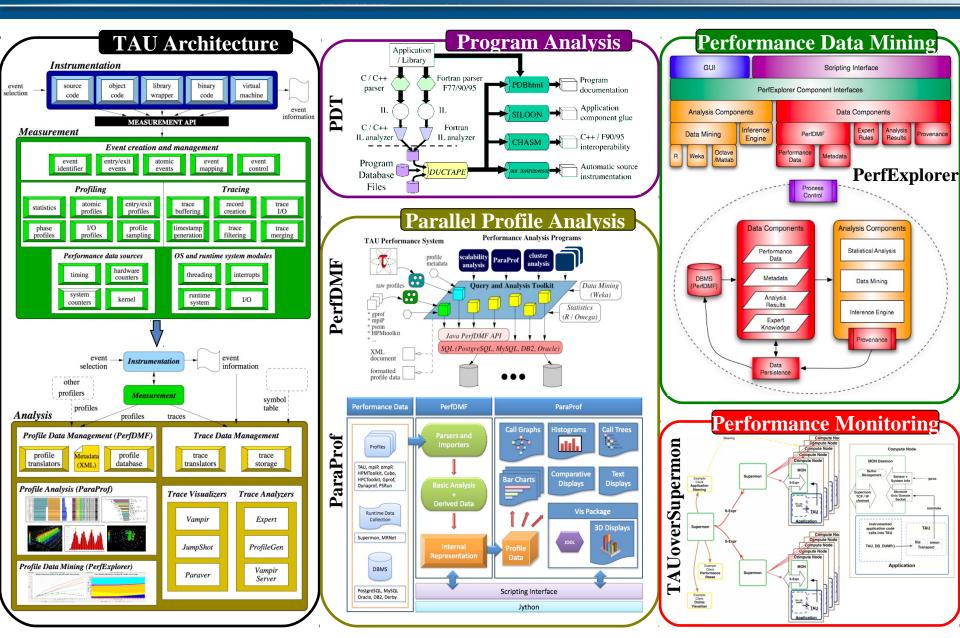
## Developed by U. Oregon/PRL

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



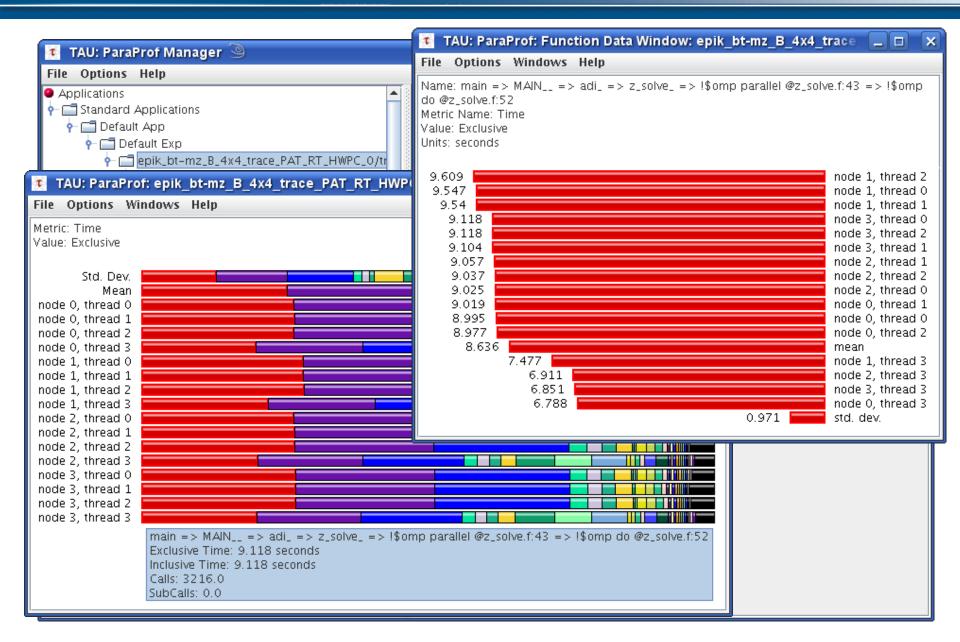
#### **TAU Performance System components**





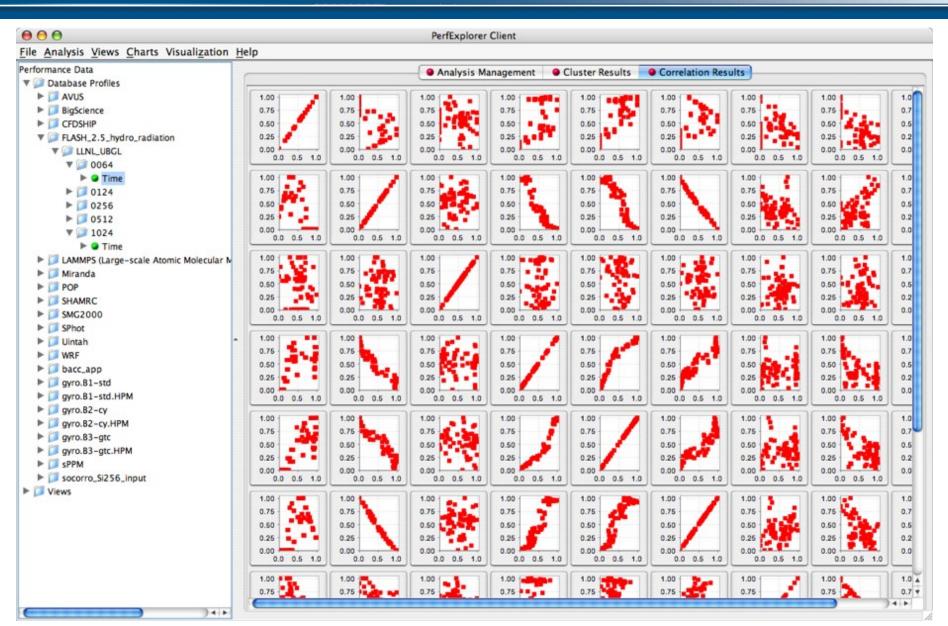
#### TAU ParaProf GUI displays (selected)





#### **TAU PerfExplorer data mining**





#### Vampir & VampirTrace



#### 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
  - ► linked displays & statistics adapt to selected time interval (zoom)
  - scalable server runs in parallel to handle larger traces

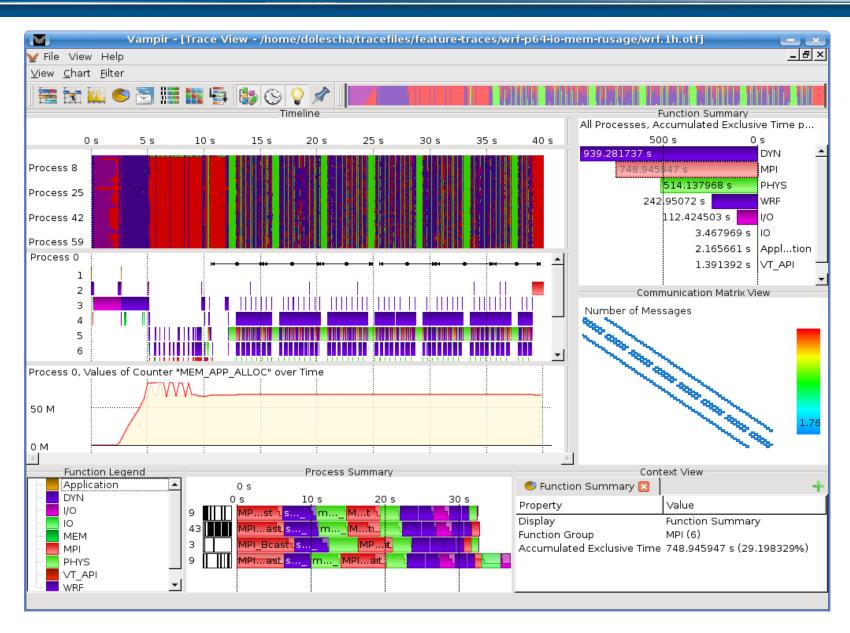
#### Developed by TU Dresden ZIH

- 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/



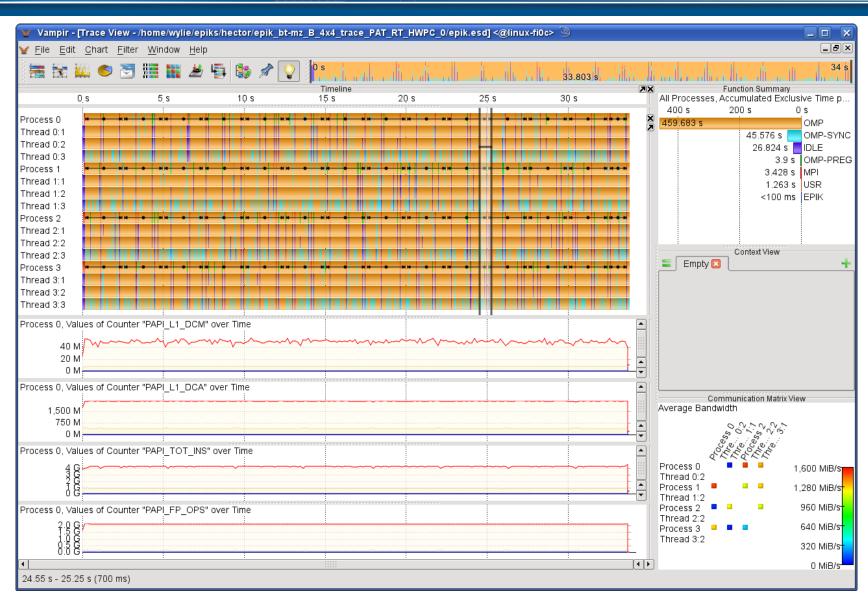
#### Vampir interactive trace analysis GUI





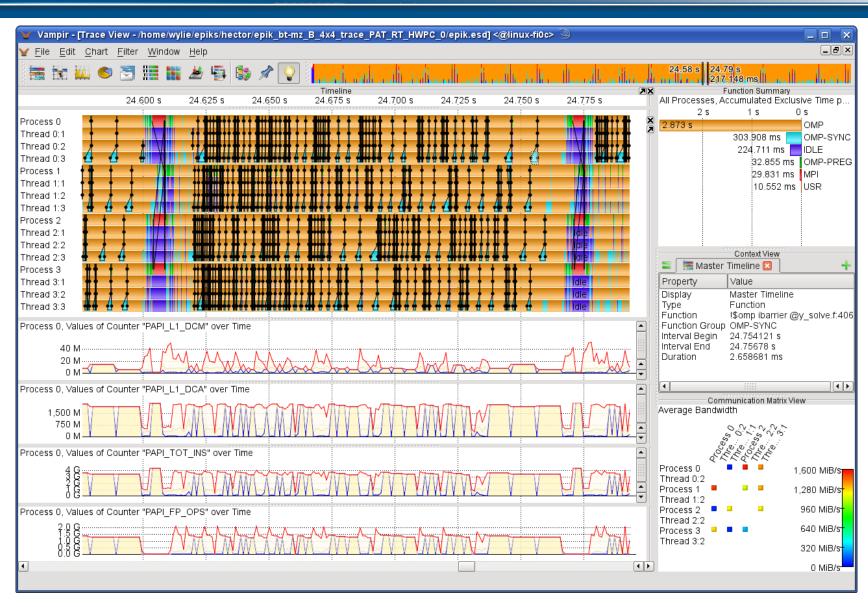
#### Vampir interactive trace analysis GUI





#### Vampir interactive trace analysis GUI (zoom)





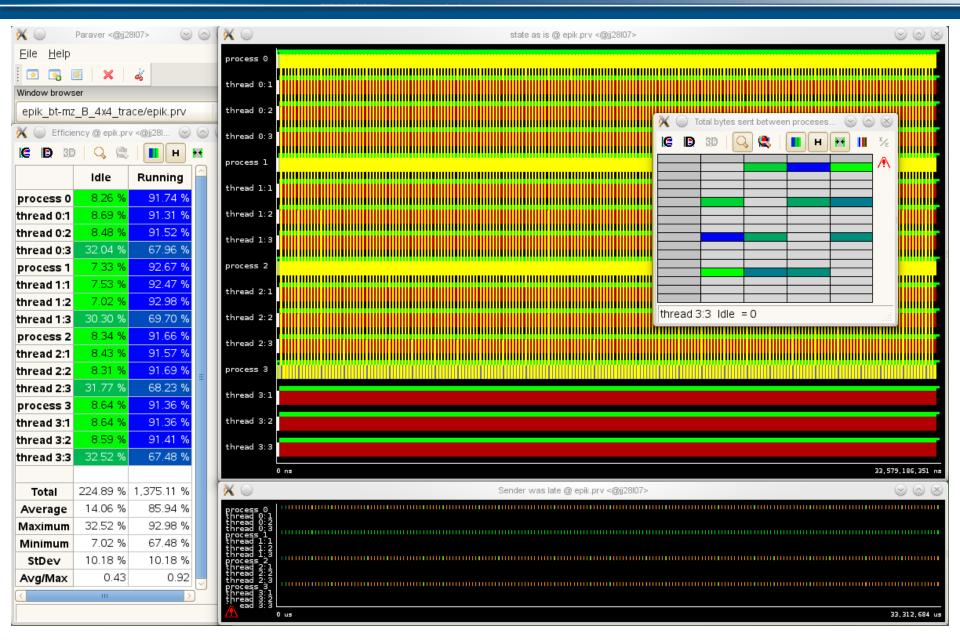
#### Paraver & Extrae



- 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





#### **VI-HPS** component technologies



#### Key tool components also provided as open-source

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



#### 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/



#### 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/