# EPCC/DiRAC/ECS MPI Tools Workshop

## Introduction

Brian Wylie[1] and Tobias Hilbrich[2]
[1]Research Center Jülich and
[2]Technische Universität Dresden

**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

HELMHOLTZ | ASSOCIATION

**http://www.vi-hps.org**

**Thursday:**

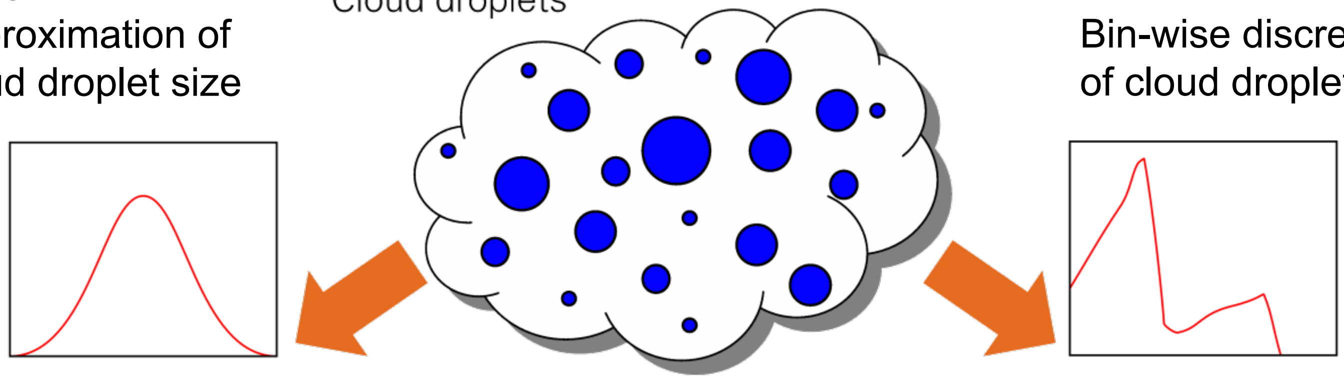
| | |
|---|---|
| *9:30am-11:00am* | Introduction, performance analysis basics, tools overview |
| *11:30am-1:00pm* | Instrumentation and profiling hands-on |
| *2:00pm-5:30pm* | Guided use with own code/examples |

**Friday:**

| | |
|---|---|
| *09:30am-11:00am* | Automatic performance analysis w/ Scalasca, correctness analysis w/ MUST, other VI-HPS tools and Vampir live demo |
| *11:30am-1:00pm* | Scalasca and MUST Hands-On |
| *2:00pm-5:30pm* | Guided use with own code/examples |

# Motivation Story 1

- COSMO-SPECS a coupling of:
  - Weather forecast model
  - Detailed cloud microphysics scheme



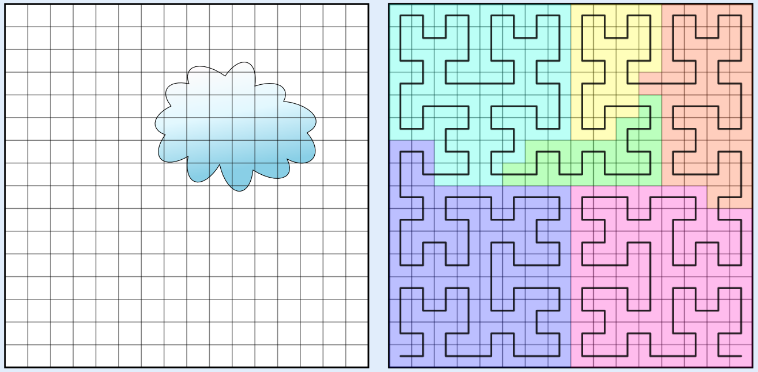

Developer observation:

***Runtime per iteration increases over time, why?***

"A hang only appeared when PF3D was scaled to half a million processes.
The user refused to debug for 6 months …"

Dong Ahn, Computer scientist at Lawrence Livermore National Laboratory, SC'13 BOF (Details in [1])

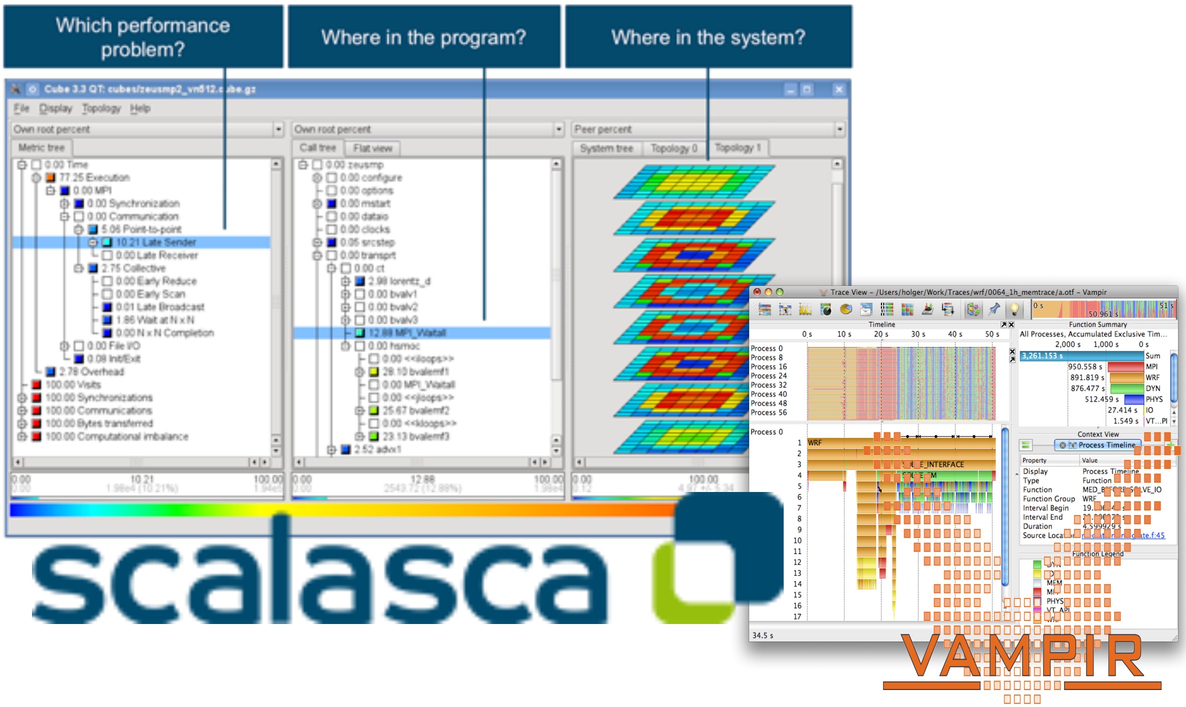
Dynamic load balancing Benchmark (Development Version):

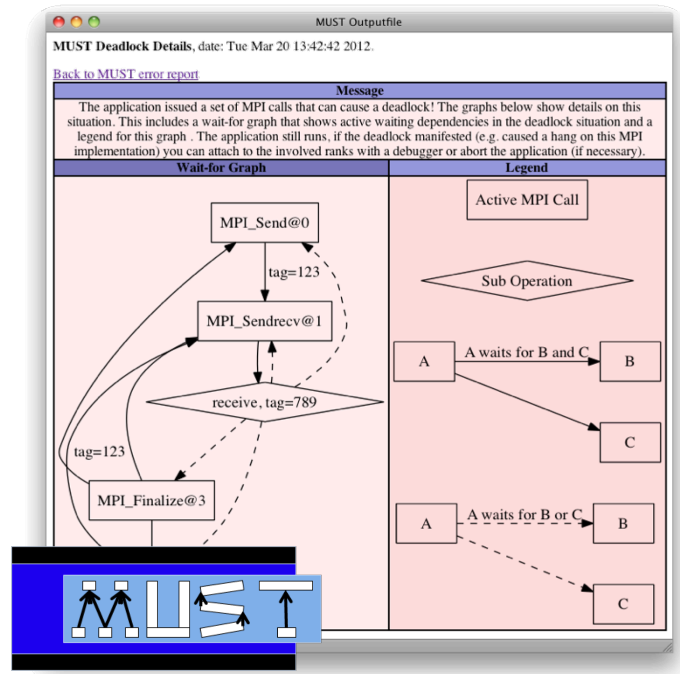


Starting at 256 processes it crashes within the MPI implementation

# Course Message

- Tools assist you in your HPC development:




Performance optimization

MUST: Correct MPI usage

VI-HPS

- Community efforts to make tools more versatile

Measurement: **Score-P**

Partners:

Technische Universität München

gns

JÜLICH FORSCHUNGSZENTRUM

TECHNISCHE UNIVERSITÄT DRESDEN

RWTH AACHEN UNIVERSITY

German Research School for Simulation Sciences

UNIVERSITY OF OREGON

Analysis:

- TAU

Tuning and Analysis Utilities

- **Vampir**

VAMPIR

- Scalasca

scalasca

- Merging runtime MPI correctness approaches

**Marmot**
Developers:
TECHNISCHE UNIVERSITÄT DRESDEN
H L R I S

Issue:
– Lack of Non-local checks

**Umpire**
Developers:
Lawrence Livermore National Laboratory

Issue:
- Scalability, local checks

**MUST**
Developers:
RWTH AACHEN UNIVERSITY
TECHNISCHE UNIVERSITÄT DRESDEN
Lawrence Livermore National Laboratory

Goal:
– Scalable, Push-button, no false positives

- Before we dive into the VI-HPS tools and their use, we:
  - Provide basic terms used in performance analysis
  - Present our performance analysis workflows
  - Highlight common pitfalls

# EPCC/DiRAC/ECS MPI Tools Workshop

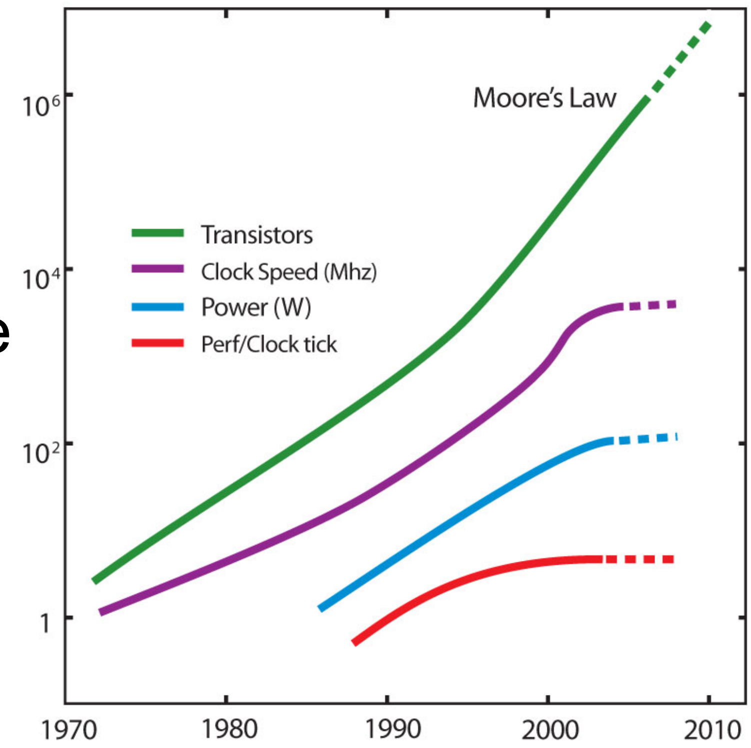
## Parallel Performance Engineering

Brian Wylie[1] and Tobias Hilbrich[2]
[1]Research Center Jülich and
[2]Technische Universität Dresden

(with content used with permission from tutorials
by Bernd Mohr/JSC and Luiz DeRose/Cray)

# Today: the “free lunch” is over

- Moore's law is still in charge, but
  - Clock rates no longer increase
  - Performance gains only through increased parallelism
- Optimizations of applications more difficult
  - Increasing application complexity
    - Multi-physics
    - Multi-scale
  - Increasing machine complexity
    - Hierarchical networks / memory
    - More CPUs / multi-core




✦ Every doubling of scale reveals a new bottleneck!

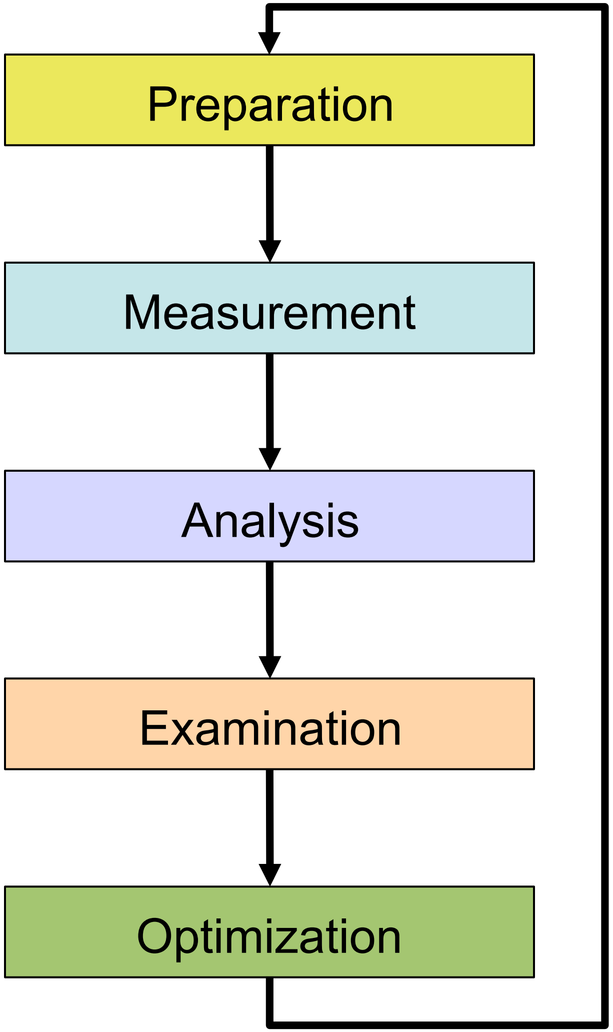
# Performance factors of parallel applications

- "Sequential" factors
  - Computation
    - ✦ Choose right algorithm, use optimizing compiler
  - Cache and memory
    - ✦ Tough! Only limited tool support, hope compiler gets it right
  - Input / output
    - ✦ Often not given enough attention
- "Parallel" factors
  - Partitioning / decomposition
  - Communication (i.e., message passing)
  - Multithreading
  - Synchronization / locking
    - ✦ More or less understood, good tool support

# Tuning basics

- Successful engineering is a combination of
  - The right algorithms and libraries
  - Compiler flags and directives
  - Thinking !!!
- Measurement is better than guessing
  - To determine performance bottlenecks
  - To compare alternatives
  - To validate tuning decisions and optimizations
    - ✦ After each step!

# Performance engineering workflow




- Prepare application (with symbols), insert extra code (probes/hooks)
- Collection of data relevant to execution performance analysis
- Calculation of metrics, identification of performance metrics
- Presentation of results in an intuitive/ understandable form
- Modifications intended to eliminate/reduce performance problems

# The 80/20 rule

- Programs typically spend 80% of their time in 20% of the code
- Programmers typically spend 20% of their effort to get 80% of the total speedup possible for the application
  - *Know when to stop!*
- Don't optimize what does not matter
  - *Make the common case fast!*

> "If you optimize everything, you will always be unhappy."
>
> Donald E. Knuth

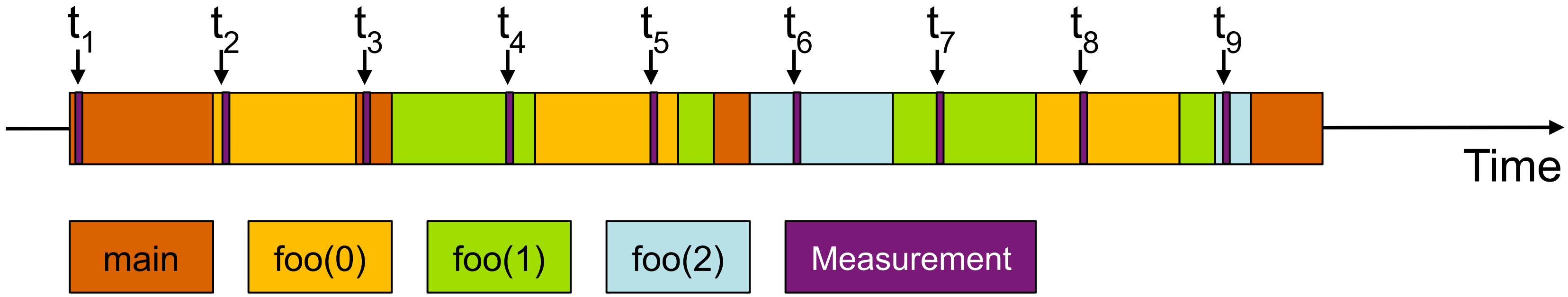
# Classification of measurement techniques

- How are performance measurements triggered?
  - Sampling
  - Code instrumentation

- How is performance data recorded?
  - Profiling / Runtime summarization
  - Tracing

- How is performance data analyzed?
  - Online
  - Post mortem

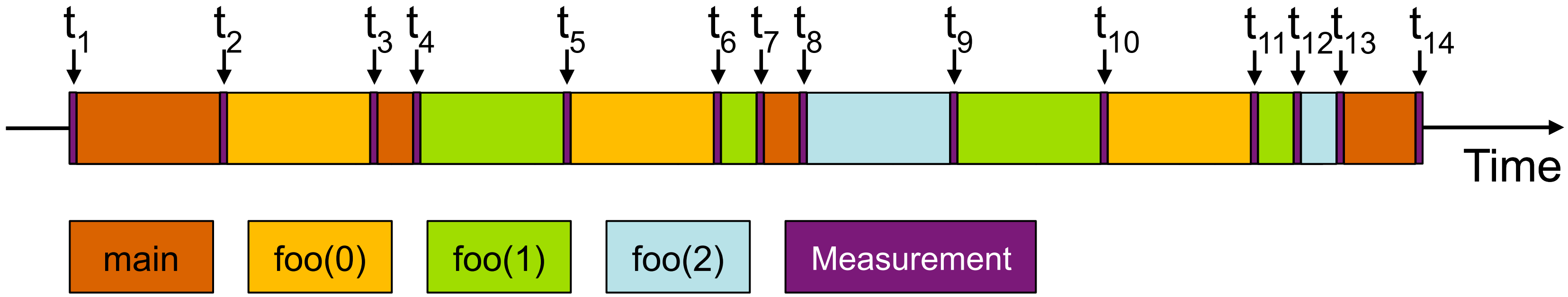
# Sampling




```
int main()
{
  int i;

  for (i=0; i < 3; i++)
    foo(i);

  return 0;
}

void foo(int i)
{

  if (i > 0)
    foo(i - 1);

}
```

- Running program is periodically interrupted to take measurement
  - Timer interrupt, OS signal, or HWC overflow
  - Service routine examines return-address stack
  - Addresses are mapped to routines using symbol table information
- **Statistical** inference of program behavior
  - Not very detailed information on highly volatile metrics
  - Requires long-running applications
- Works with unmodified executables

# Instrumentation




```
int main()
{
  int i;
  Enter("main");
  for (i=0; i < 3; i++)
    foo(i);
  Leave("main");
  return 0;
}

void foo(int i)
{
  Enter("foo");
  if (i > 0)
    foo(i – 1);
  Leave("foo");
}
```

- Measurement code is inserted such that every event of interest is captured **directly**
  - Can be done in various ways
- Advantage:
  - Much more detailed information
- Disadvantage:
  - Processing of source-code / executable necessary
  - Large relative overheads for small functions

# Instrumentation techniques

- Static instrumentation
  - Program is instrumented prior to execution
- Dynamic instrumentation
  - Program is instrumented at runtime
- Code is inserted
  - Manually
  - Automatically
    - By a preprocessor / source-to-source translation tool
    - By a compiler
    - By linking against a pre-instrumented library / runtime system
    - By binary-rewrite / dynamic instrumentation tool

# Critical issues

- Accuracy
  - Intrusion overhead
    - Measurement itself needs time and thus lowers performance
  - Perturbation
    - Measurement alters program behaviour
    - E.g., memory access pattern
  - Accuracy of timers & counters
- Granularity
  - How many measurements?
  - How much information / processing during each measurement?

✦ *Tradeoff: Accuracy vs. Expressiveness of data*

# Profiling / Runtime summarization

- Recording of aggregated information
  - Total, maximum, minimum, …
- For measurements
  - Time
  - Counts
    - Function calls
    - Bytes transferred
    - Hardware counters
- Over program and system entities
  - Functions, call sites, basic blocks, loops, …
  - Processes, threads

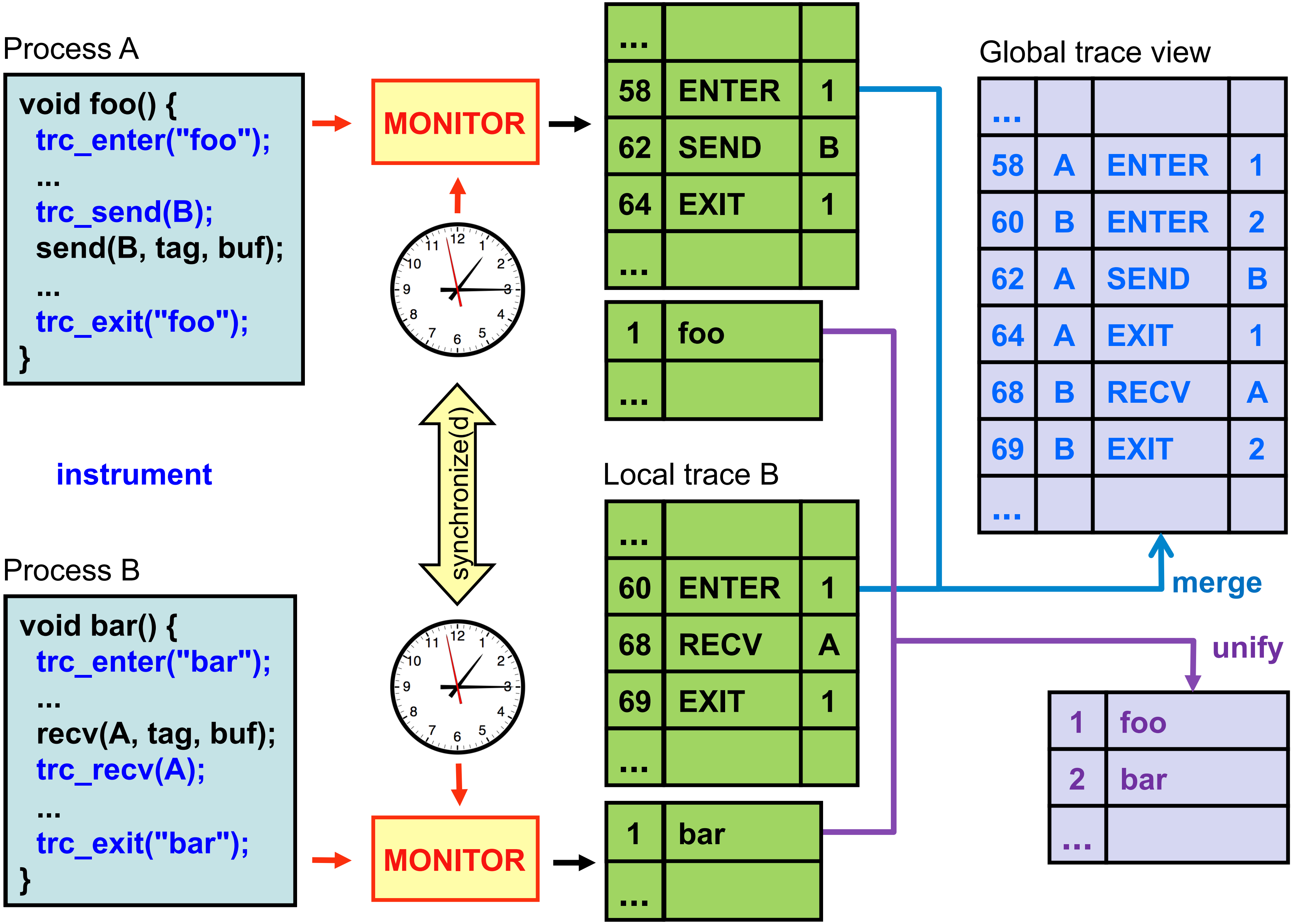
✦ *Profile = summarization of events over execution interval*

# Tracing

- Recording information about significant points (events) during execution of the program
  - Enter / leave of a region (function, loop, …)
  - Send / receive a message, …
- Save information in event record
  - Timestamp, location, event type
  - Plus event-specific information (e.g., communicator, sender / receiver, …)
- Abstract execution model on level of defined events

✦ *Event trace = Chronologically ordered sequence of event records*

# Event tracing



# Tracing vs. Profiling

- Tracing advantages
  - Event traces preserve the **temporal** and **spatial** relationships among individual events (✦ context)
  - Allows reconstruction of **dynamic** application behaviour on any required level of abstraction
  - Most general measurement technique
    - Profile data can be reconstructed from event traces
- Disadvantages
  - Traces can very quickly become extremely large
  - Writing events to file at runtime causes perturbation
  - Writing tracing software is complicated
    - Event buffering, clock synchronization, ...

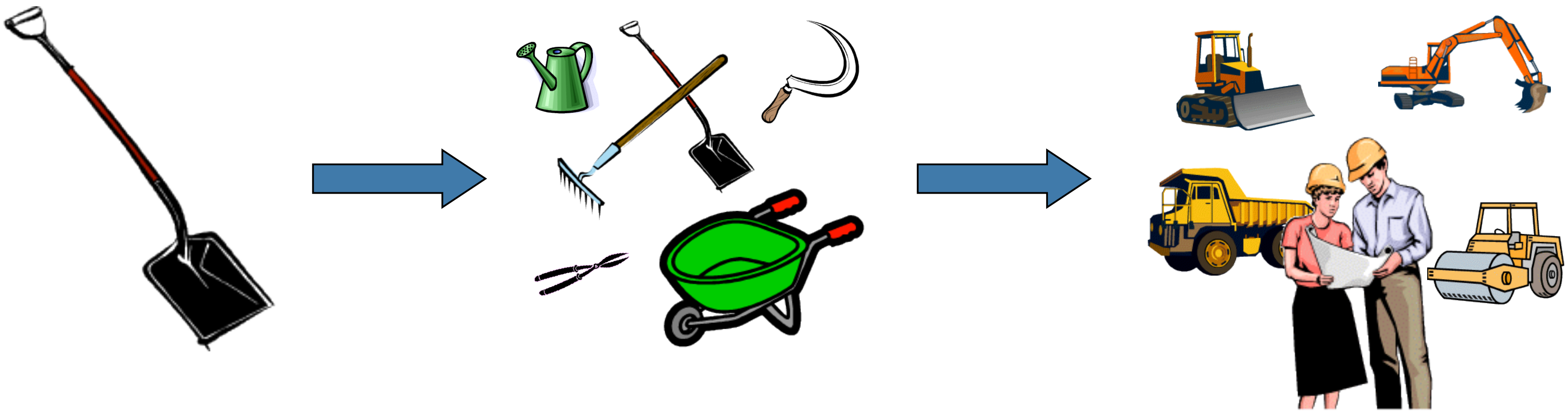
# Online analysis

- Performance data is processed during measurement run
  - Process-local profile aggregation
  - More sophisticated inter-process analysis using
    - “Piggyback” messages
    - Hierarchical network of analysis agents
- Inter-process analysis often involves application steering to interrupt and re-configure the measurement

# Post-mortem analysis

- Performance data is stored at end of measurement run
- Data analysis is performed afterwards
  - Automatic search for bottlenecks
  - Visual trace analysis
  - Calculation of statistics

# No single solution is sufficient!



✦ *A combination of different methods, tools and techniques is typically needed!*

- Analysis
  - Statistics, visualization, automatic analysis, data mining, ...
- Measurement
  - Sampling / instrumentation, profiling / tracing, ...
- Instrumentation
  - Source code / binary, manual / automatic, ...

# Typical performance analysis procedure

- Do I have a performance problem at all?
  - Time / speedup / scalability measurements
- What is the key bottleneck (computation / communication)?
  - MPI / OpenMP / flat profiling
- Where is the key bottleneck?
  - Call-path profiling, detailed basic block profiling
- Why is it there?
  - Hardware counter analysis, trace selected parts to keep trace size manageable
- Does the code have scalability problems?
  - Load imbalance analysis, compare profiles at various sizes function-by-function

# EPCC/DiRAC/ECS MPI Tools Workshop

## VI-HPS Tools and Workshop Tools

Brian Wylie[1] and Tobias Hilbrich[2]
[1]Research Center Jülich and
[2]Technische Universität Dresden

# Execution monitoring, checking & debugging

- system/batchqueue monitoring (PTP/**SysMon**)
- lightweight execution monitoring/screening (**LWM2**)
- portable performance counter access (**PAPI**)
- MPI library profiling (**mpiP**)
- MPI execution outlier detection (AutomaDeD)
- MPI memory usage checking (**memchecker**)
- MPI correctness checking (**MUST**)
- lightweight stack trace debugging (**STAT**)
- task dependency debugging (**Temanejo**)

# Integrated appl. execution profile & trace analysis

- instrumentation & measurement (**Score-P**, Extrae)
- profile analysis examination (**CUBE**, **ParaProf**)
- execution trace exploration (**(Vampir)**, **Paraver**)
- automated trace analysis (**Scalasca**)
- on-line automated analysis (**Periscope**)

# Complementary tools & utilities

- parallel performance frameworks (O|SS, **TAU**)
- performance analysis data-mining (**PerfExplorer**)
- parallel execution parametric studies (**Dimemas**)
- cache usage analysis (**kcachegrind**)
- assembly code optimization (**MAQAO**)
- process mapping generation/optimization (Rubik)
- parallel file I/O optimization (**SIONlib**)
- uniform tool/utility installation/access (**UNITE**)

# Application execution monitoring, checking & debugging

# Execution monitoring, checking & debugging

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- MPI runtime error detection tool
- Open source (BSD license) https://doc.itc.rwth-aachen.de/display/CCP/Project+MUST
- Wide range of checks, strength areas:
  - Overlaps in communication buffers
  - Errors with derived datatypes
  - Deadlocks
- Largely distributed, can scale with the application
- Developed by RWTH Aachen, TU Dresden, LLNL & LANL

VI-HPS

- C code:

```
...
MPI_Type_contiguous (2, MPI_INTEGER,
&newtype);
MPI_Send (buf, count, newtype, target,
          tag, MPI_COMM_WORLD)
...
```

Use of uncommitted type

- Tool Output:

MUST Outputfile

14:11 2014.

Who?

What?

Where?

Details

| Rank(s) | Type | Message | From | References |
|---|---|---|---|---|
| 0 | Error | Argument 3 (datatype) is not commited for transfer, call MPI_Type_commit before using the type for transfer! (Information on datatypeDatatype created at reference 1 is for Fortran, based on the following type(s): { MPI_INTEGER}Typemap = {(MPI_INTEGER, 0), (MPI_INTEGER, 4)}) | Representative location: **MPI_Send** (1st occurrence) called from: #0 main@test.c:17 | References of a representative process: reference 1 rank 0: **MPI_Type_contiguous** (1st occurrence) called from: #0 main@test.c:14 |

# Need for runtime error checking

- Programming MPI is error-prone
- Interfaces often define requirements for function arguments
  - non-MPI Example: *memcpy* has undefined behaviour for overlapping memory regions

- MPI-2.2 Standard specification has 676 pages
  - Who remembers all requirements mentioned there?
- For performance reasons MPI libraries run no checks

- Runtime error checking pinpoints incorrect, inefficient & unsafe function calls

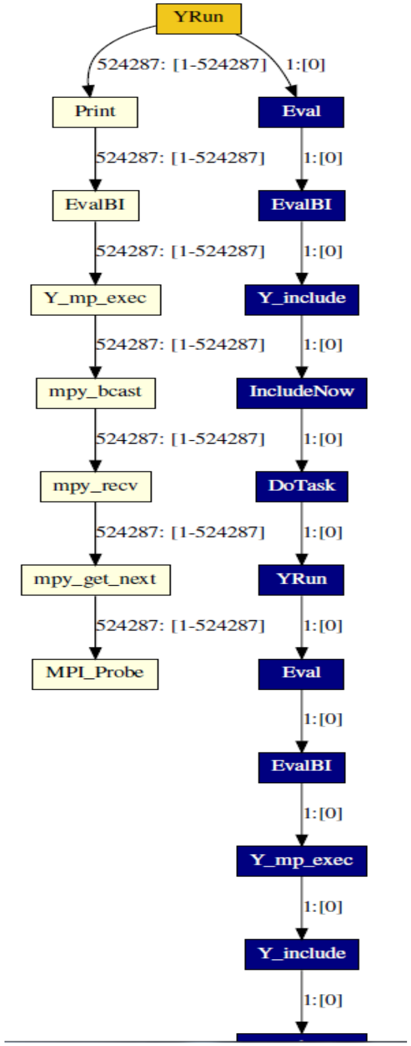
# MUST features

- Local checks:
  - Integer validation
  - Integrity checks (pointer validity, etc.)
  - Operation, Request, Communicator, Datatype & Group object usage
  - Resource leak detection
  - Memory overlap checks
- Non-local checks:
  - Collective verification
  - Lost message detection
  - Type matching (for P2P and collectives)
  - Deadlock detection (with root cause visualization)

# STAT

- Stack trace analysis tool
  - highly scalable, lightweight debugging
  - merges stack traces from a parallel application's processes
    - calling sequences of routines leading to current point of execution
  - groups similar processes at suspicious points of execution
    - automatically identifies equivalence classes and outliers
  - presents 2D spatial and 3D spatial-temporal call graphs
    - prefix tree with nodes labeled by routine names
    - edges labeled with the number and set of associated processes
- Supports BlueGene, Cray & Linux clusters
  - Built on portable, open-source infrastructure
- Developed by LLNL, UWM & UNM
  - Open source with BSD license
  - http://www.paradyn.org/STAT/STAT.html

# STAT Example




- A hang only appeared only when pf3d is scaled to *half a million processes*.
- User refused to debug for *6 months*…
- Incorrect message mismatches due to *non-deterministic communication patterns*.
- Non-deterministic concurrency errors are increasingly common and painful.
- Demand for scalable—yet effective—techniques and tools for this class of errors.

# Integrated application execution profiling and trace analysis

# Integrated appl. execution profile & trace analysis

- instrumentation & measurement (**Score-P**, Extrae)
- profile analysis examination (**CUBE**, **ParaProf**)
- execution trace exploration (**Vampir**, **Paraver**)
- automated trace analysis (**Scalasca**)
- on-line automated analysis (**Periscope**)

- Community efforts to make tools more versatile

Measurement: **Score-P**

Partners:

Technische Universität München
gns
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Analysis:

- TAU

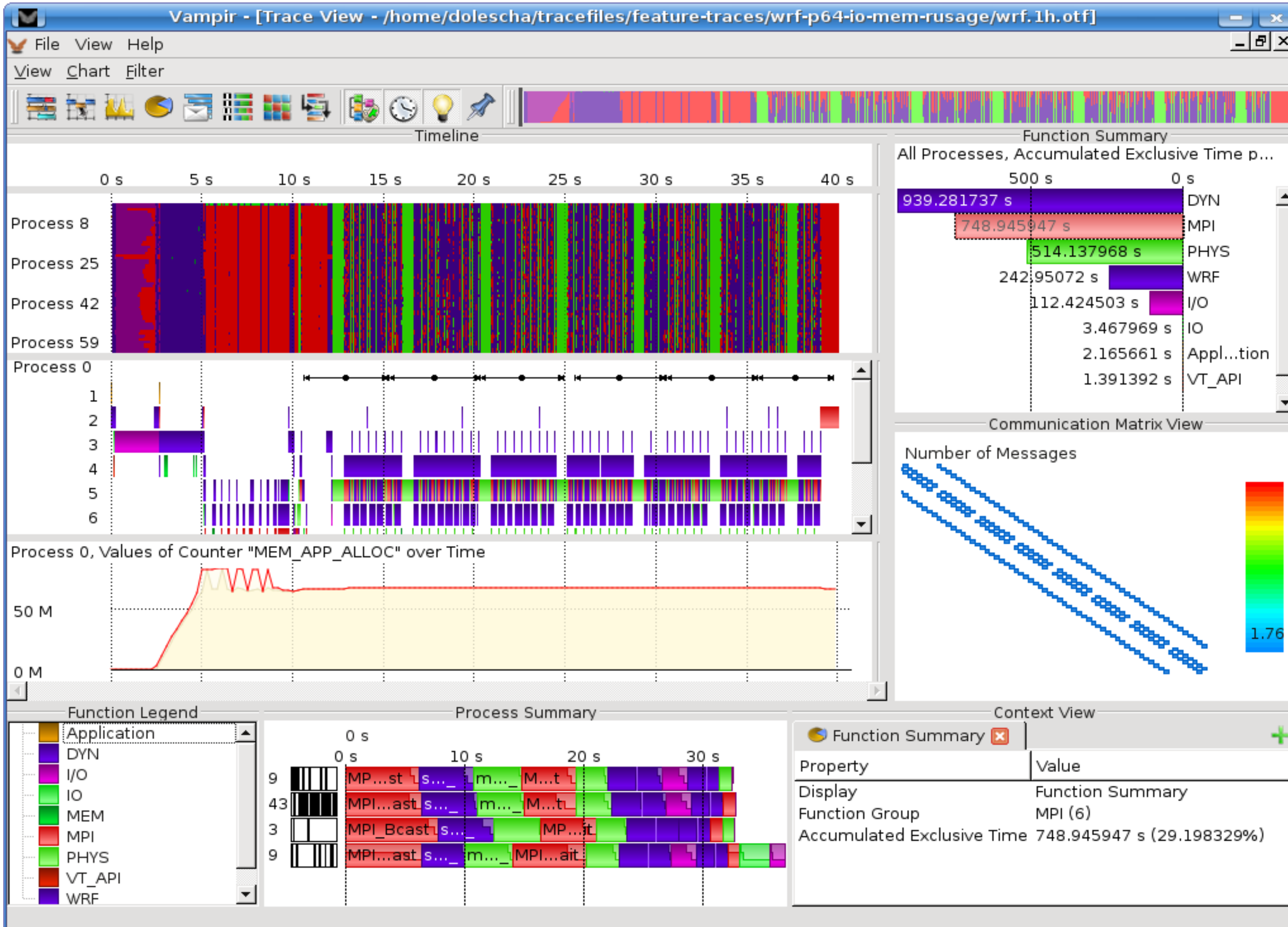
Tuning and Analysis Utilities

- **Vampir**
- Scalasca

# Vampir

- 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/

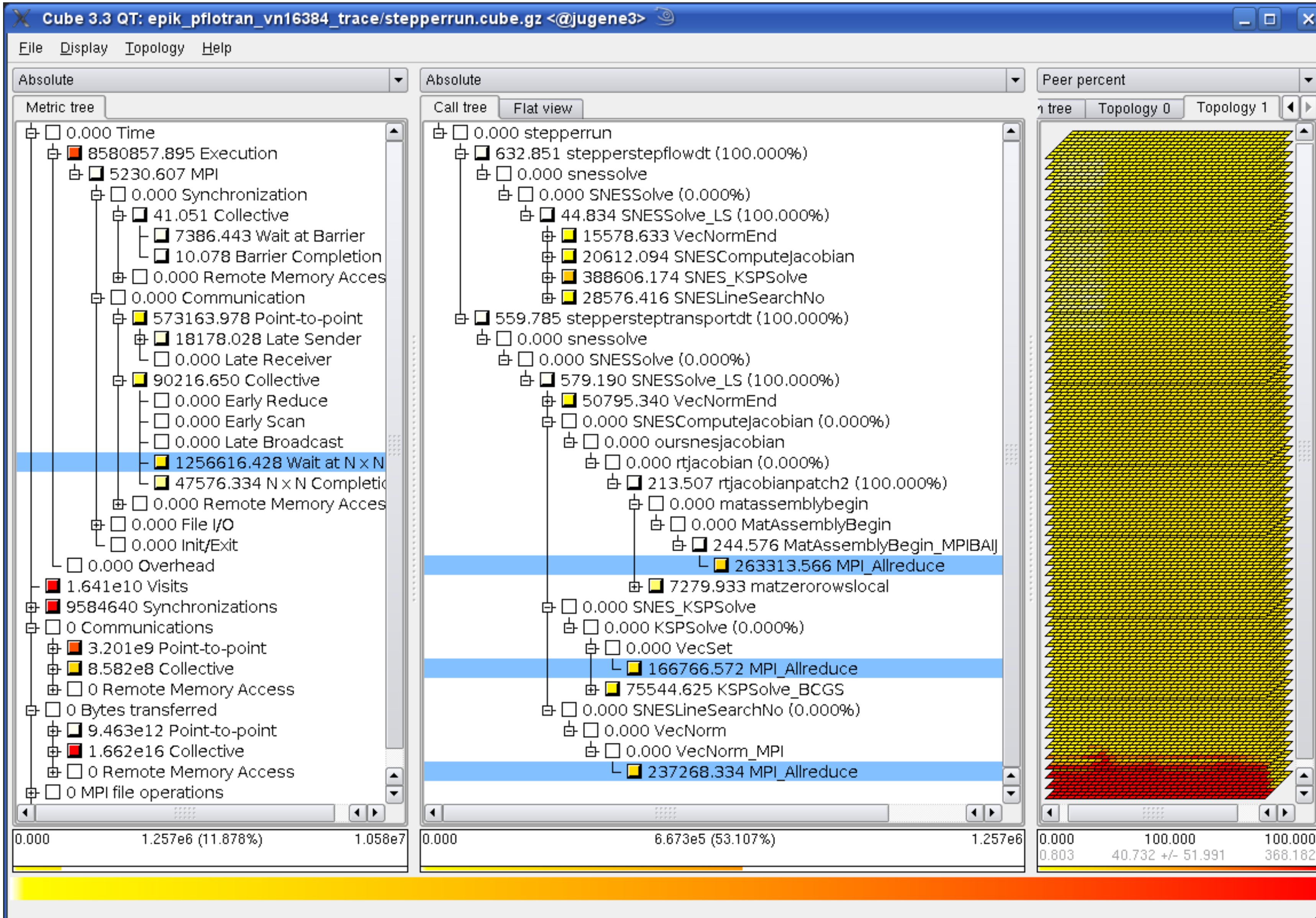
# Vampir interactive trace analysis GUI



# Scalasca

- 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



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