scalasca

Performance analysis & tuning case studies

Brian Wylie & Markus Geimer
Jülich Supercomputing Centre
scalasca@fz-juelich.de
March 2010

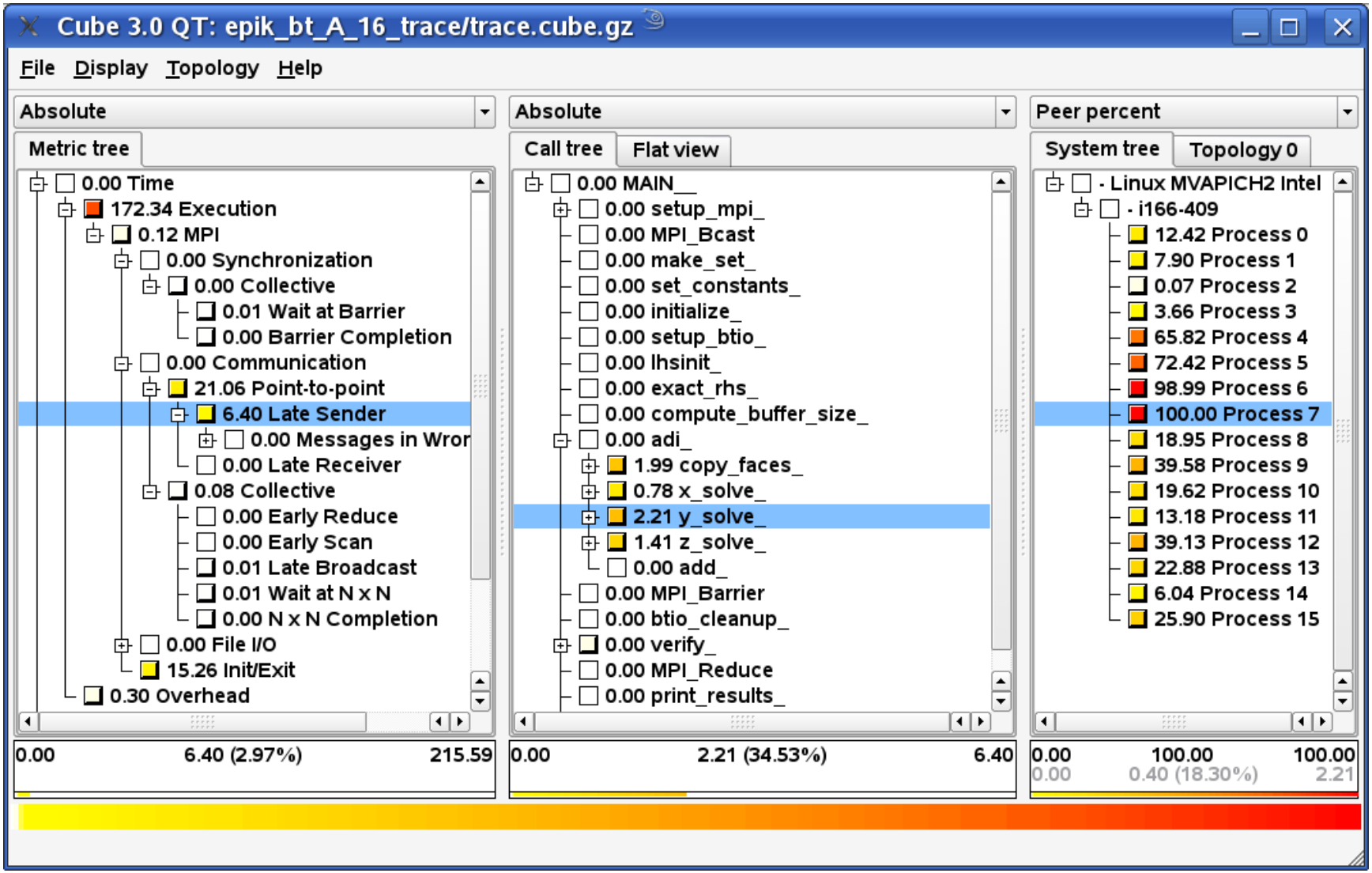
Additional Live-DVD example experiments

- Example experiment archives provided for examination:
  - jugene_sweep3d
    - 294,912 & 65,536 MPI processes on BG/P (trace)
  - jump_zeusmp2
    - 512 MPI processes on p690 cluster (summary & trace)
  - marenostrum_wrf-nmm
    - 1600 MPI processes on JS21 blade cluster, solver extract
    - summary analysis with 8 PowerPC hardware counters
    - trace analysis showing NxN completion problem on some blades
  - neptun_jacobi
    - 12 MPI processes, or 12 OpenMP threads, or 4x3 hybrid parallelizations implemented in C, C++ & Fortran on SGI Altix
  - ranger_smg2000
    - 12,288 MPI processes on Sun Constellation cluster, solve extract

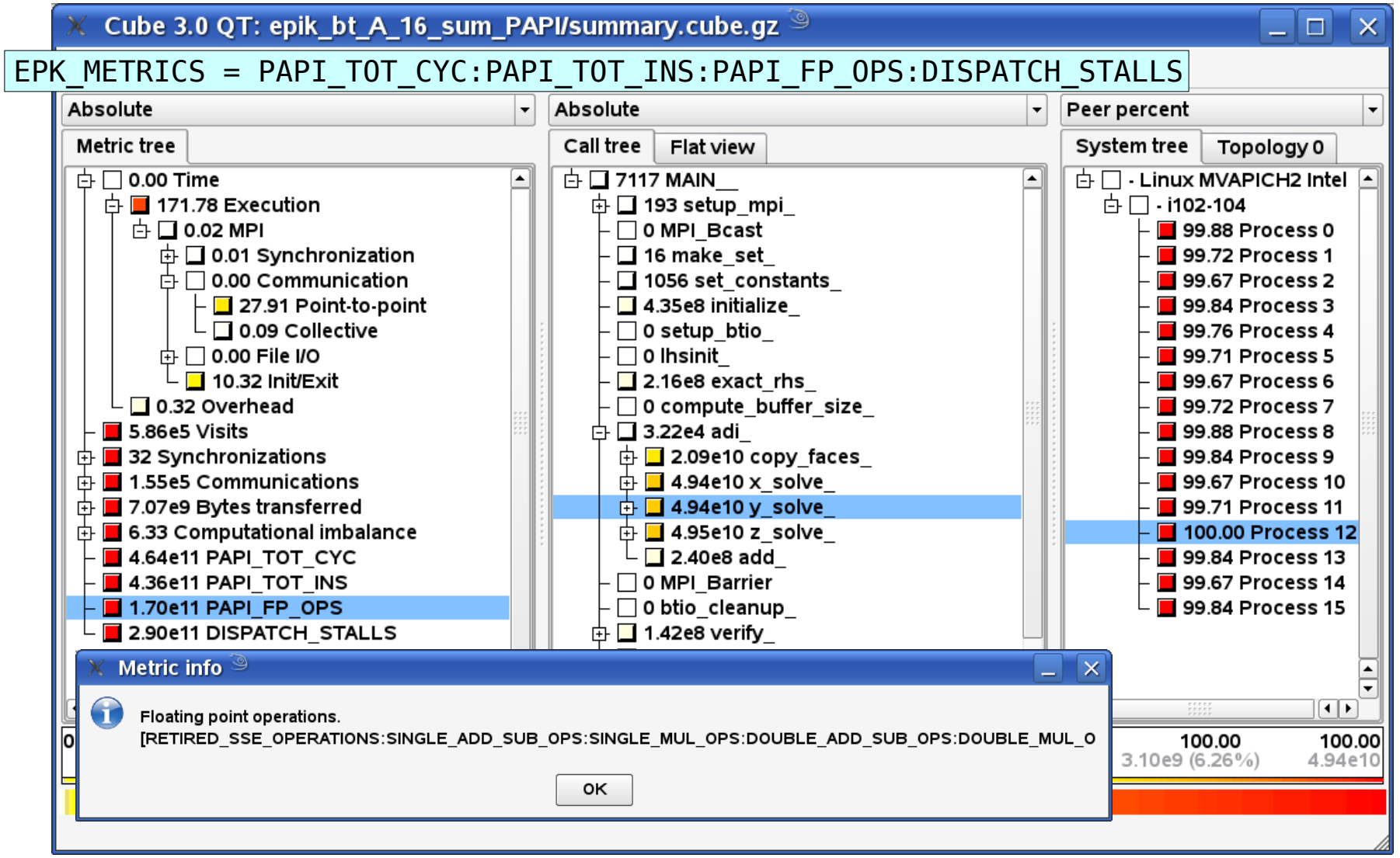
Scalasca NPB-BT experiments

- Comparison of NPB-BT class A in various configurations run on a single dedicated 16-core cluster compute node
  - 16 MPI processes
    - optionally built using MPI File I/O (e.g., SUBTYPE=full)
    - optionally including PAPI counter metrics in measurement (e.g., EPK_METRICS=PAPI_FP_OPS:DISPATCH_STALLS)
  - 16 OpenMP threads
  - 4 MPI processes each with 4 OpenMP threads (MZ-MPI)
- NPB-BT-MZ class B on Cray XT5 (8-core compute nodes)
  - 32 MPI processes with OMP_NUM_THREADS=8
    - More threads created on some processes (and fewer on others) as application attempts to balance work distribution
- NPB-MPI-BT on BlueGene/P with 144k processes
  - 1536x1536x1536 gridpoints distributed on 384x384 processes

16-process trace analysis

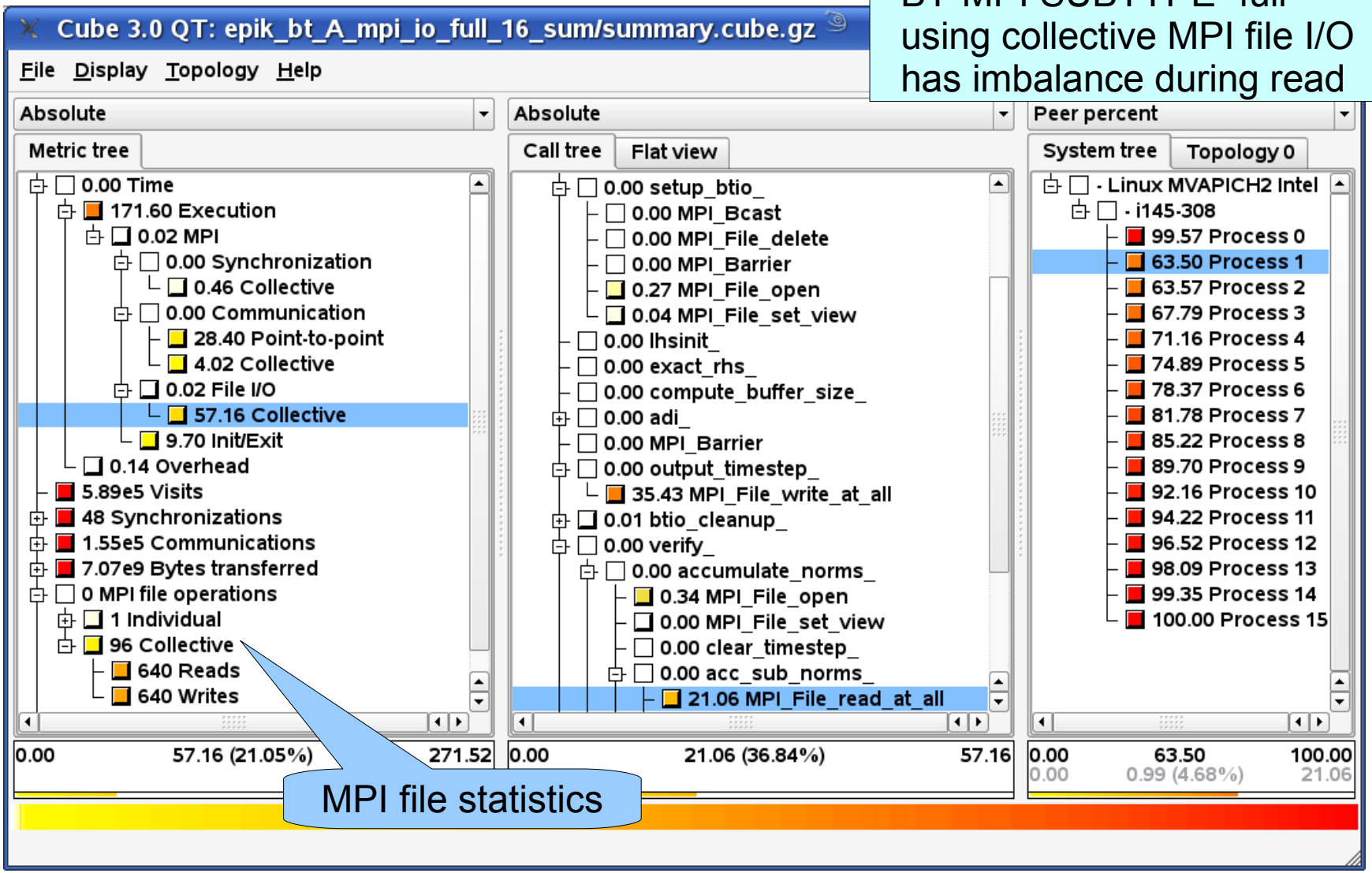


16-process summary analysis with HWC metrics



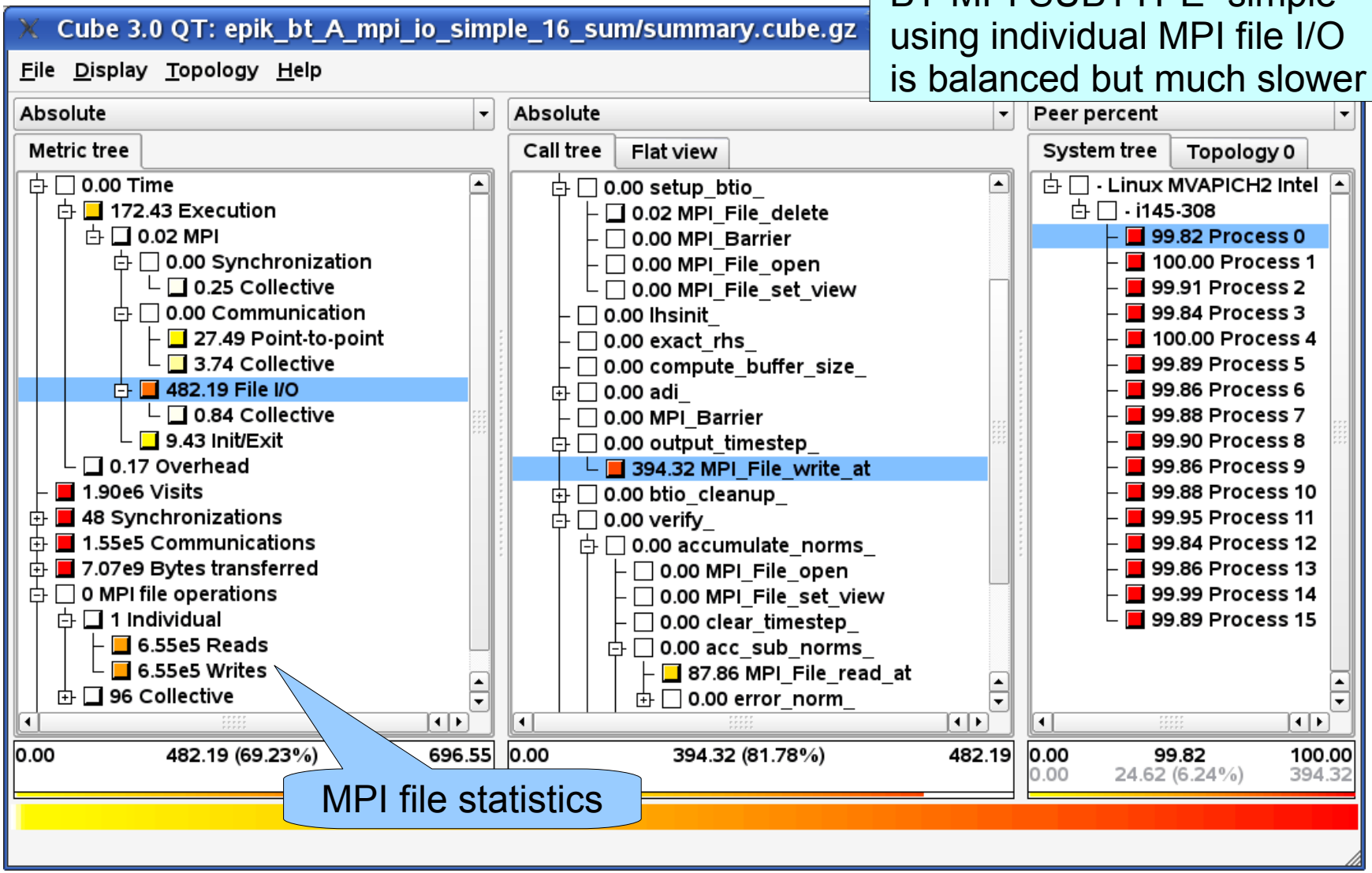
16-process summary analysis: MPI File I/O time

BT-MPI SUBTYPE=full
using collective MPI file I/O
has imbalance during read

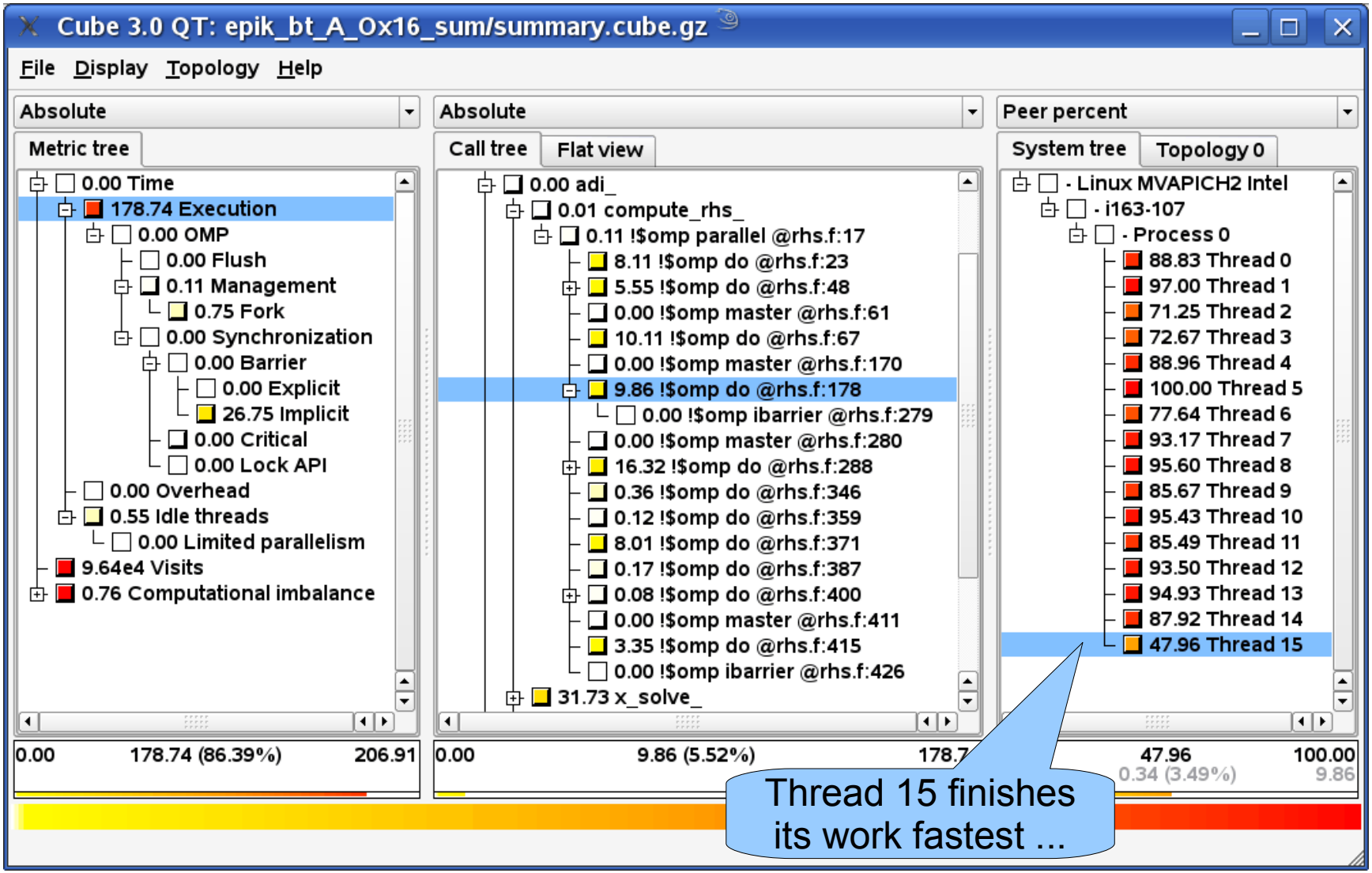


16-process summary analysis: MPI File I/O time

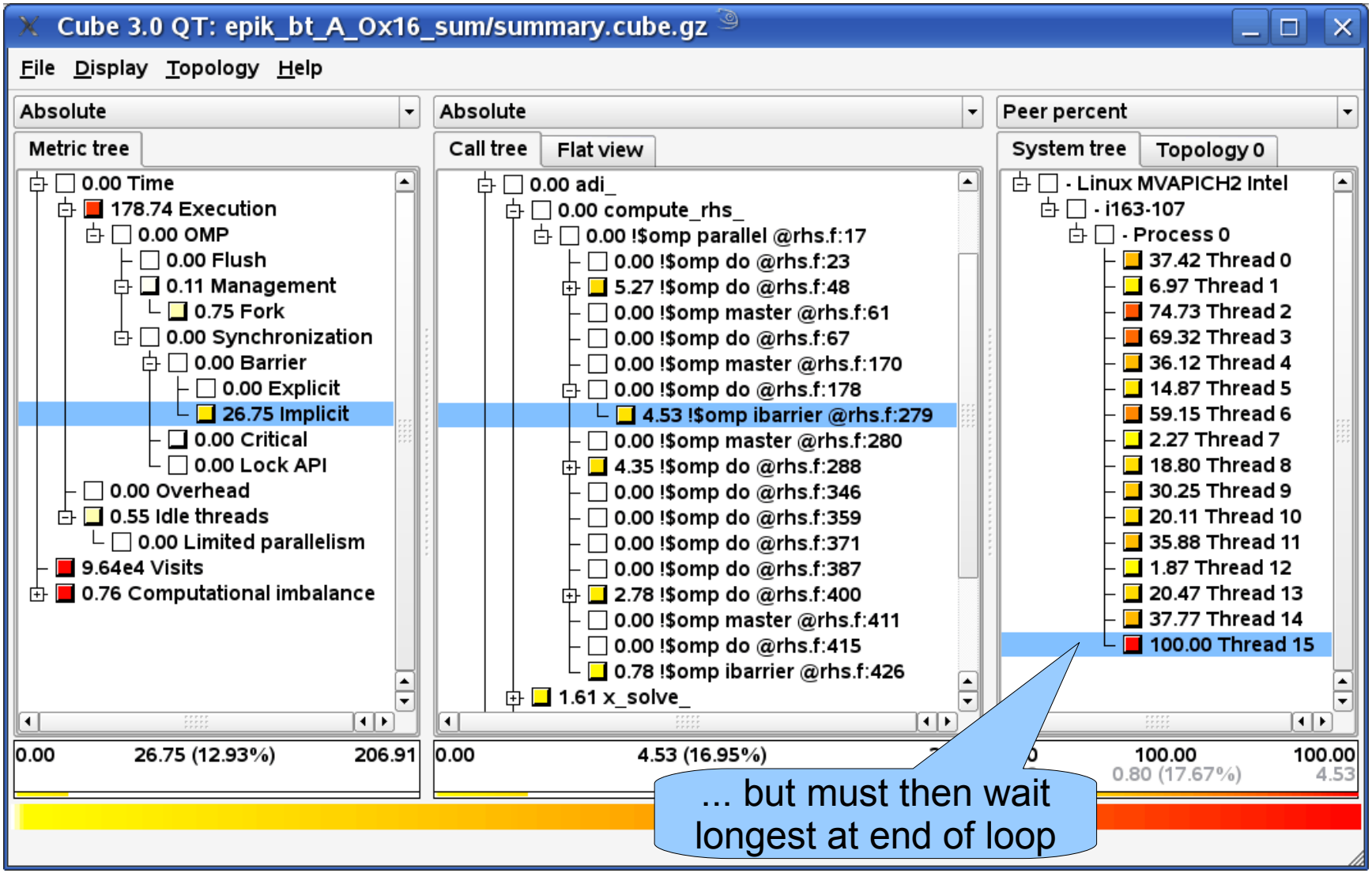
BT-MPI SUBTYPE=simple using individual MPI file I/O is balanced but much slower



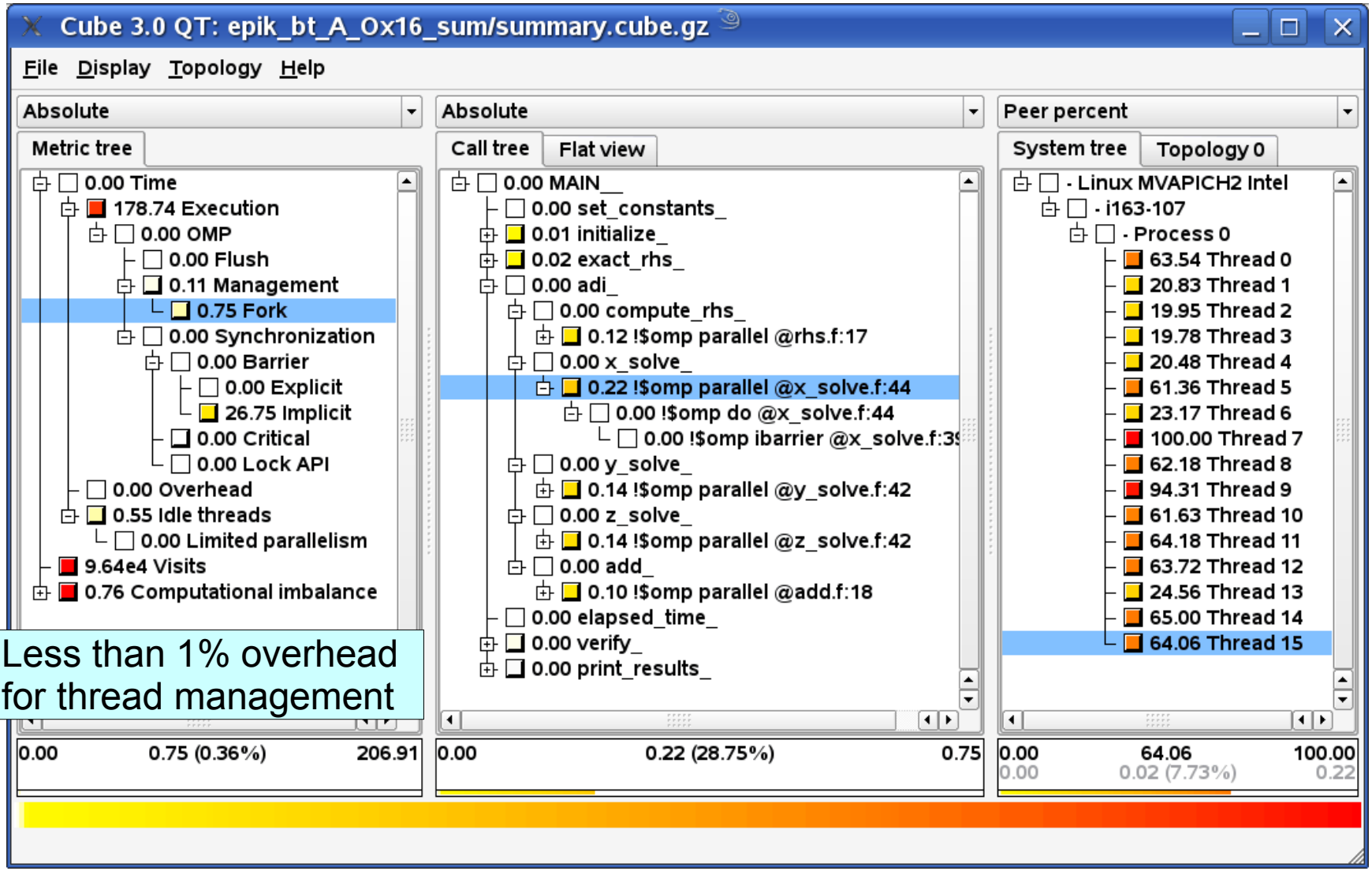
16-thread summary analysis: Execution time



16-thread summary analysis: Implicit barrier time

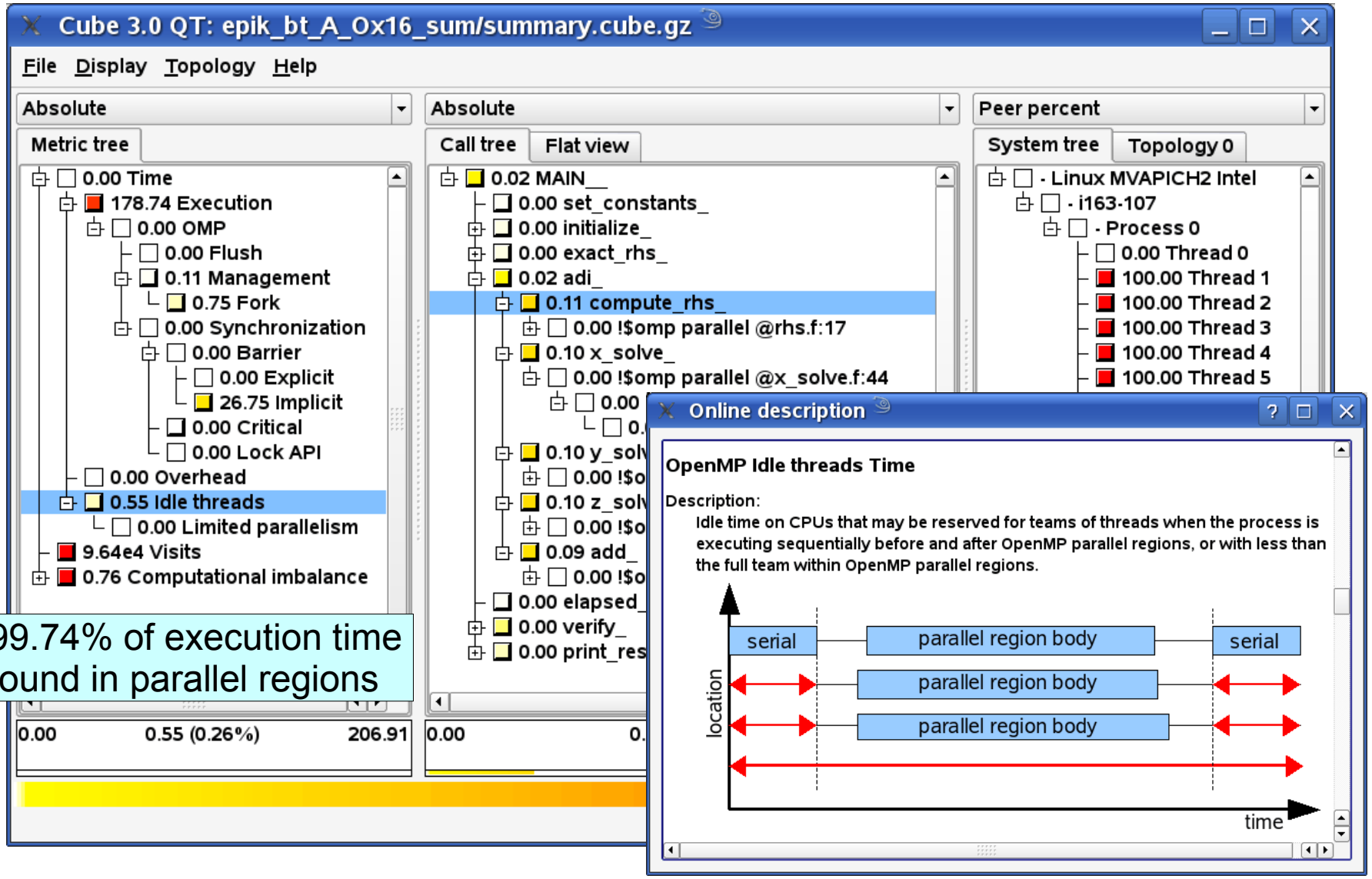


16-thread summary analysis: Thread fork time



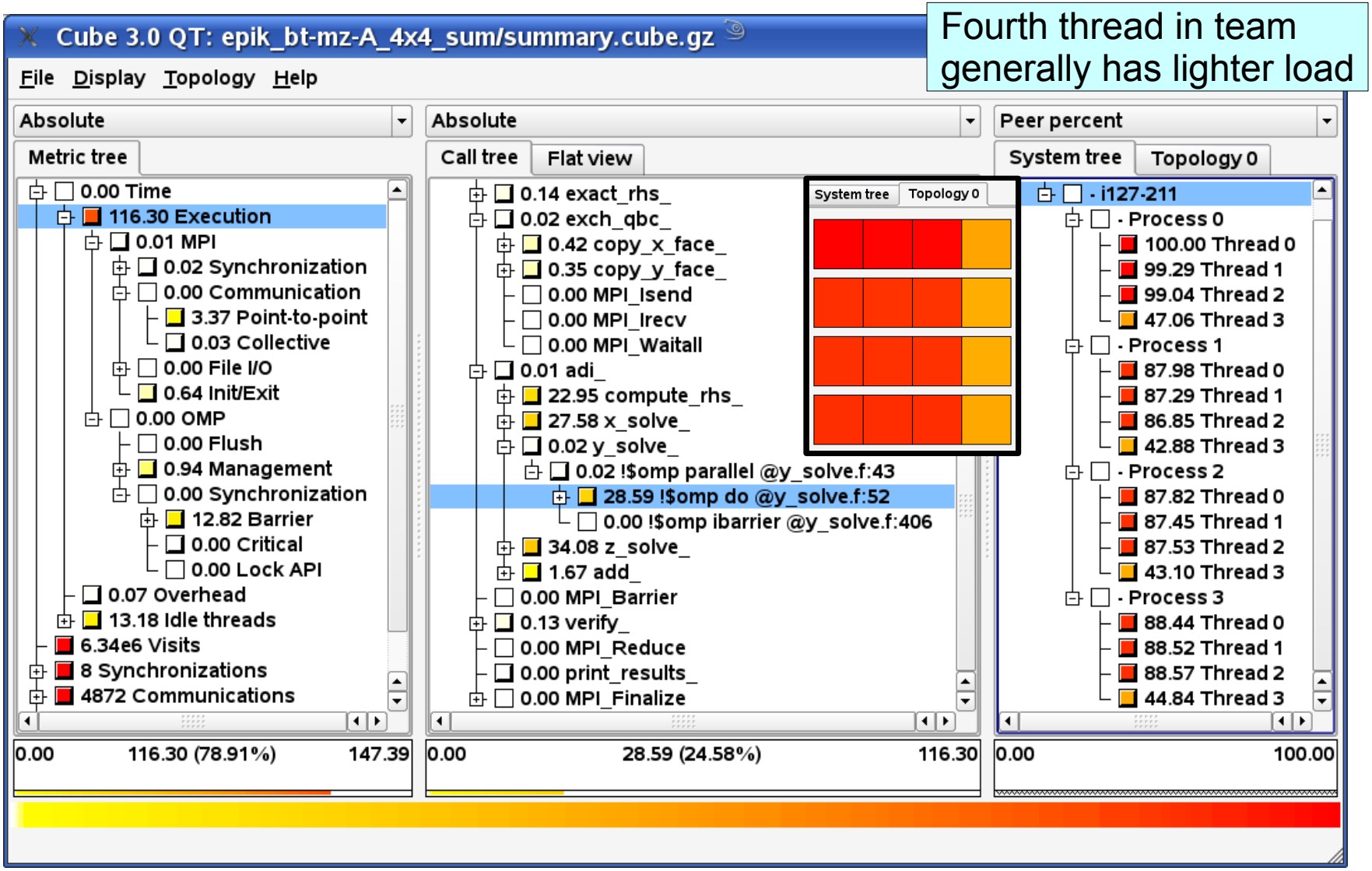
Less than 1% overhead for thread management

16-thread summary analysis: Idle threads time



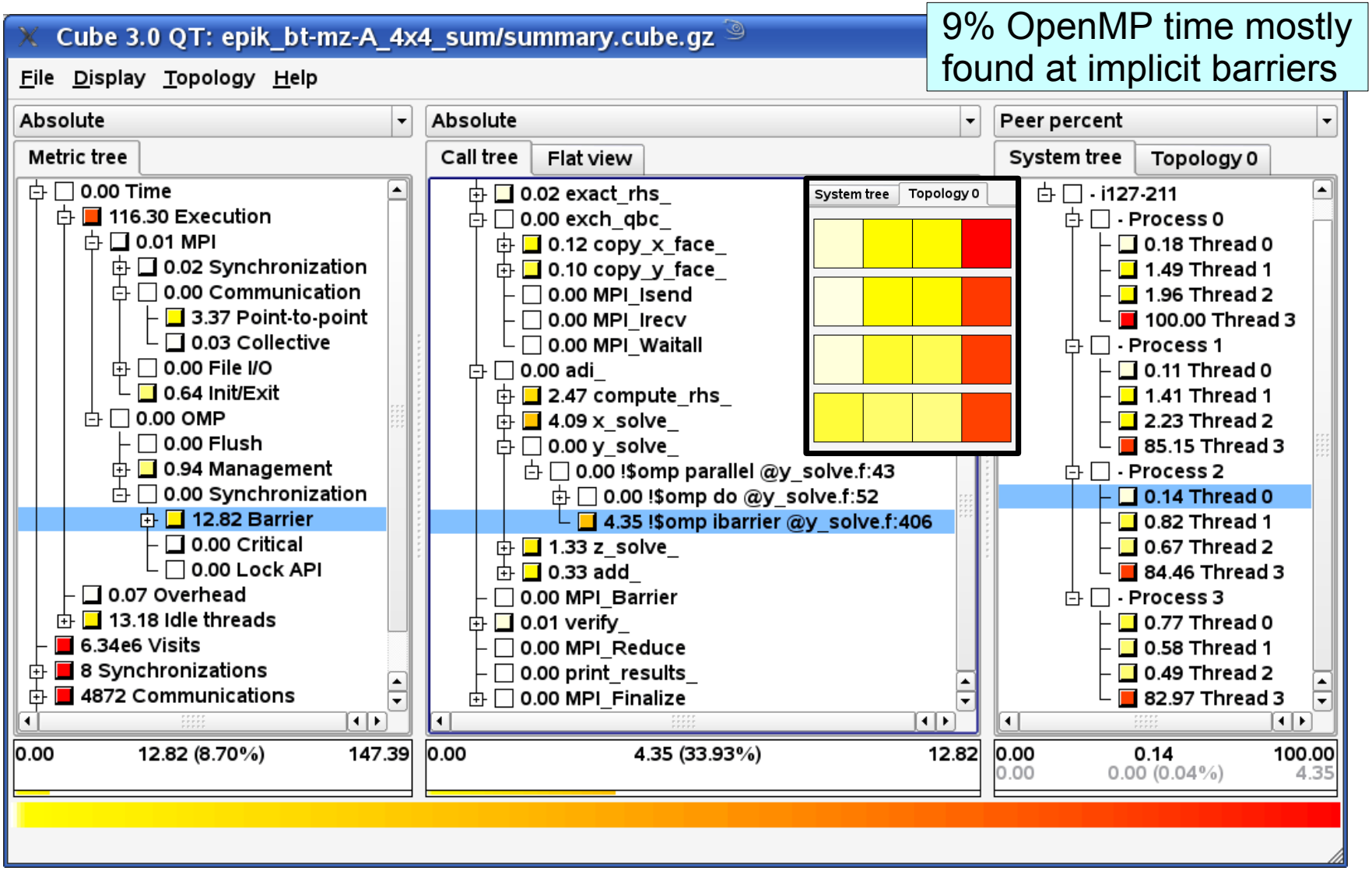
99.74% of execution time found in parallel regions

4x4 summary analysis: Execution time



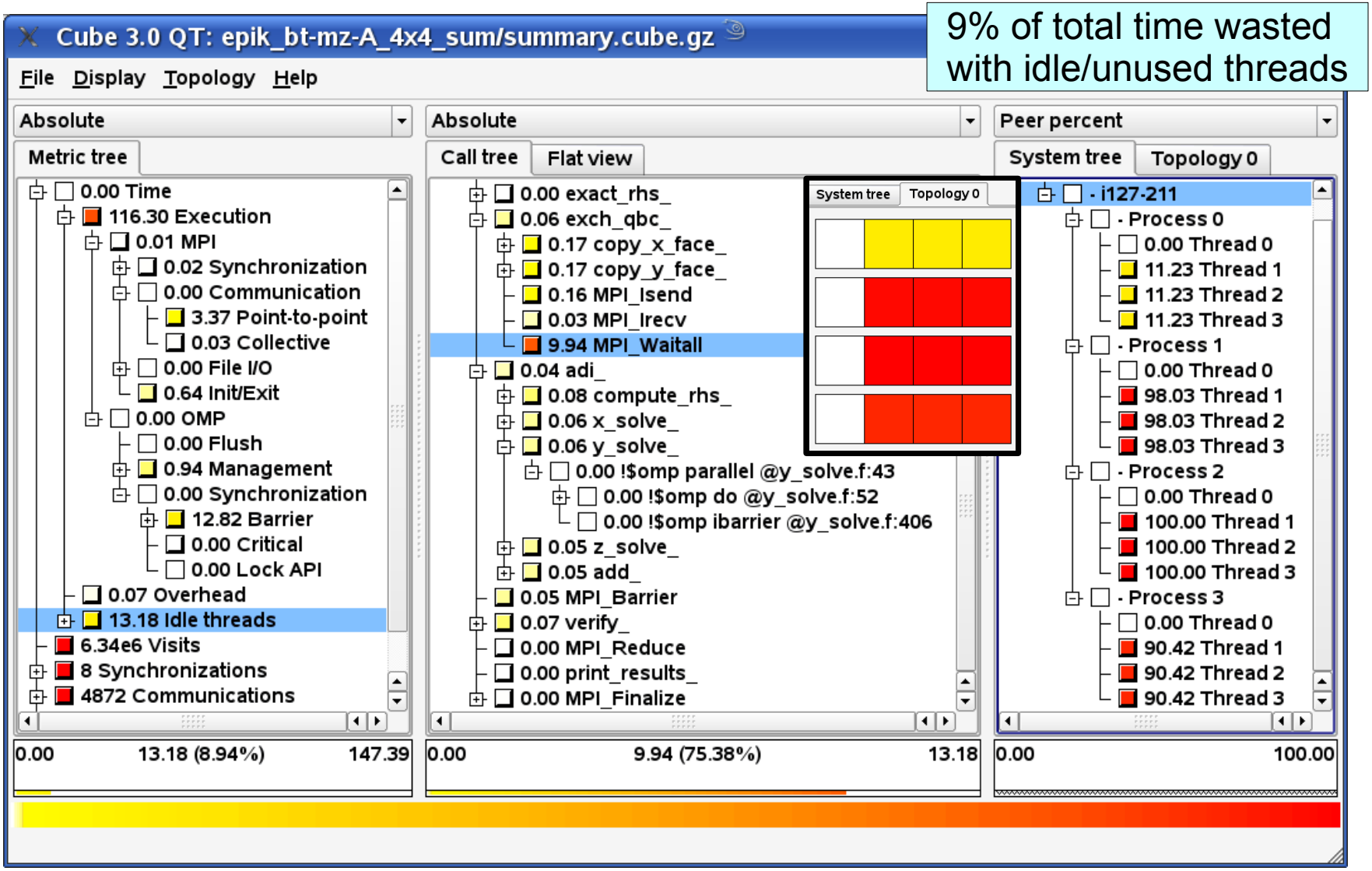
Fourth thread in team generally has lighter load

4x4 summary analysis: OpenMP time



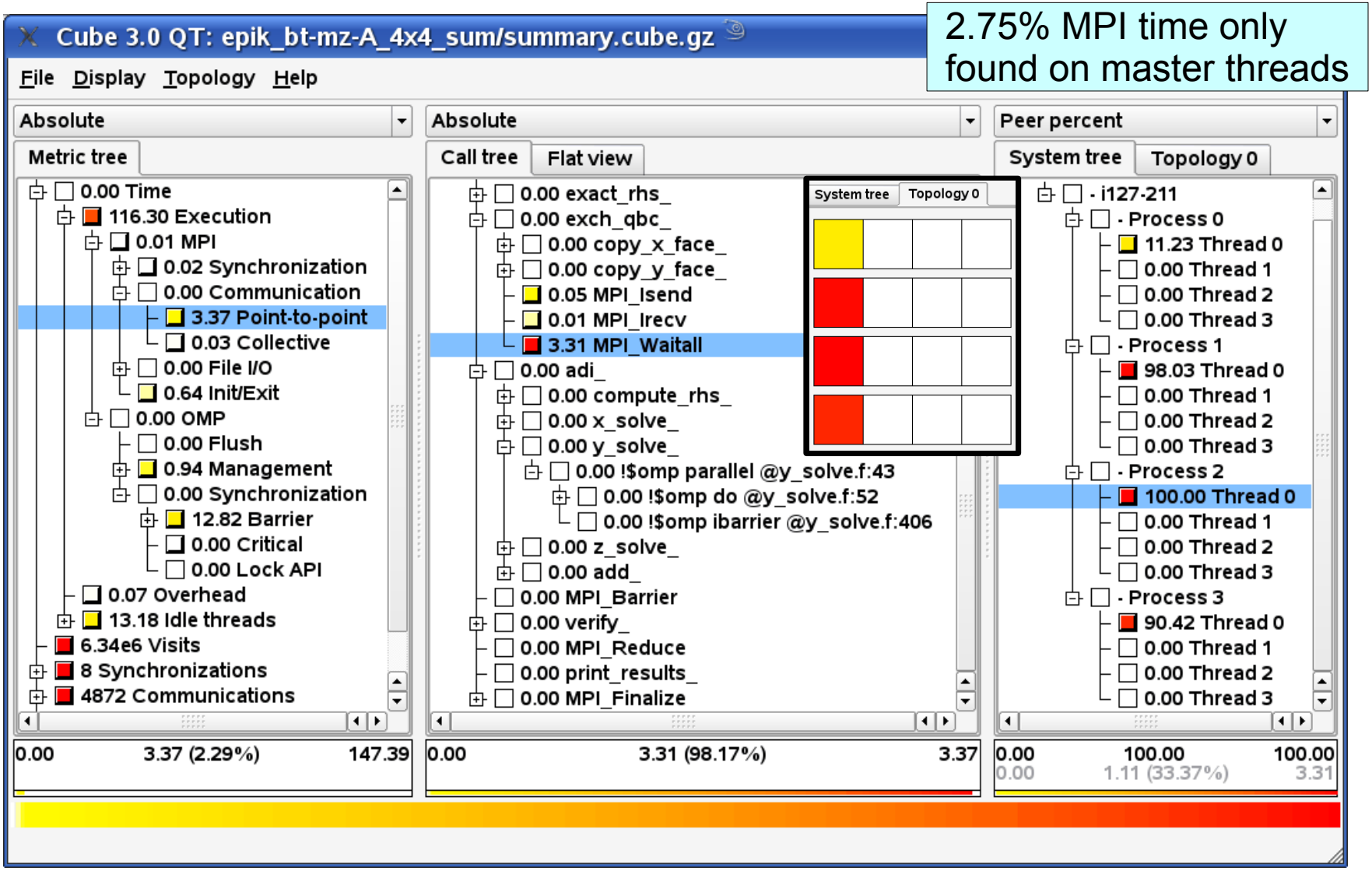
9% OpenMP time mostly found at implicit barriers

4x4 summary analysis: Idle threads time



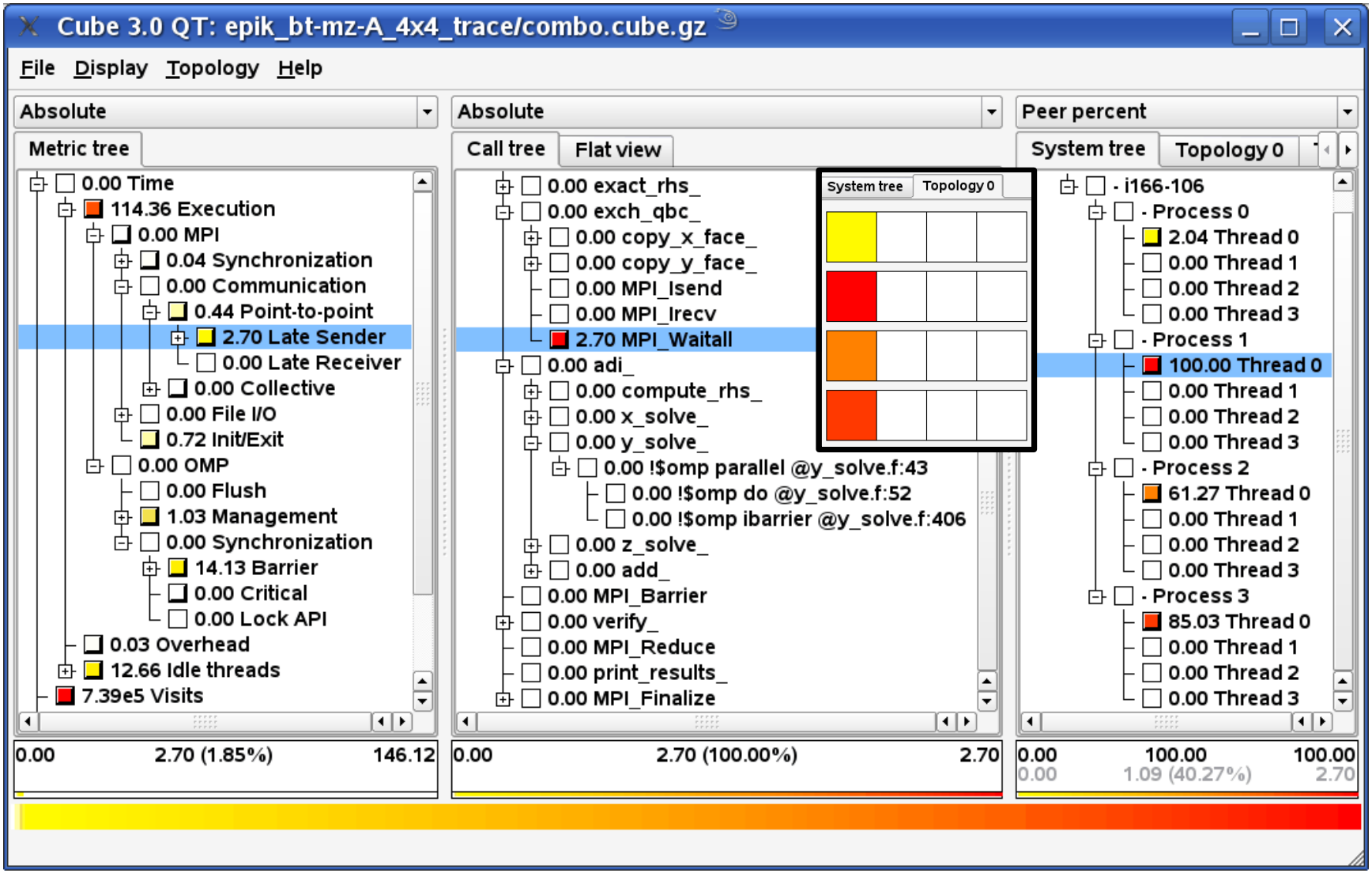
9% of total time wasted with idle/unused threads

4x4 summary analysis: MPI time

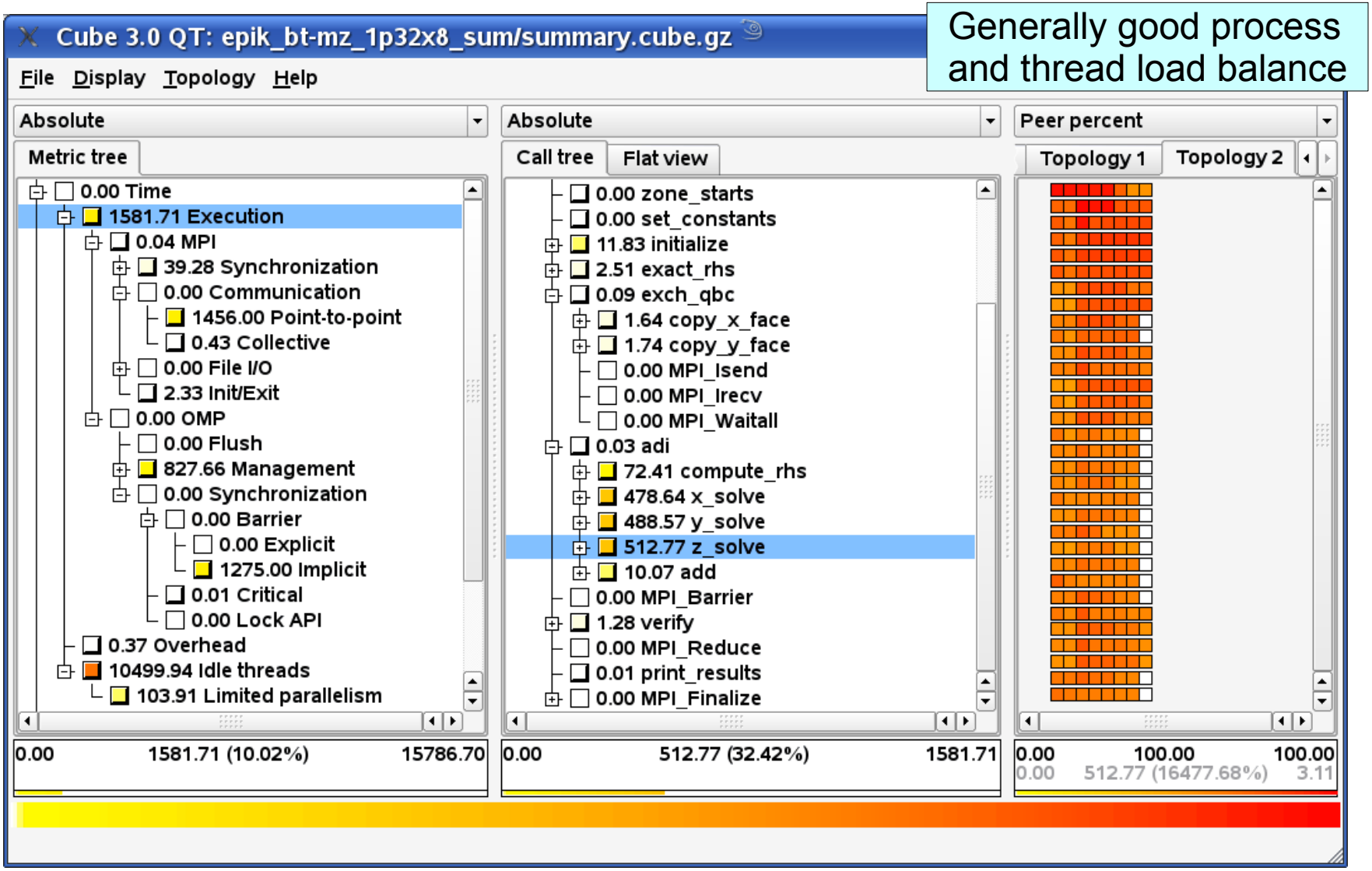


2.75% MPI time only found on master threads

4x4 combined summary & trace analysis

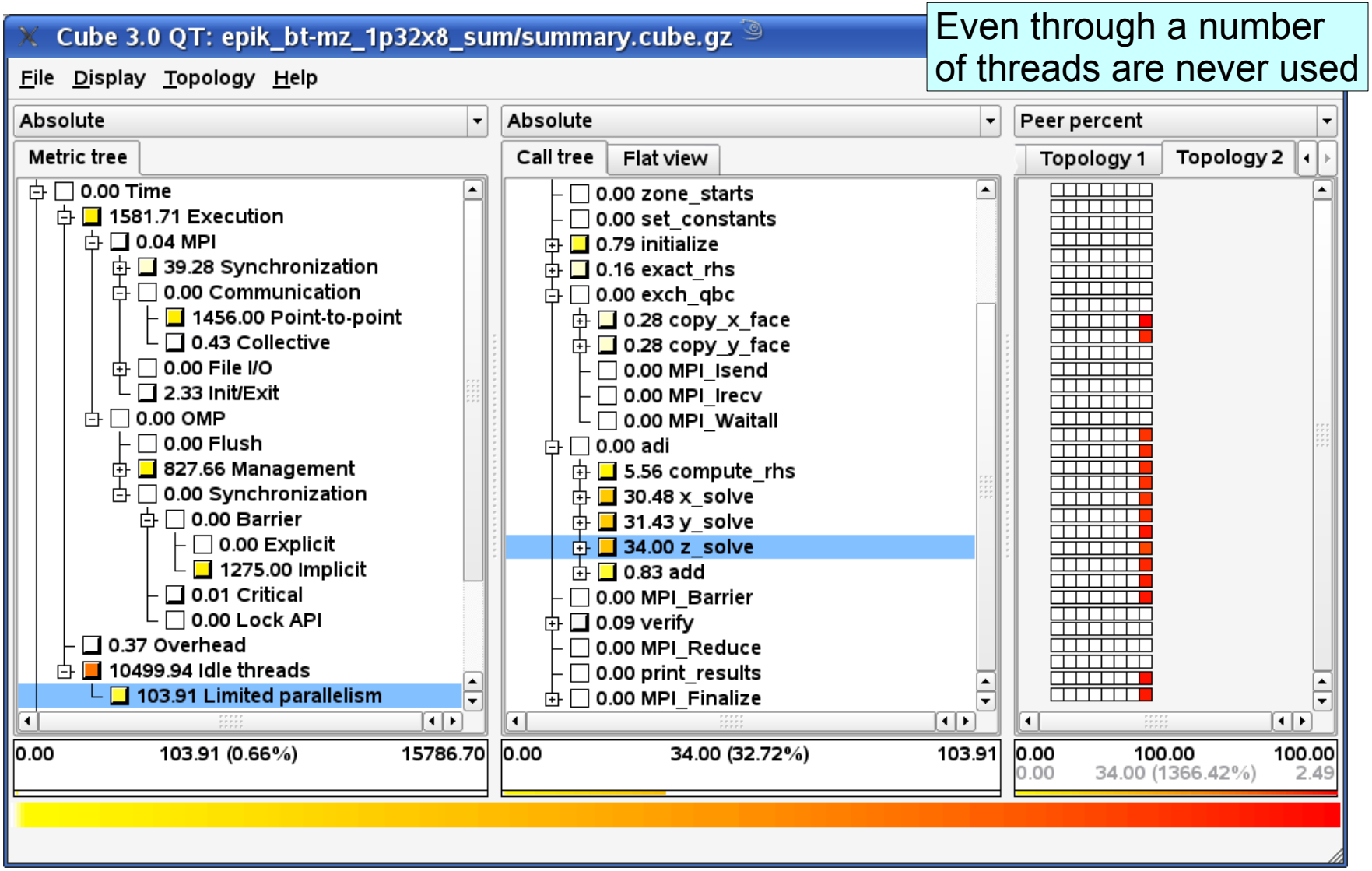


32x8 summary analysis: Excl. execution time

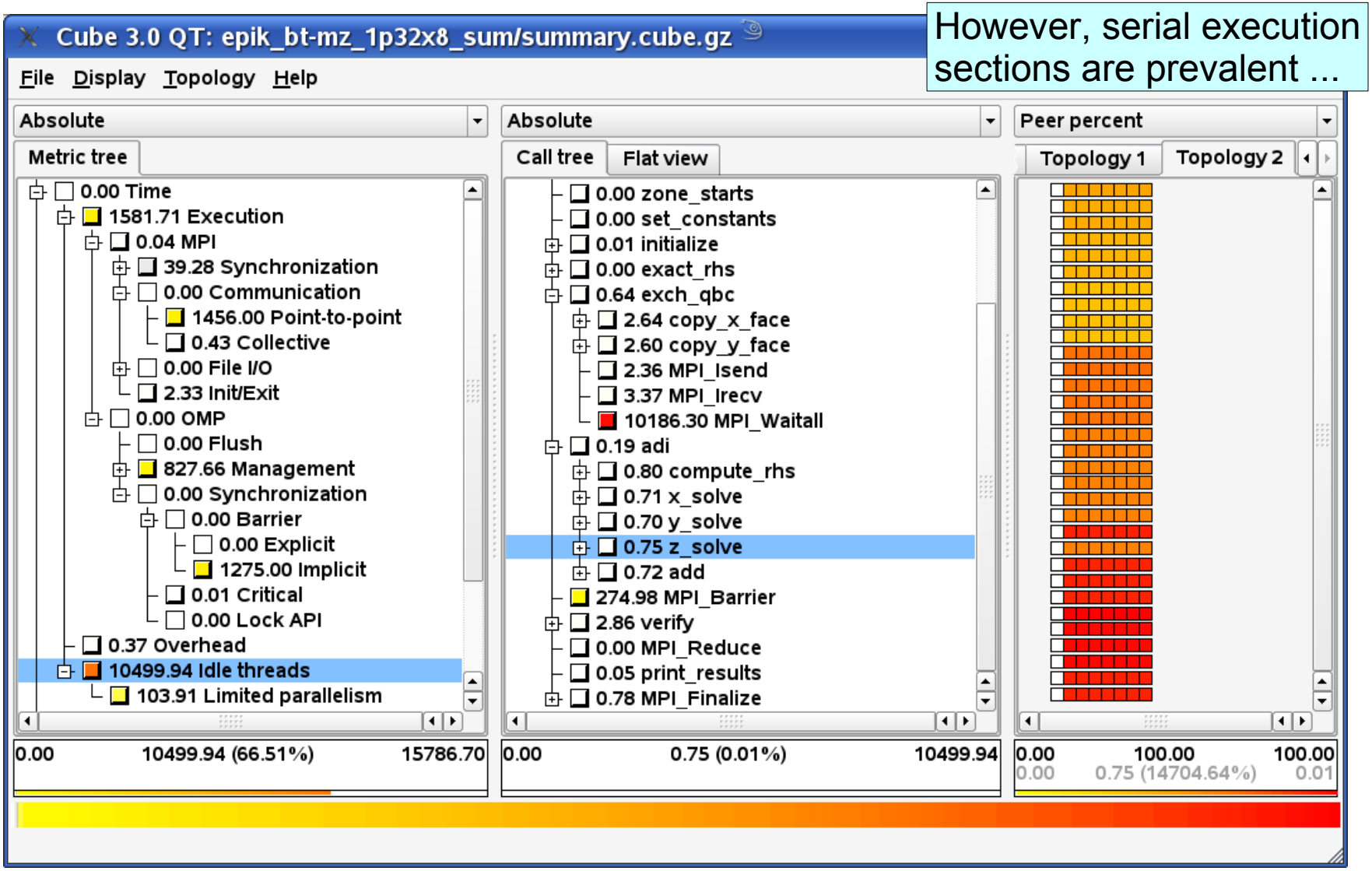


Generally good process and thread load balance

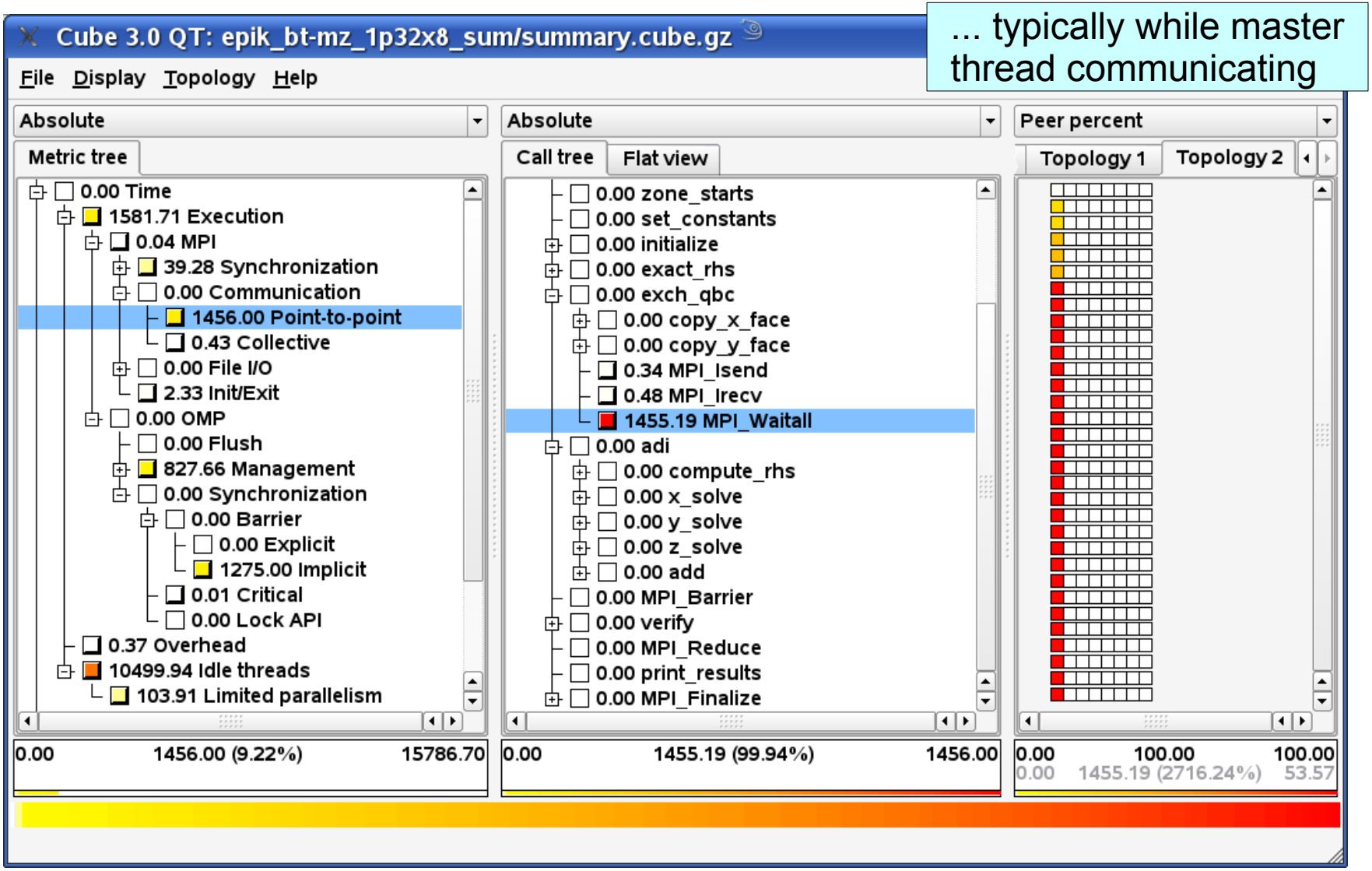
32x8 summary analysis: Limited parallelism



32x8 summary analysis: Idle threads time

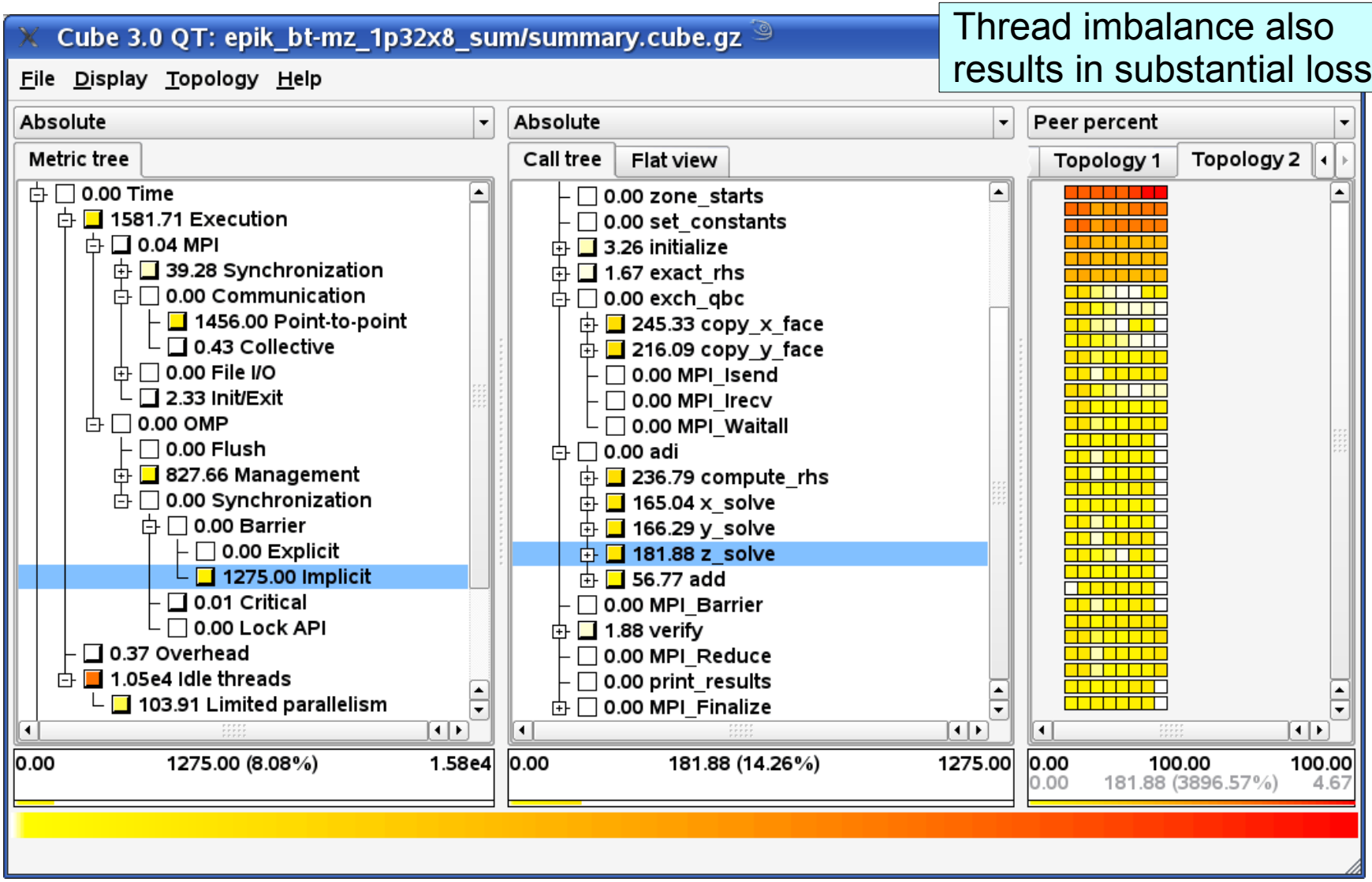


32x8 summary analysis: MPI communication time



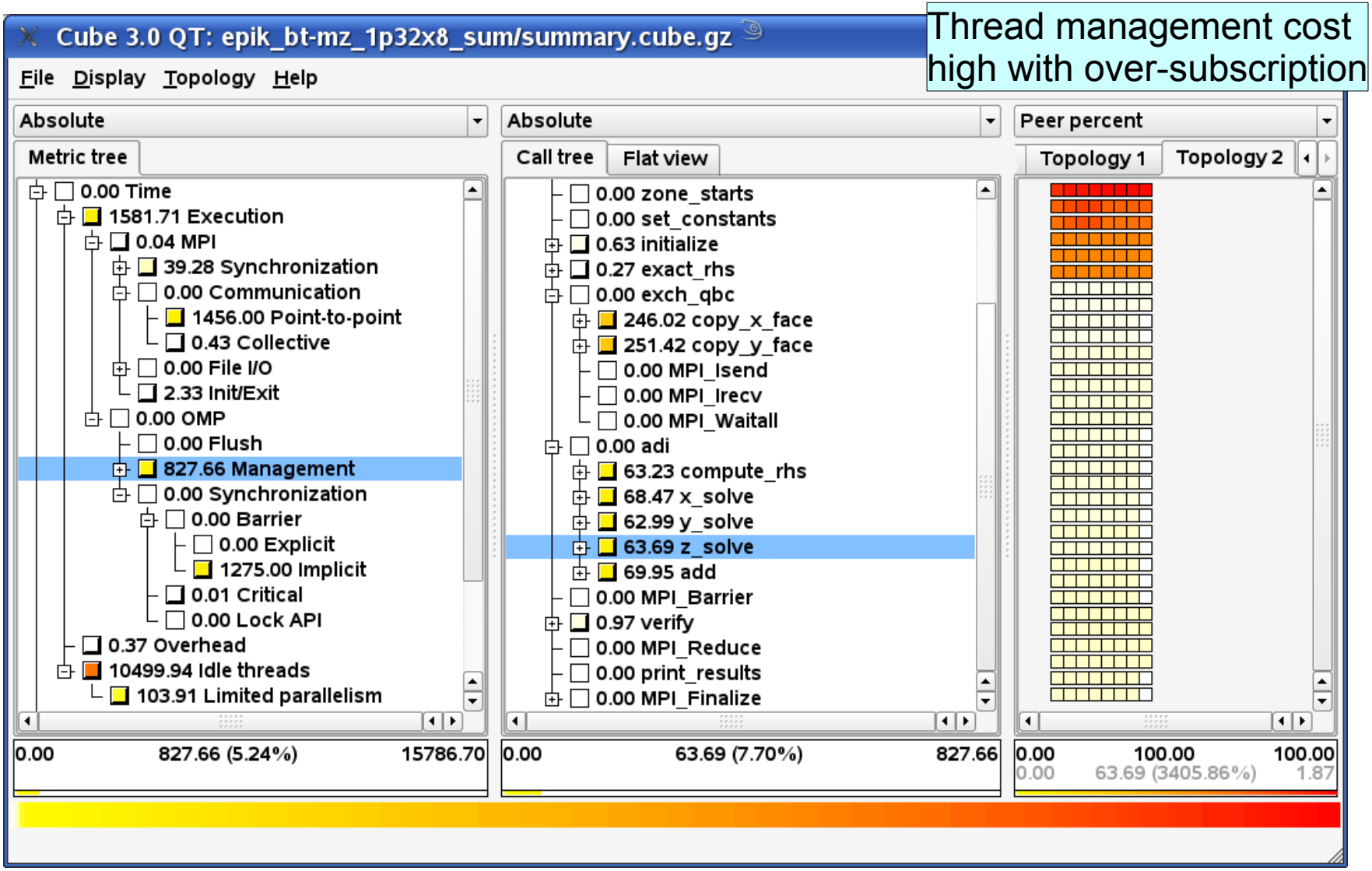
... typically while master thread communicating

32x8 summary analysis: Implicit barrier time



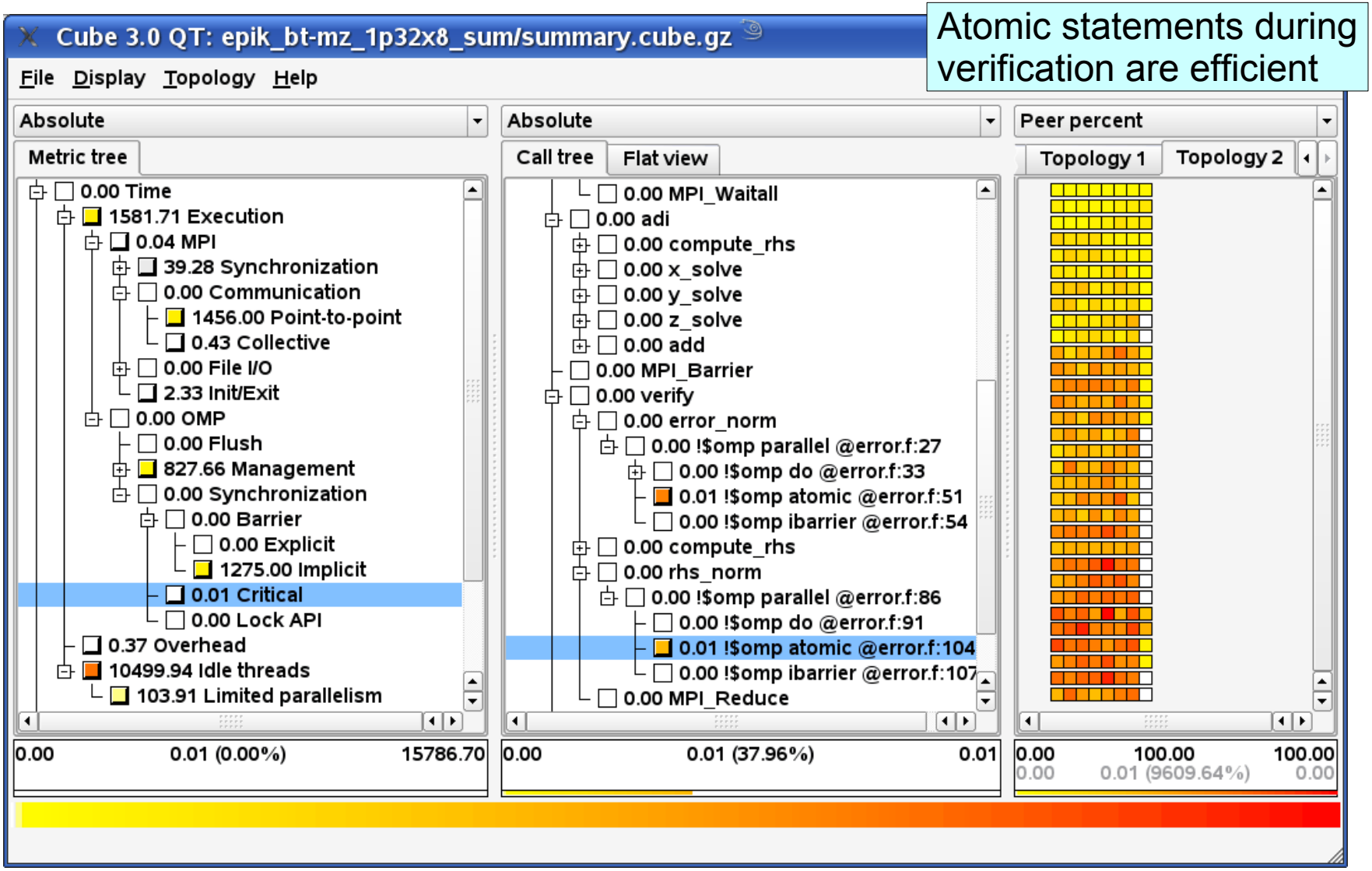
Thread imbalance also results in substantial loss

32x8 summary analysis: Thread management



Thread management cost high with over-subscription

32x8 summary analysis: Critical section time

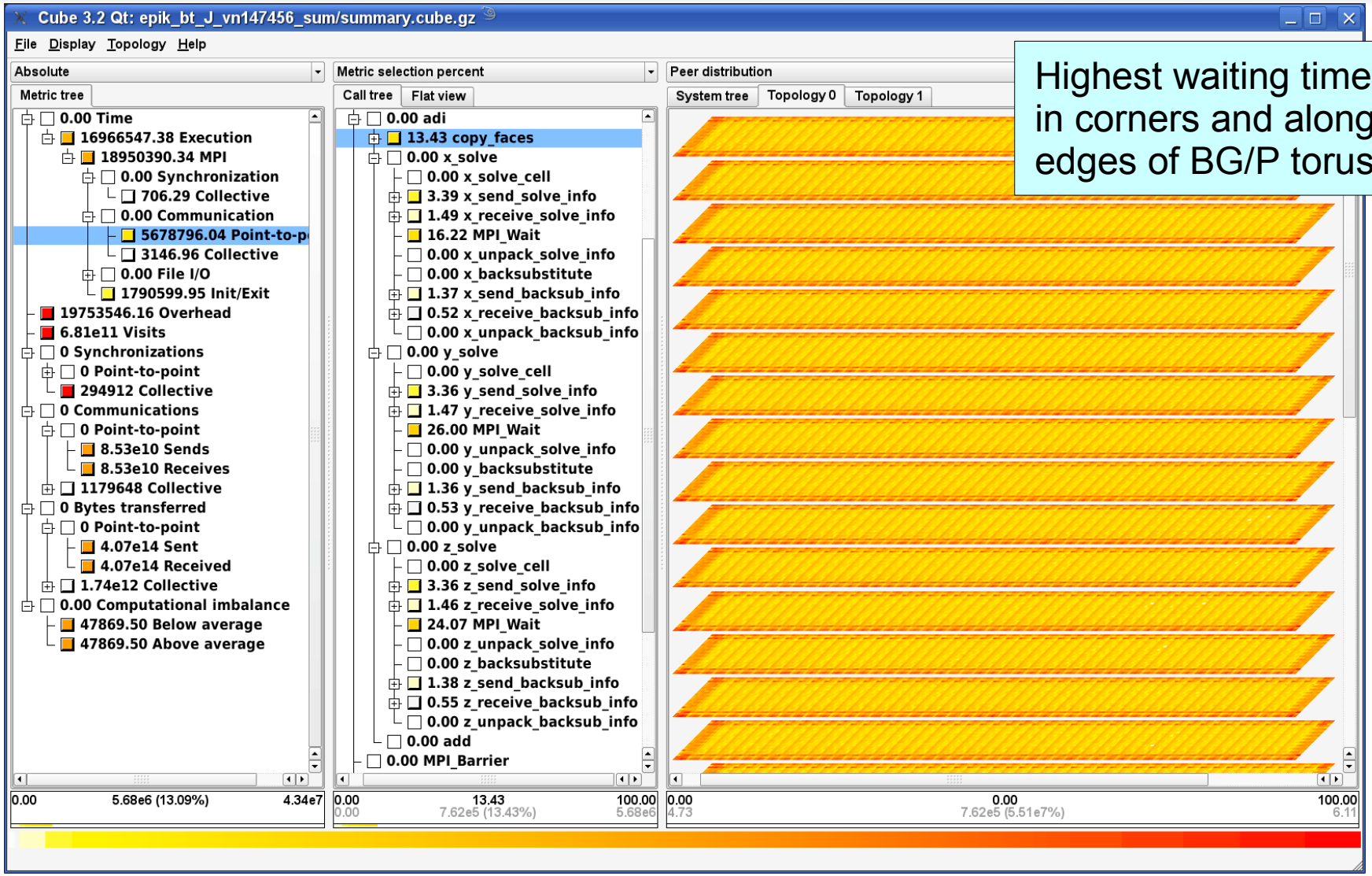


Atomic statements during verification are efficient

NPB-MPI-BT on BlueGene/P case study

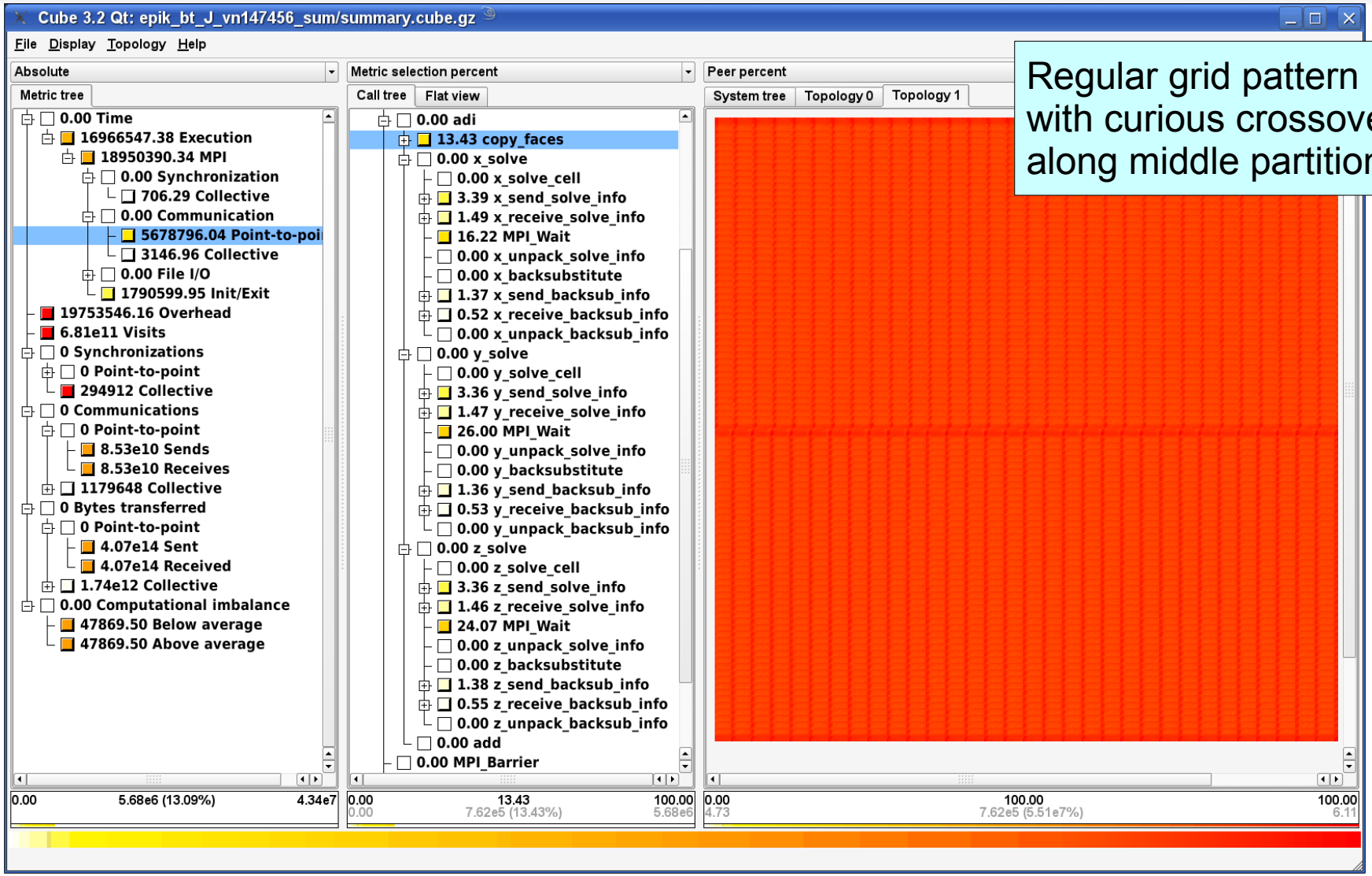
- 3D solution of unsteady, compressible Navier-Stokes eqs
  - NASA NAS parallel benchmark suite Block-Tridiagonal solver
  - series of ADI solve steps in X, Y & Z dimensions
  - ~9,500 lines (20 source modules), mostly Fortran77
- Run on IBM BlueGene/P in VN mode with 144k processes
  - Good scaling when problem size matched to architecture
    - 1536x1536x1536 gridpoints mapped onto 384x384 processes
  - Measurement collection took 53 minutes
  - 38% dilation for summarization measurement compared to uninstrumented execution (using 10 function filter)
  - MPI trace size would be 18.6TB
  - 25% of time in ADI is point-to-point communication time
    - 13% copy_faces, 23% x_solve, 33% y_solve, 31% z_solve
  - 128s for a single MPI_Comm_split during setup!

NPB-MPI-BT on jugene@144k summary analysis



Highest waiting times in corners and along edges of BG/P torus

NPB-MPI-BT on jugene@144k summary analysis



Regular grid pattern with curious crossover along middle partition

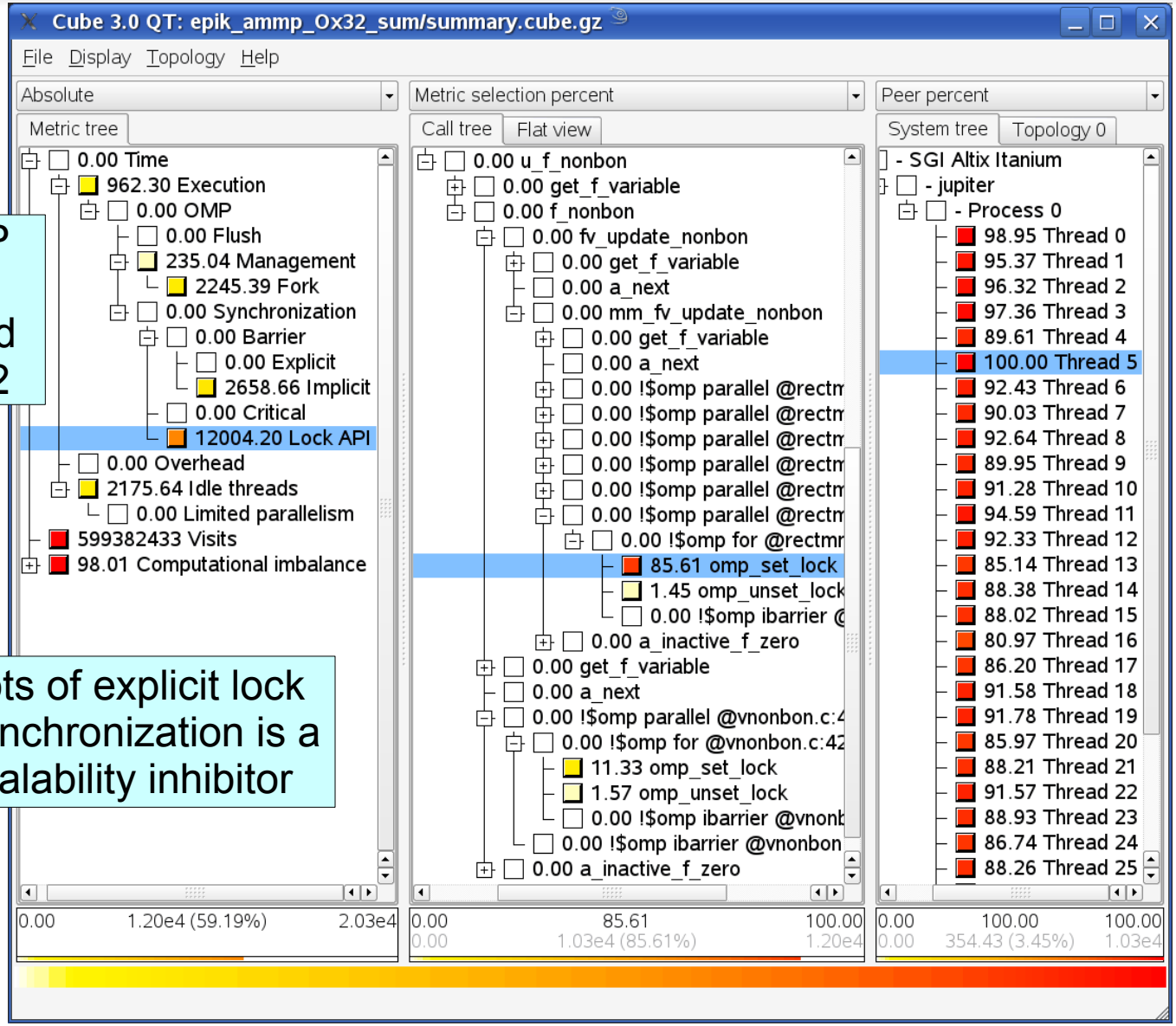
AMMP on Altix case study

- Molecular mechanics simulation
  - original version developed by Robert W. Harrison
- SPEC OMP benchmark parallel version
  - ~14,000 lines (in 28 source modules): 100% C
- Run with 32 threads on SGI Altix 4700 at TUD-ZIH
  - Built with Intel compilers
  - 333 simulation timesteps for 9,582 atoms
- Scalasca summary measurement
  - Minimal measurement dilation
  - 60% of total time lost in synchronization with lock API
  - 12% thread management overhead

ammp on jupiter@32 OpenMP lock analysis

OpenMP metrics reworked with v1.2

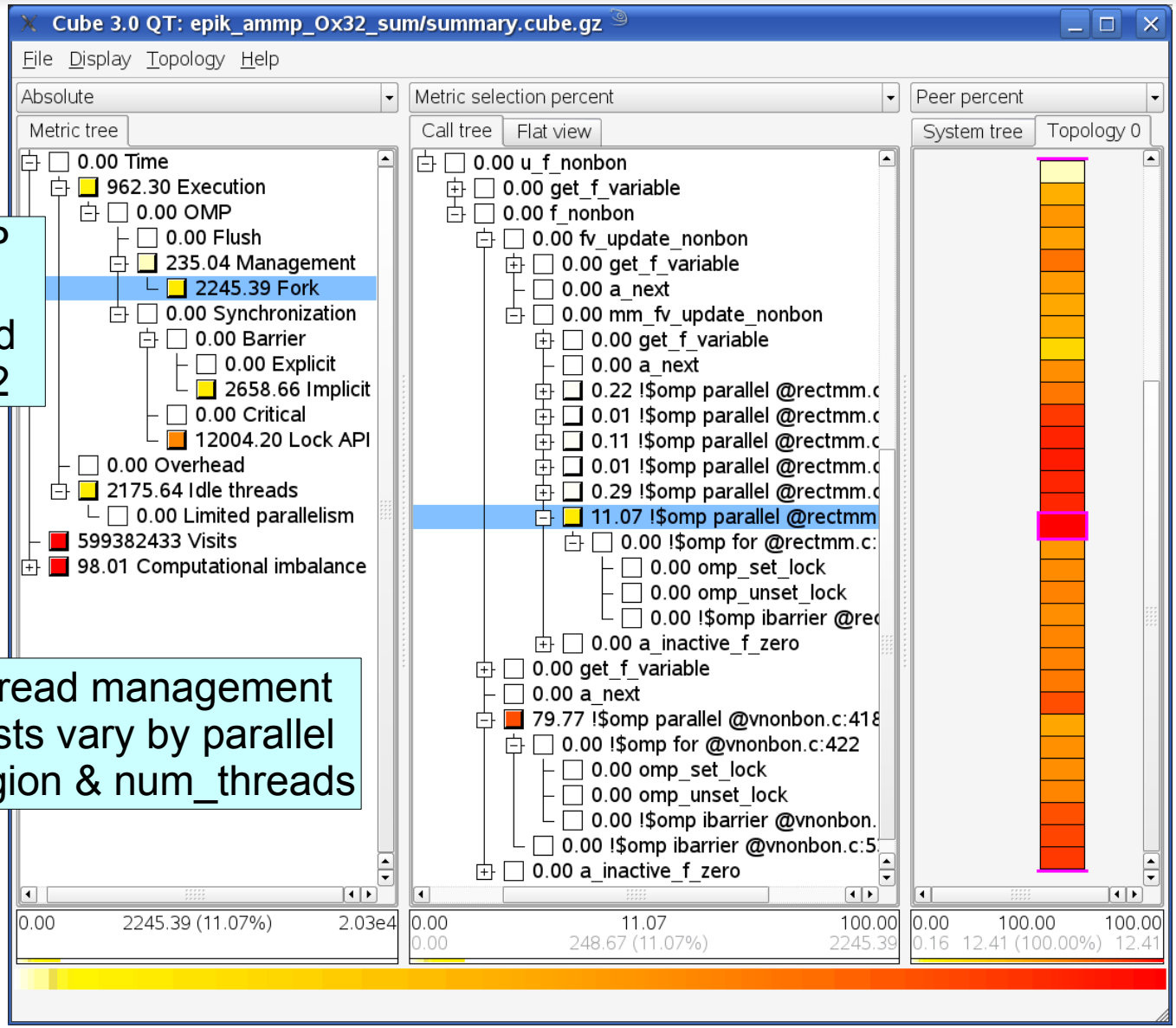
Lots of explicit lock synchronization is a scalability inhibitor



ammp on jupiter@32 OpenMP fork analysis

OpenMP metrics reworked with v1.2

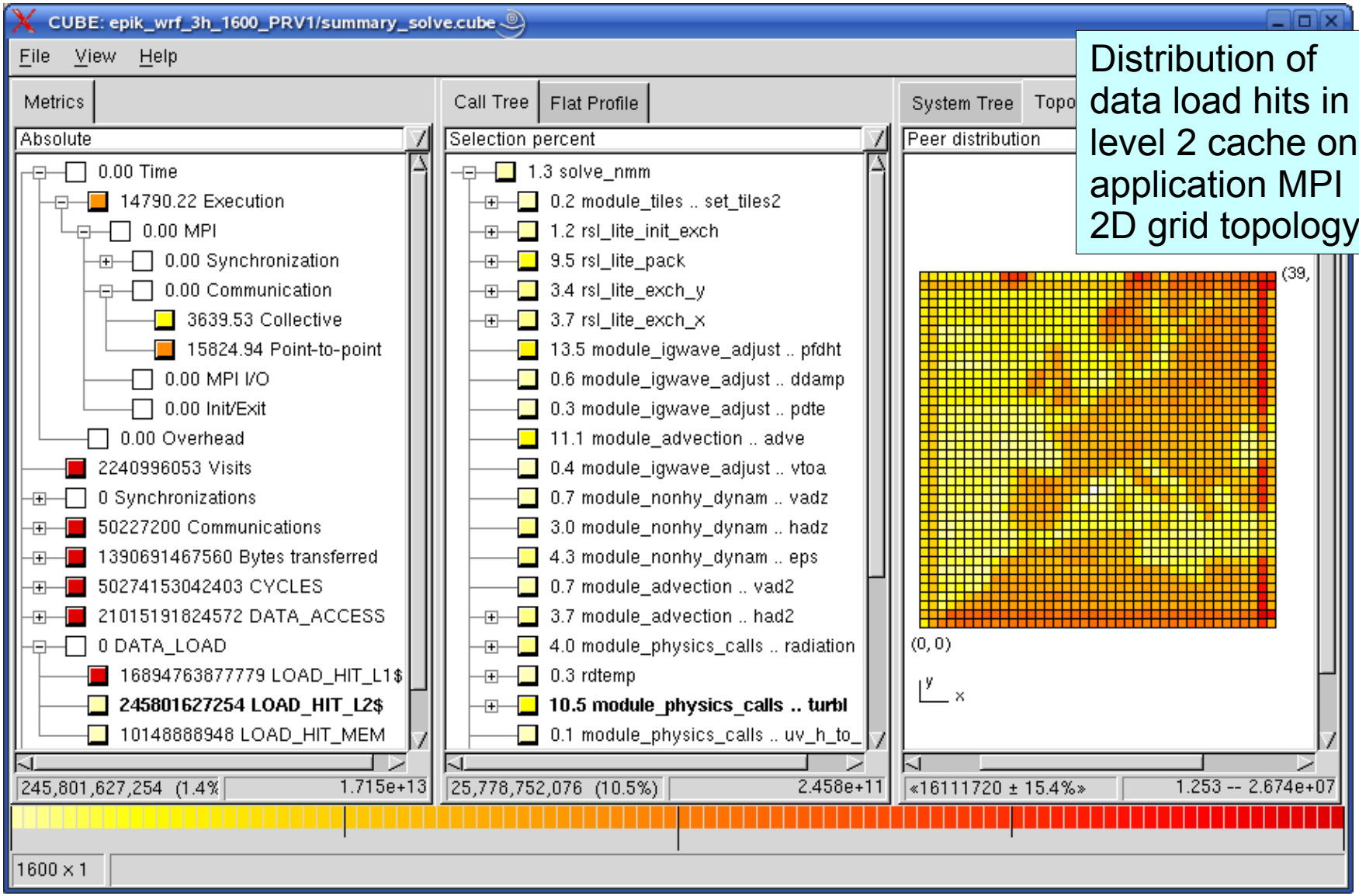
Thread management costs vary by parallel region & num_threads



WRF/MareNostrum case study

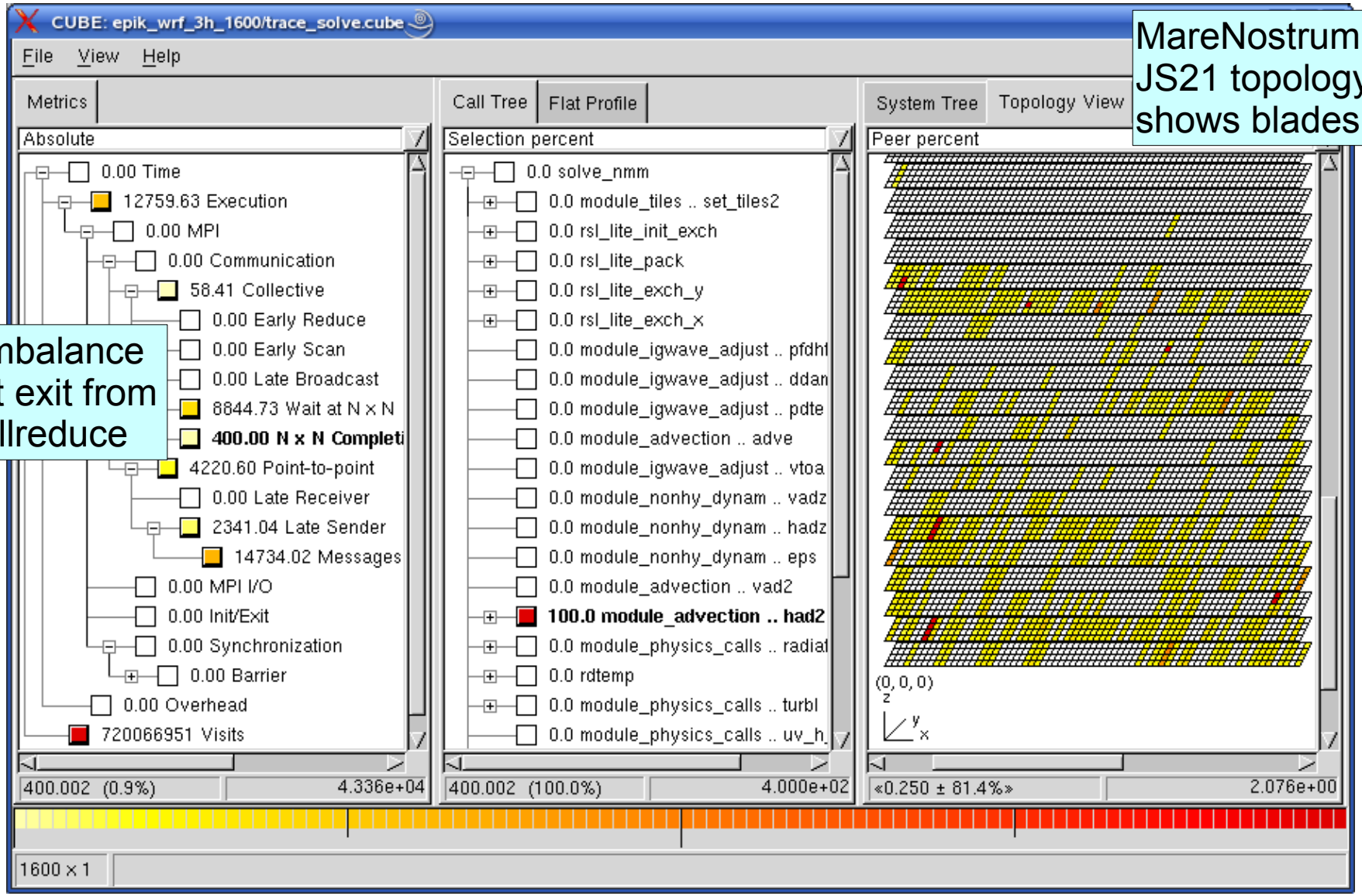
- Numerical weather prediction
  - public domain code developed by US NOAA
  - flexible, state-of-the-art atmospheric simulation
  - Non-hydrostatic Mesoscale Model (NMM)
- MPI parallel version 2.1.2 (Jan-2006)
  - >315,000 lines (in 480 source modules): 75% Fortran, 25% C
- Eur-12km dataset configuration
  - 3-hour forecast (360 timesteps) with checkpointing disabled
- Run with 1600 processes on MareNostrum
  - IBM BladeCenter cluster at BSC
- Scalasca summary and trace measurements
  - 15% measurement dilation with 8 hardware counters
  - 23GB trace analysis in 5 mins

WRF on MareNostrum@1600 with HWC metrics



Distribution of data load hits in level 2 cache on application MPI 2D grid topology

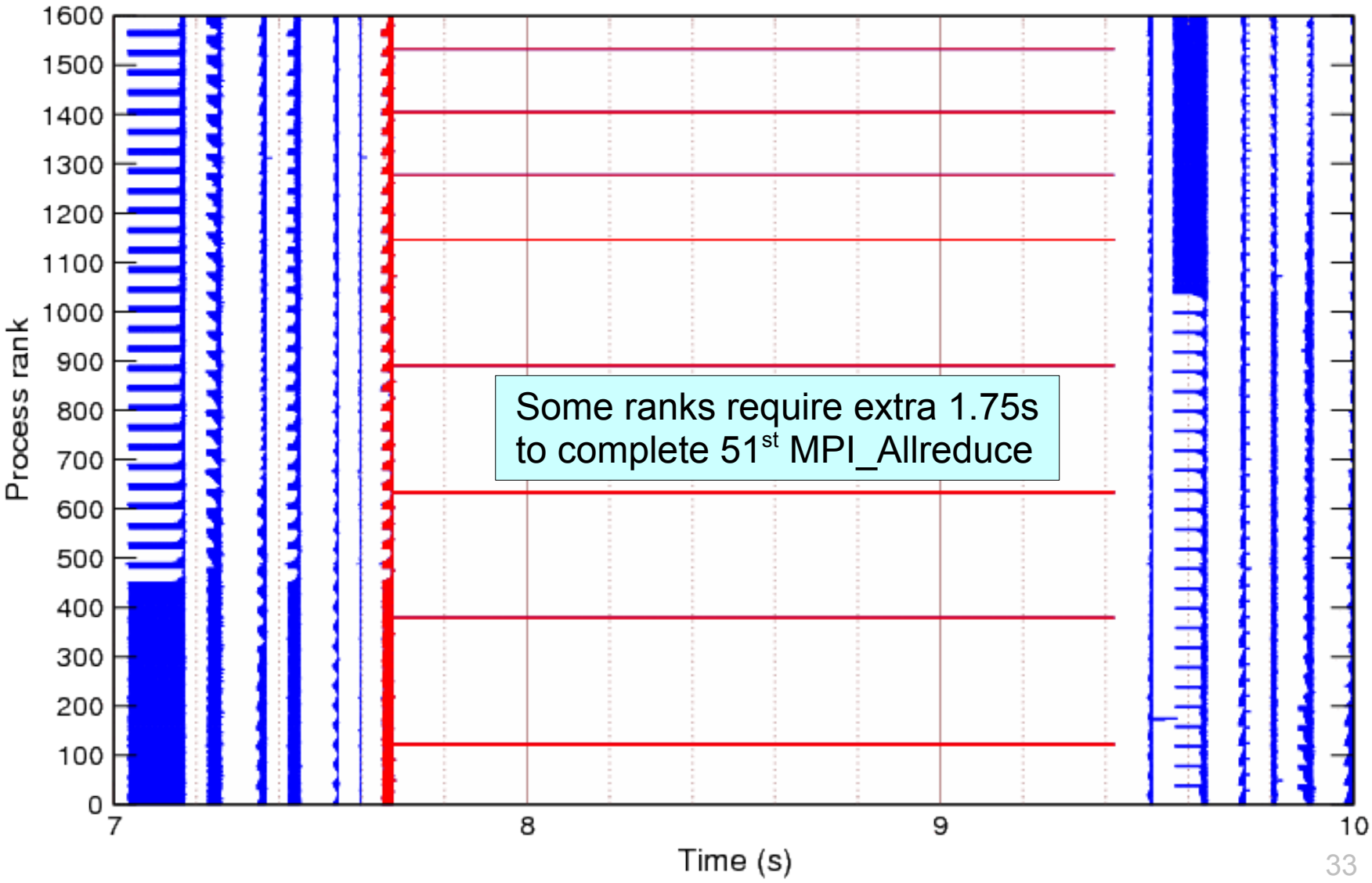
WRF on MareNostrum@1600 trace analysis



Imbalance at exit from Allreduce

MareNostrum JS21 topology shows blades

WRF on MareNostrum@1600 time-line extract

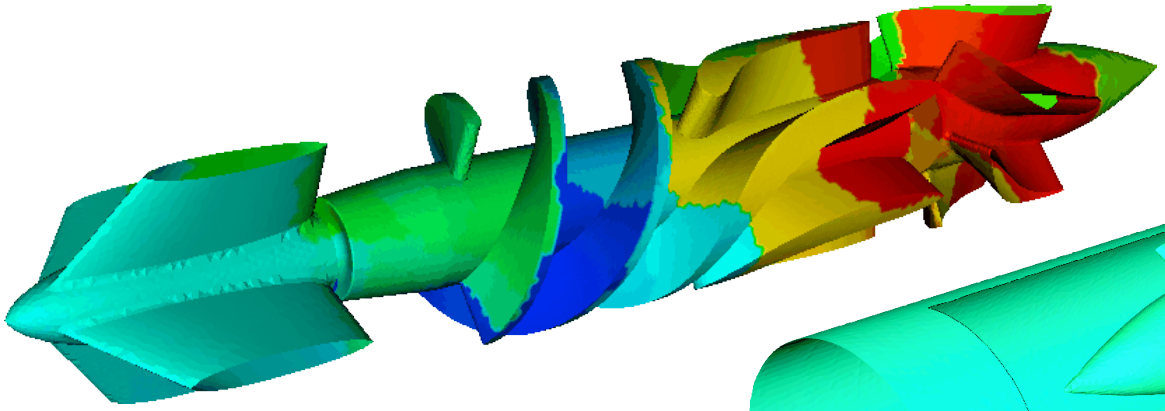


WRF/MareNostrum experience

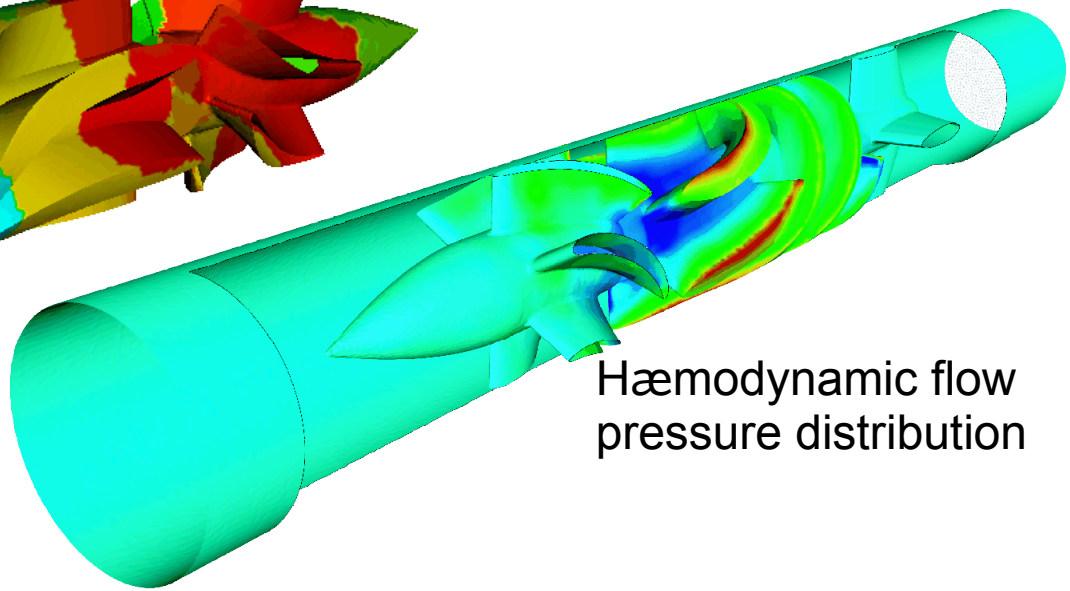
- Limited system I/O requires careful management
  - Selective instrumentation and measurement filtering
- PowerPC hardware counter metrics included in summary
  - Memory/cache data access hierarchy constructed
- Automated trace analysis quantified impact of imbalanced exit from MPI_Allreduce in “NxN completion time” metric
  - Intermittent but serious MPI library/system problem, that restricts application scalability
  - Only a few processes directly impacted, however, communication partners also quickly blocked
- Presentation using logical and physical topologies
  - MPI Cartesian topology provides application insight
  - Hardware topology helps localize system problems

XNS on BlueGene/L case study

- CFD simulation of unsteady flows
  - developed by RWTH CATS group of Marek Behr
  - exploits finite-element techniques, unstructured 3D meshes, iterative solution strategies
- MPI parallel version (Dec-2006)
  - >40,000 lines of Fortran & C
  - DeBakey blood-pump dataset (3,714,611 elements)

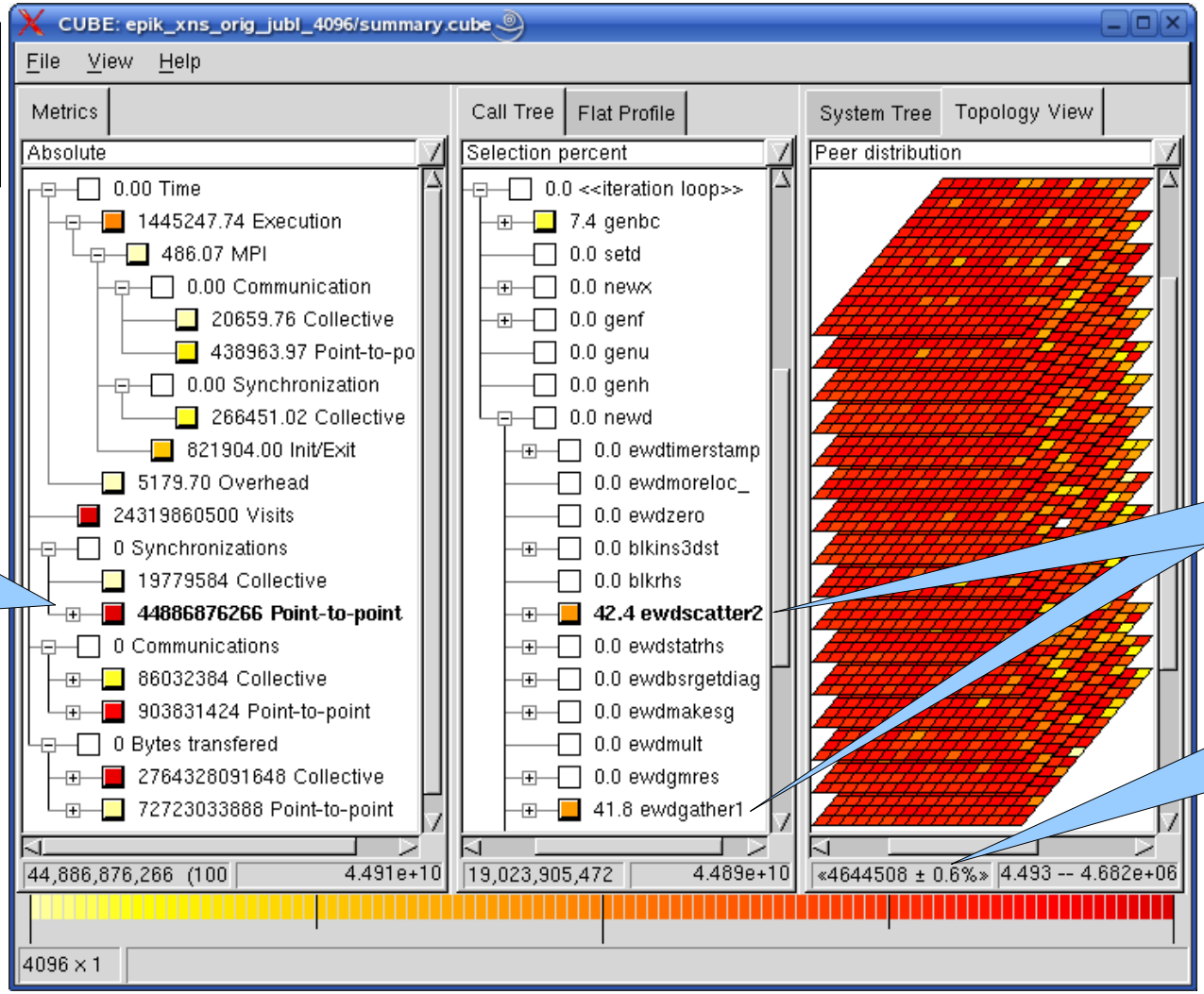


Partitioned finite-element mesh



Hæmodynamic flow pressure distribution

XNS-DeBakey on jubl@4096 summary analysis



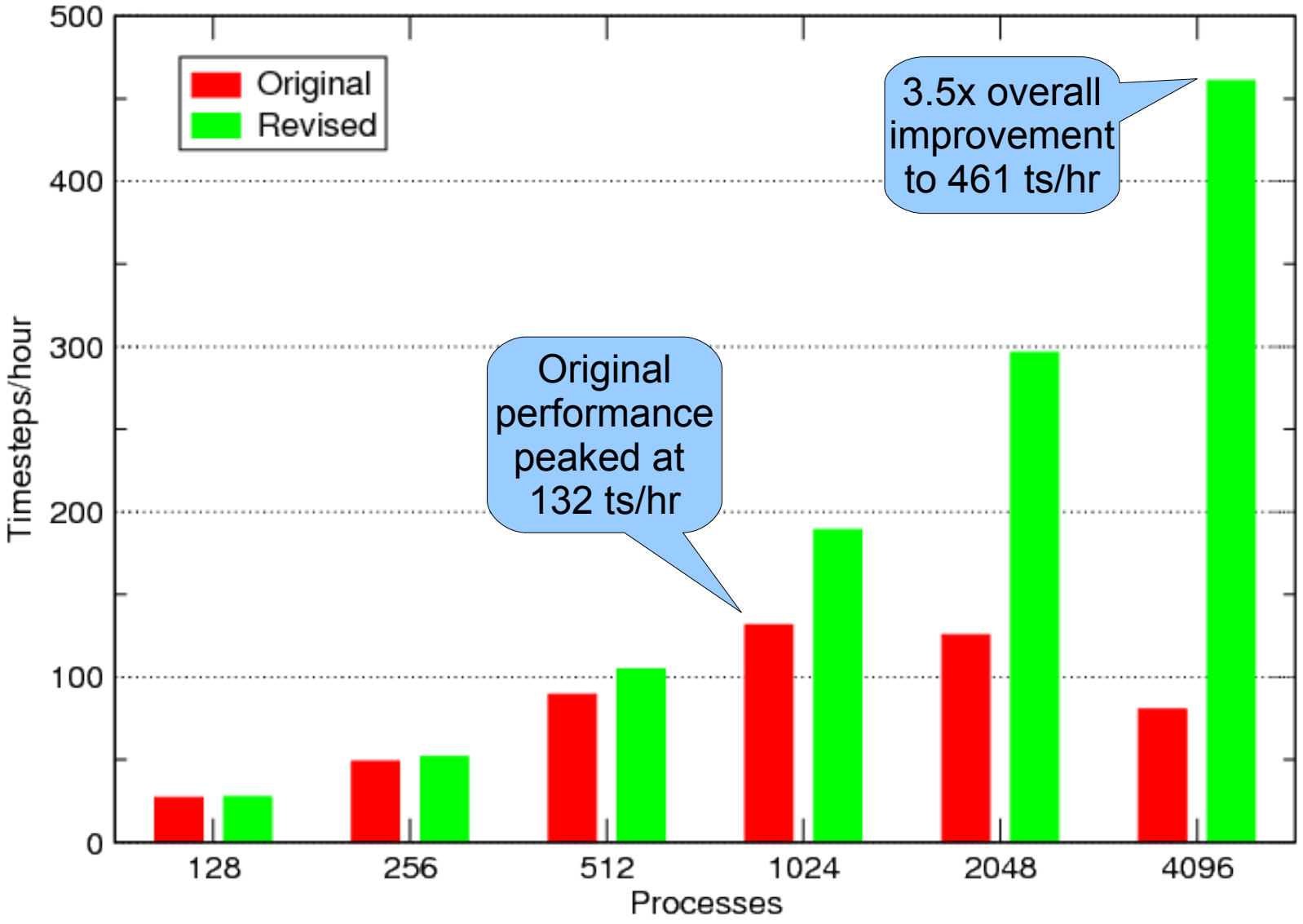
Point-to-point msgs w/o data

Masses of P2P synch operations

Primarily in scatter & gather

Processes all equally responsible

XNS-DeBakey scalability on BlueGene/L



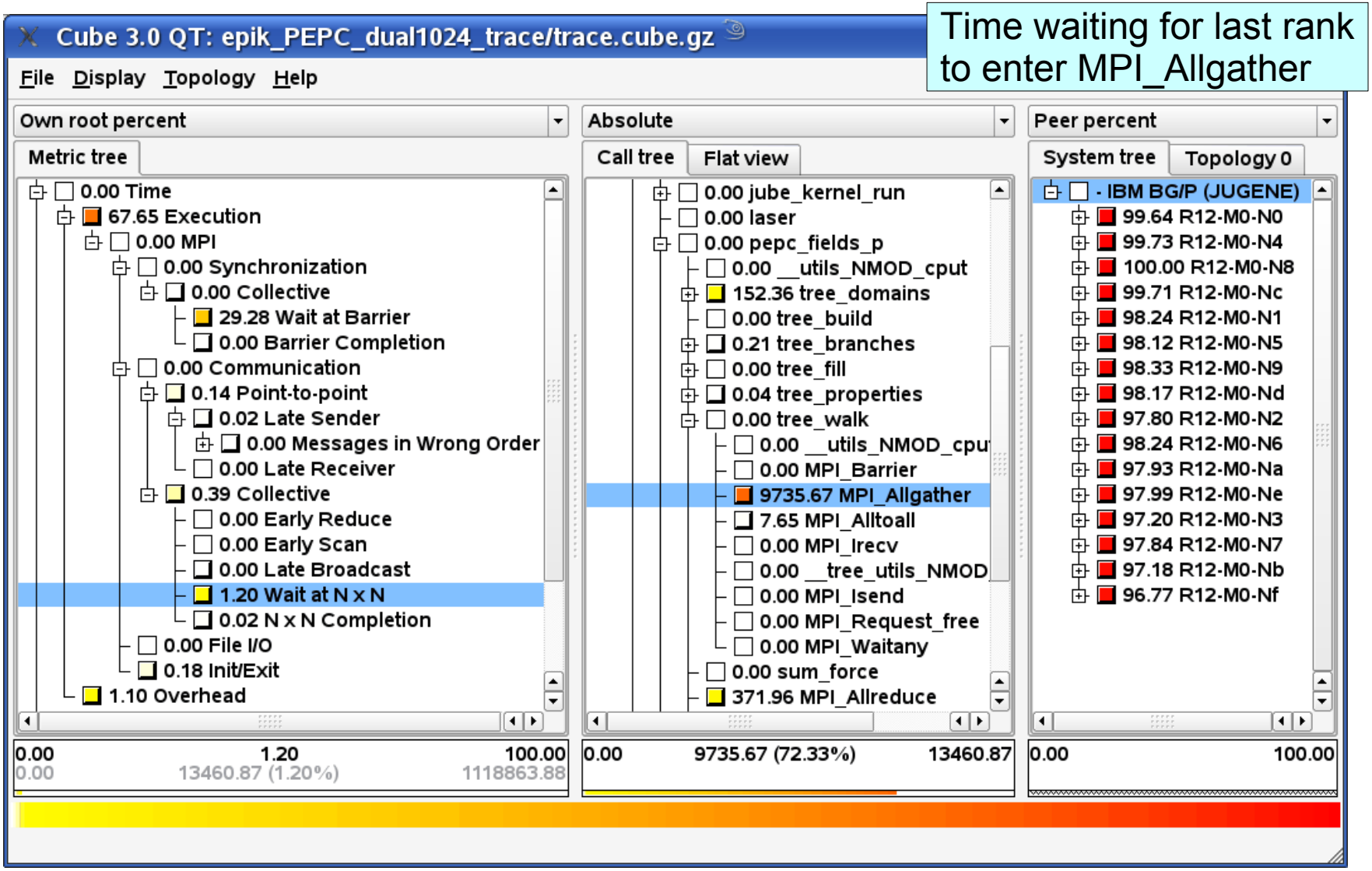
XNS on BlueGene/L experience

- Globally synchronized high-resolution clock facilitates efficient measurement & analysis
- Restricted compute node memory limits trace buffer size and analyzable trace size
- Summarization identified bottleneck due to unintended P2P synchronizations (messages with zero-sized payload)
- 4x solver speedup after replacing MPI_Sendrecv operations with size-dependant separate MPI_Send and MPI_Recv
- Significant communication imbalance remains due to mesh partitioning and mapping onto processors
- MPI_Scan implementation found to contain implicit barrier
  - responsible for 6% of total time with 4096 processes
  - decimated when substituted with simultaneous binomial tree

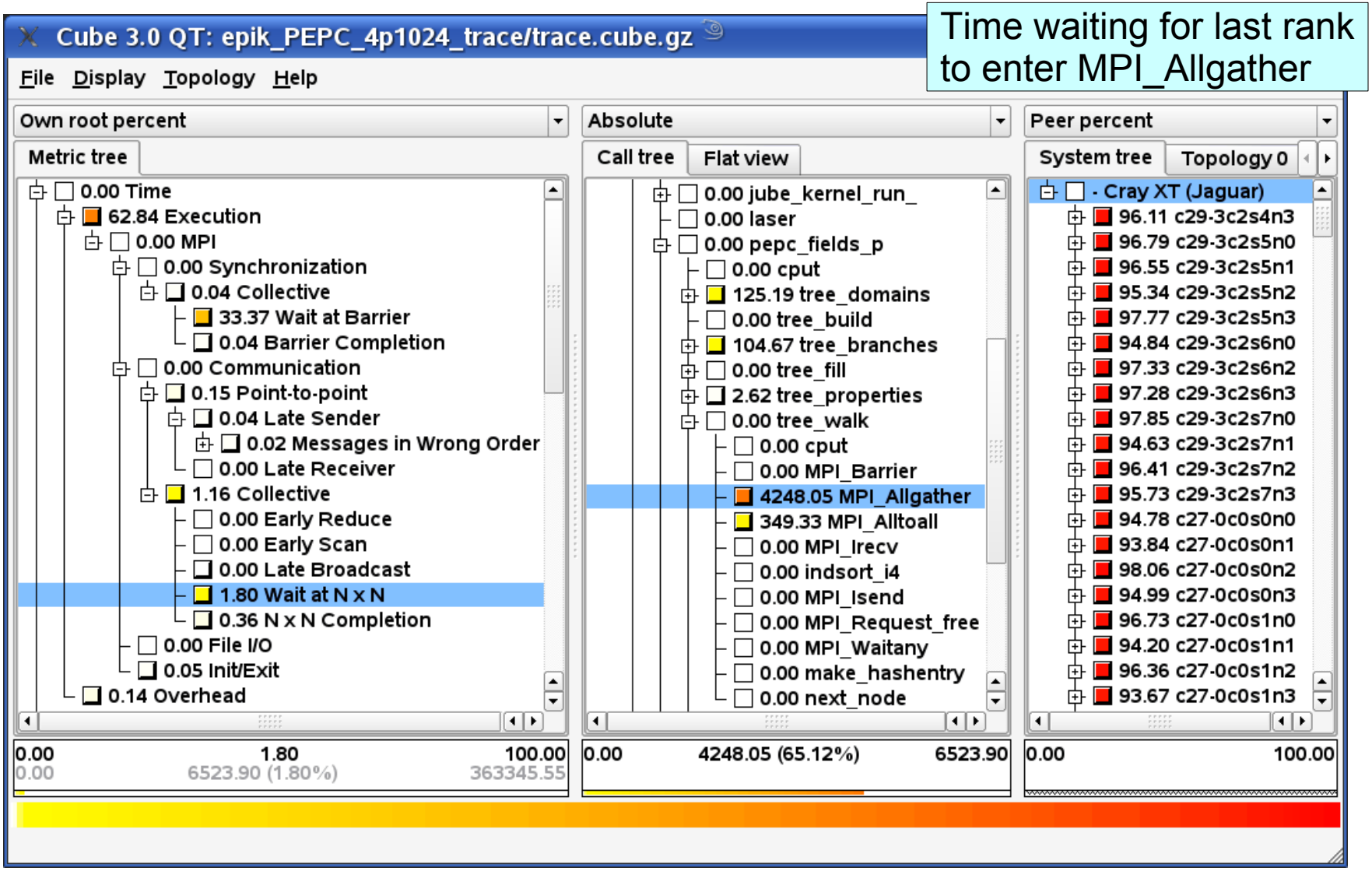
PEPC-B on BG/P & Cray XT case study

- Coulomb solver used for laser-plasma simulations
  - Developed by Paul Gibbon (JSC)
  - Tree-based particle storage with dynamic load-balancing
- MPI version
  - PRACE benchmark configuration, including file I/O
- Run on BlueGene/P in dual mode with 1024 processes
  - 2 processes per quad-core PowerPC node, 1100 seconds
  - IBM XL compilers, MPI library and torus/tree interconnect
- Run on Cray XT in VN (4p) mode with 1024 processes
  - 4 processes per quad-core Opteron node, 360 seconds
  - PGI compilers and Cray MPI, CNL, SeaStar interconnect

PEPC@1024 on BlueGene/P: Wait at NxN time



PEPC@1024 on Cray XT4: Wait at NxN time



Time waiting for last rank to enter MPI_Allgather

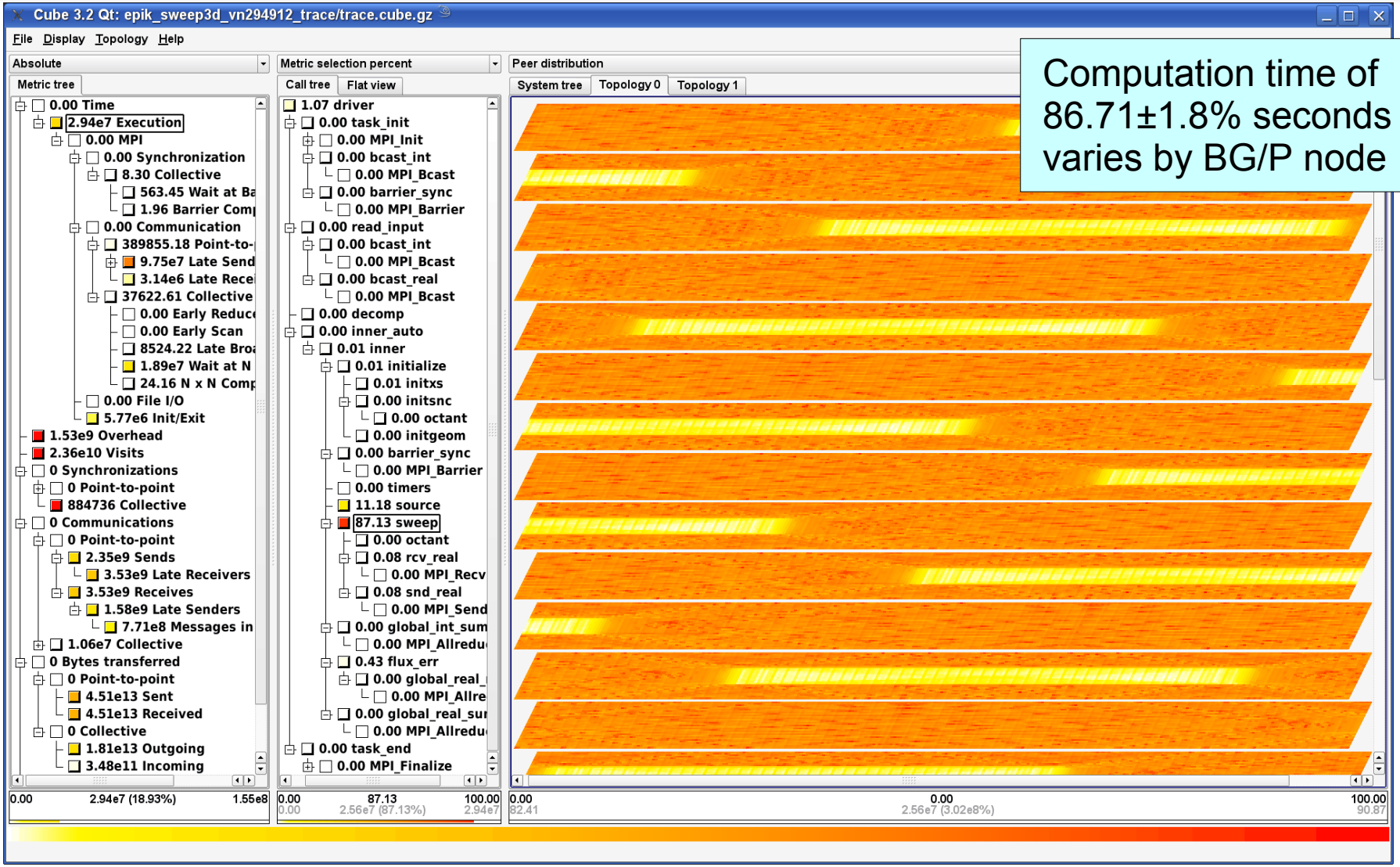
PEPC-B on BG/P & Cray XT experience

- Despite very different processor and network performance, measurements and analyses can be easily compared
  - different compilers affect function naming & in-lining
- Both spend roughly two-thirds of time in computation
  - tree_walk has expensive computation & communication
- Both waste 30% of time waiting to enter MPI_Barrier
  - not localized to particular processes, since particles are regularly redistributed
- Most of collective communication time is also time waiting for last ranks to enter MPI_Allgather & MPI_Alltoall
  - imbalance for MPI_Allgather twice as severe on BlueGene/P, however, almost 50x less for MPI_Alltoall
  - collective completion times also notably longer on Cray XT

Sweep3d on BlueGene/P case study

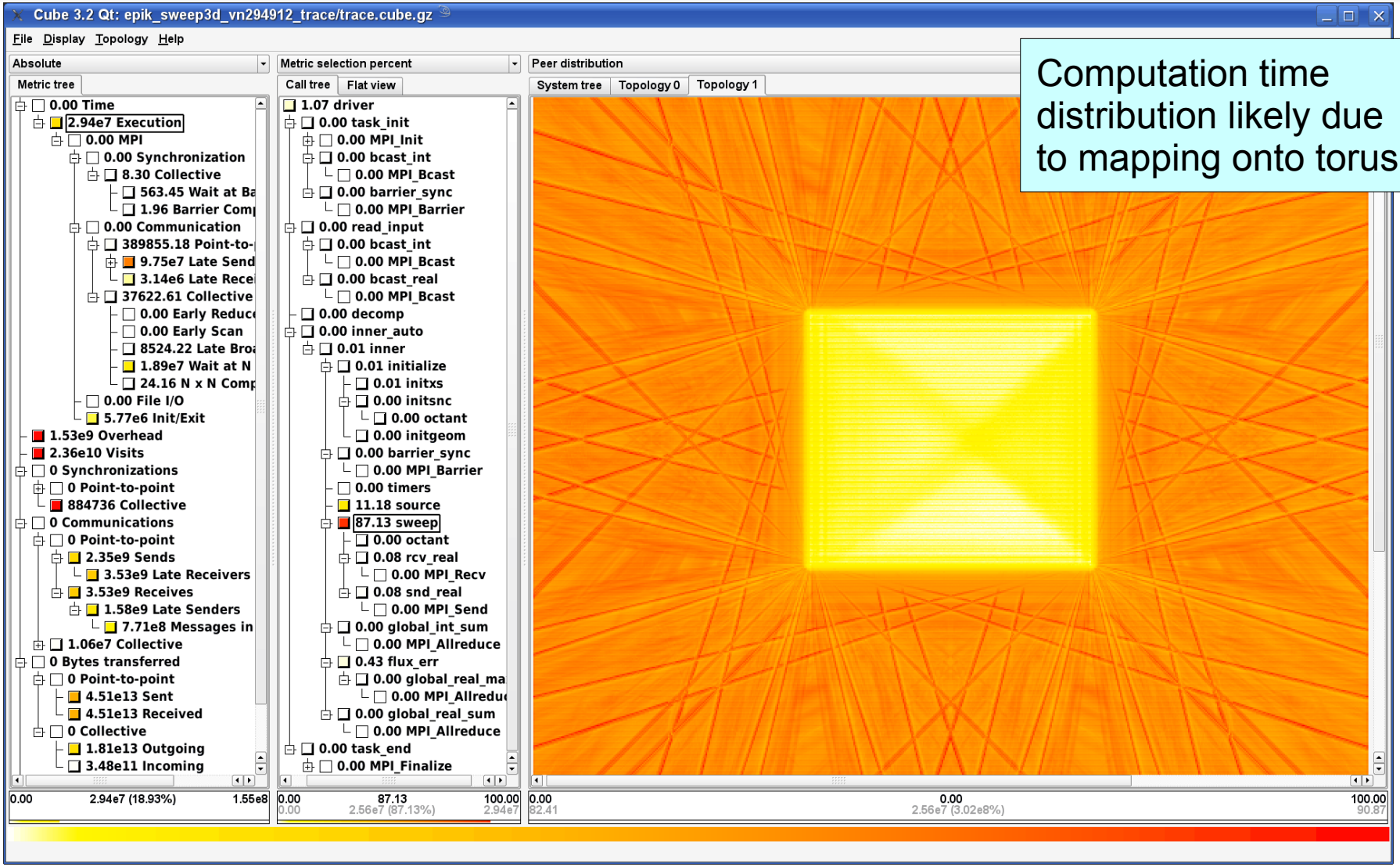
- 3D neutron transport simulation
  - ASC benchmark
  - direct order solve uses diagonal sweeps through grid cells
- MPI parallel version 2.2b using 2D domain decomposition
  - ~2,000 lines (12 source modules), mostly Fortran77
- Run on IBM BlueGene/P in VN mode with 288k processes
  - 790GB trace written in 47 minutes, analyzed in 7 minutes
    - plus 86 minutes just to create 294,912 files (one per MPI rank)
    - SIONlib being developed to address management of sets of files
  - Mapping of 576x512 grid of processes onto 3D physical torus results in regular pattern of performance artifacts

sweep3d on jugene@288k trace analysis



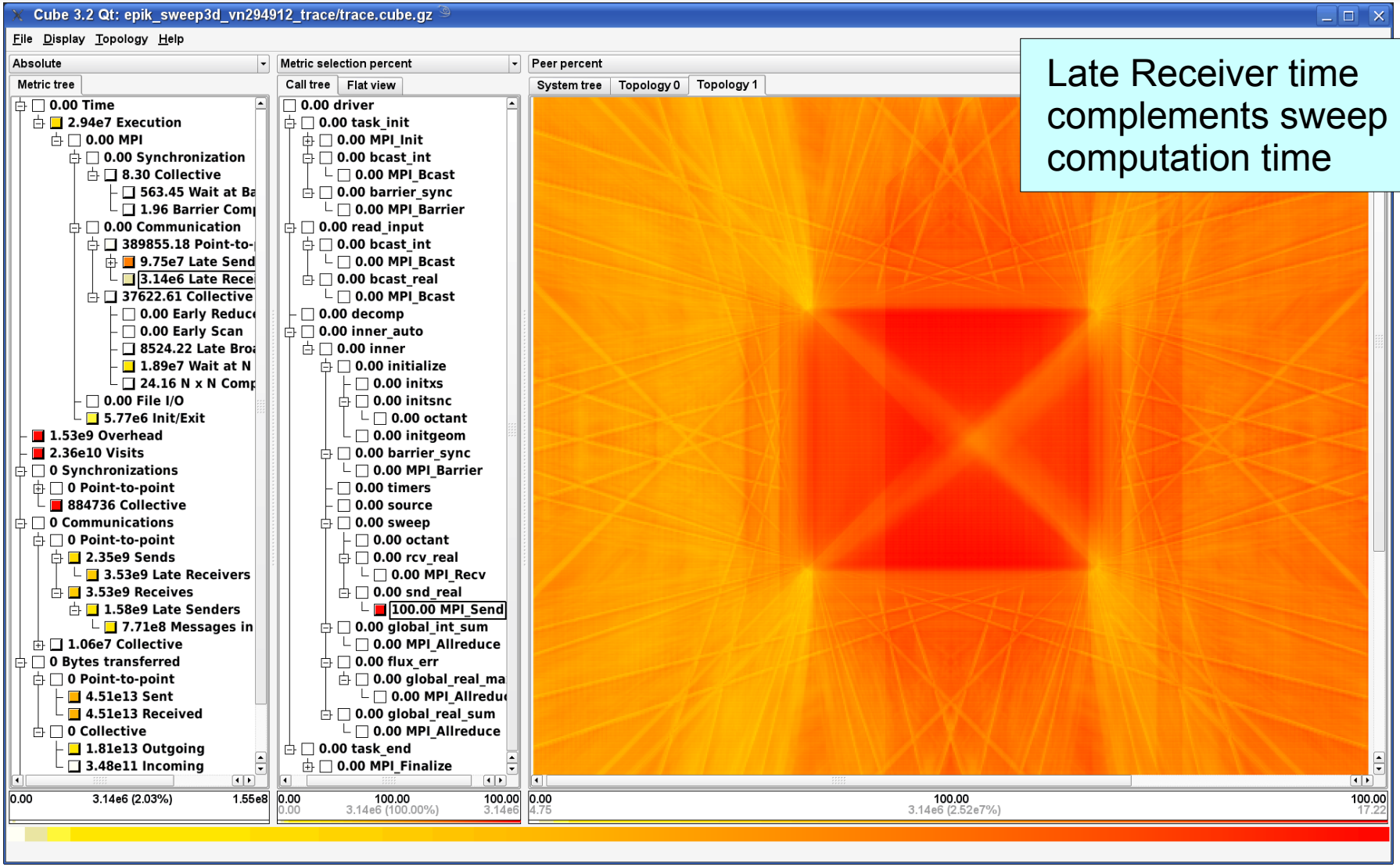
Computation time of 86.71±1.8% seconds varies by BG/P node

sweep3d on jugene@288k trace analysis



Computation time distribution likely due to mapping onto torus

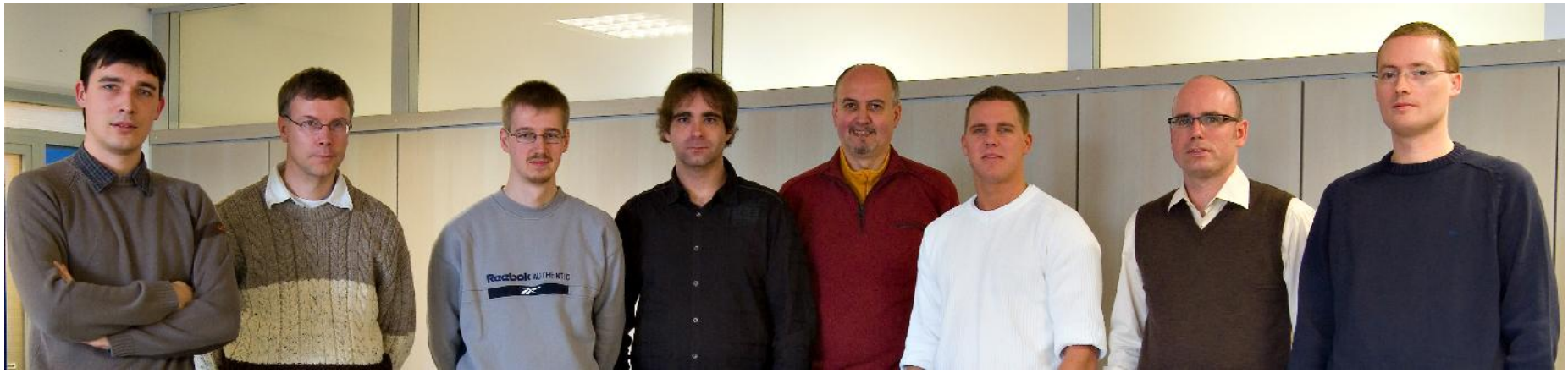
sweep3d on jugene@288k trace (wait) analysis



Late Receiver time complements sweep computation time

Acknowledgements

- The application and benchmark developers who generously provided their codes and/or measurement archives
- The facilities who made their HPC resources available and associated support staff who helped us use them effectively
  - ALCF, BSC, CSC, CSCS, EPCC, JSC, HLRN, HLRS, ICL, LRZ, NCAR, NCCS, NICS, RWTH, RZG, SARA, TACC, ZIH
    - Access & usage supported by European Union, German and other national funding organizations
- The Scalasca development team



Scalable performance **a**nalysis of **la**rge-**sc**ale parallel **a**pplications

- toolset for scalable performance measurement & analysis of MPI, OpenMP & hybrid parallel applications
- supporting most popular HPC computer systems
- available under New BSD open-source license
- sources, documentation & publications:
  - http://www.scalasca.org
  - mailto: scalasca@fz-juelich.de