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Extreme-Scale In-Situ Visualization of Turbulent Flows on IBM Blue Gene/Q JUQUEEN

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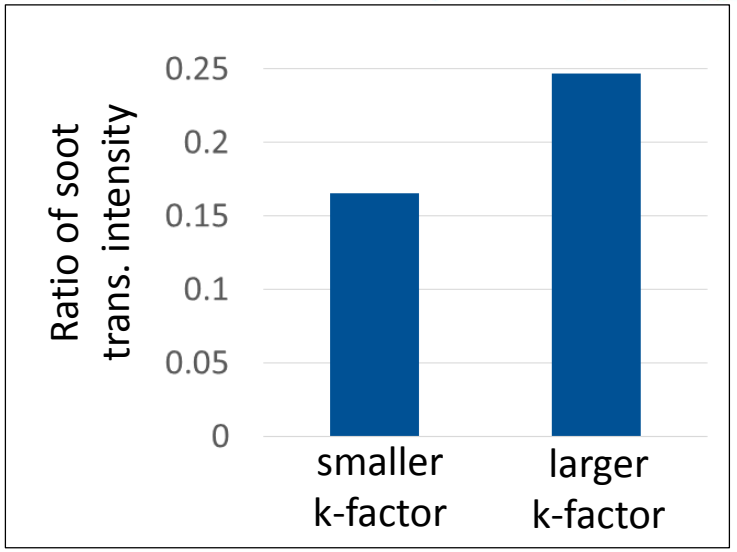
June 23th, 2016 Workshop on Exascale Multi/Many Core Computing Systems (E-MuCoCoS)

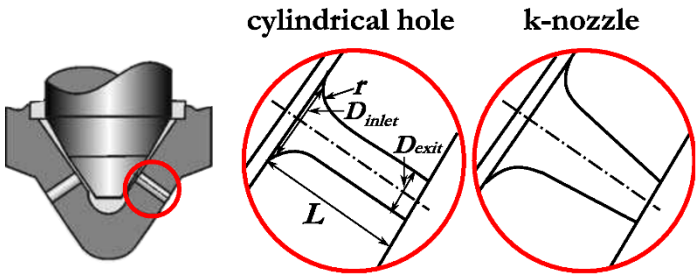
Motivation

spray injection & droplet formation

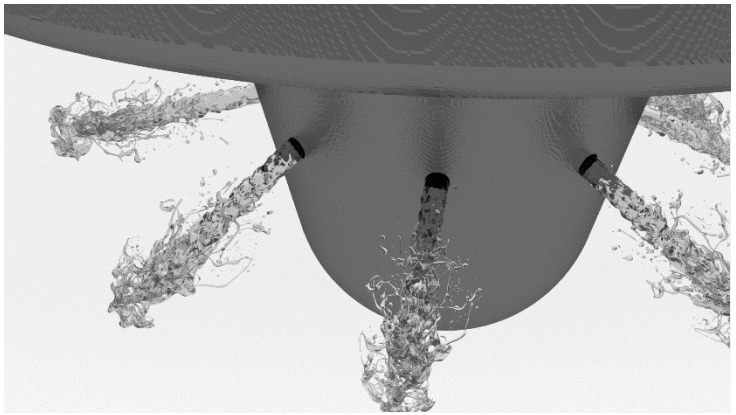
- Geometry of injection systems increasingly complex
- Emission and pollutant formation strongly depend on injection systems
- Experimental investigation of geometry impact very challenging



High-fidelity spray simulations required!



Baumgarten, C., Mixture formation in internal combustion engines, Springer, 2006.

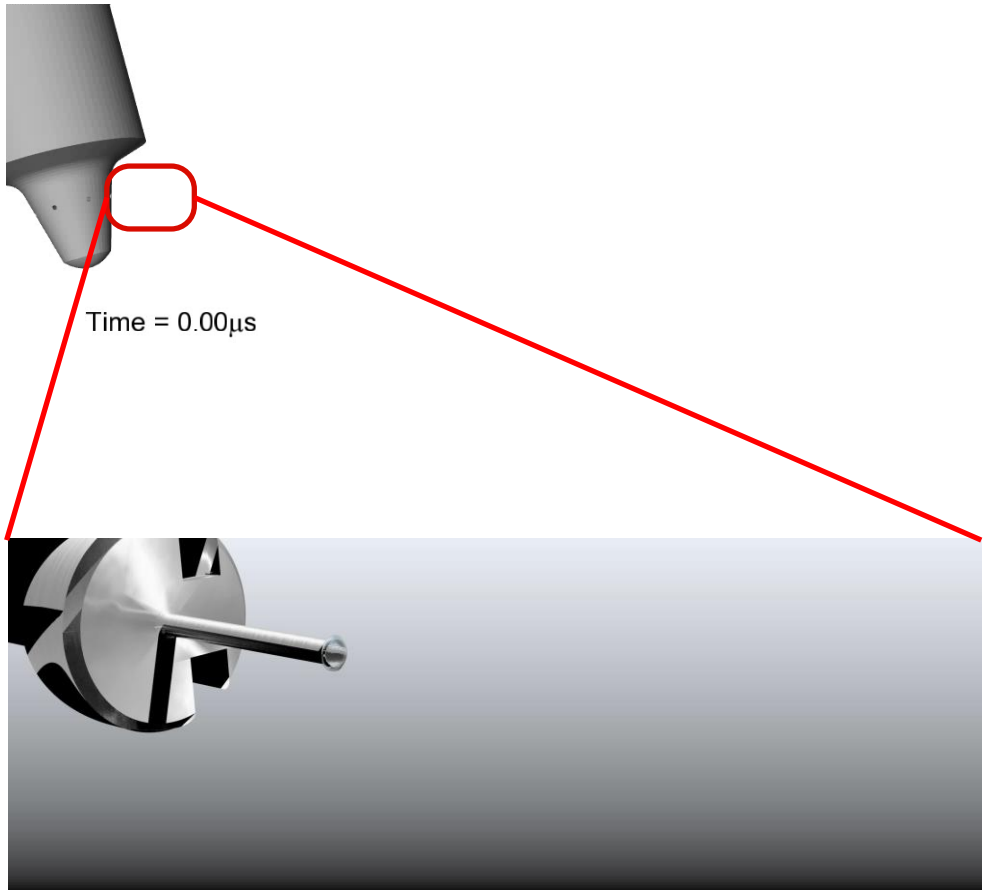


Aye, M.M. et al., Studying the influence of k-factor of different nozzles on spray and combustion under diesel engine-like conditions in a high pressure spray chamber (submitted).

Motivation

spray injection & droplet formation

- Experimental investigation of injection systems very challenging due to small length (~100 µm) and high velocity scales (~600 m/s).
- Highly resolved simulations result in large amount of data which can be reduced with in-situ visualization.
- Predictive simulations using in-situ visualization and studying injection systems and resulting cavitation give more insight.

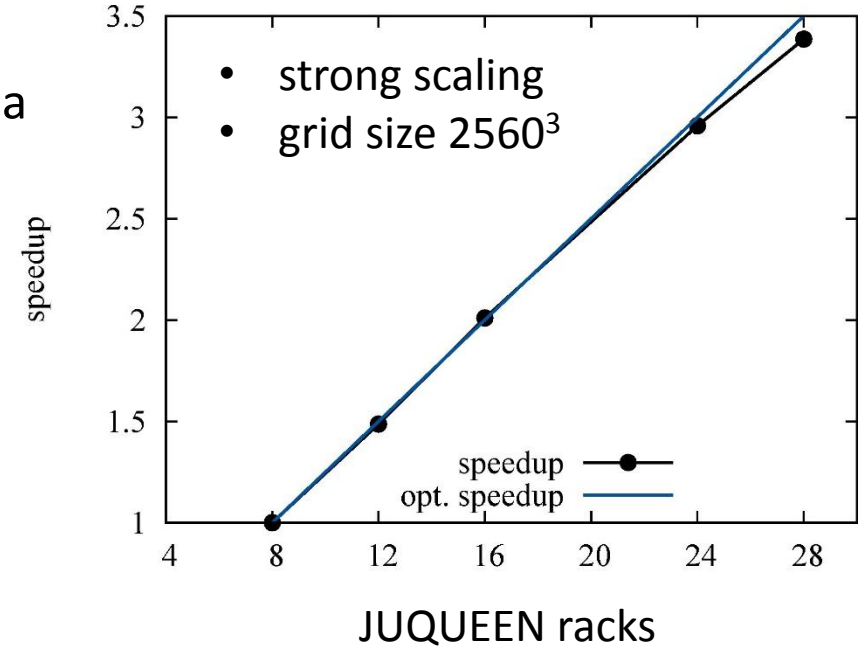


Le Chenadec, V. and Pitsch, H., "A 3D Unsplit Forward/Backward Volume-of-Fluid Approach and Coupling to the Level Set Method," Journal of Computational Physics 233:10-33, 2013
Le Chenadec, V. and Pitsch, H., "A monotonicity preserving conservative sharp interface flow solver for high density ratio two-phase flows," Journal of Computational Physics 249:185-203, 2013

Numerical Simulation

CIAO – multiphysics solver

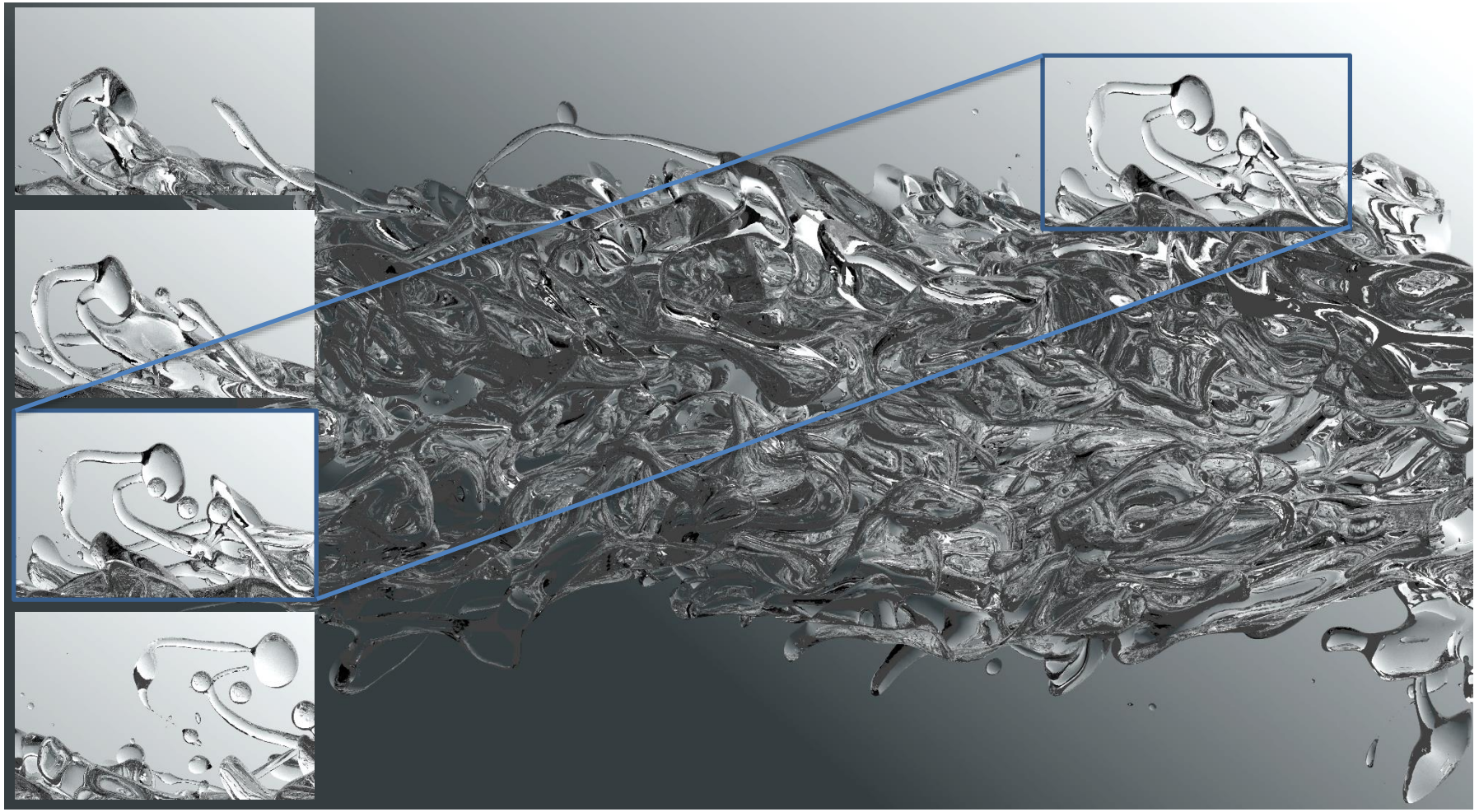
- **C**ompressible/**I**ncompressible **A**RTS with **O**verset-meshes
  - ARTS: **A**dvanced **R**eactive **T**urbulent **S**imulation
- Multiphysics, multiscale Navier-Stokes solver (LES and DNS) for turbulent reacting flows in complex geometries
- Low Mach & Compressible
- Structured Finite Difference Schema
- Fortran & MPI
- Main applicatoin developer
  - Prof. Heinz Pitsch
    Mathis Bode, Tobias Falkenstein
    Institute for Combustion Technology
    RWTH Aachen University, Germany
  - Prof. Seongwon Kang
    Department of Mechanical Engineering
    Sogang University, Korea



JUQUEEN HiQ-Club http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/_node.html
JUQUEEN Extreme Scaling Workshop 2016: http://hdl.handle.net/2128/9990

Numerical Simulation

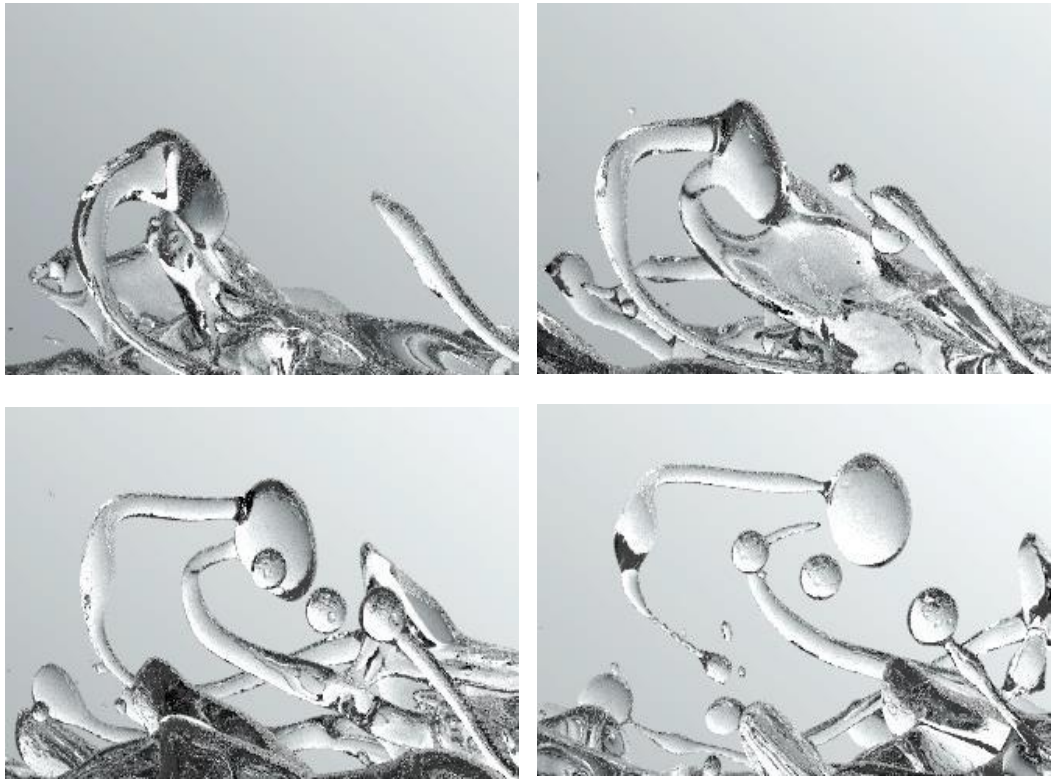
CIAO – multiphysics solver



Numerical Simulation

CIAO – multiphysics solver

- Single droplets are identified with VoF and LS fields
- A complete droplet formation evolves over 3000 time steps.
- To follow the evolution of a droplet formation, every 100 time step has to be visualized



Challenges …

why not stick to the established workflow

JÜLICH FORSCHUNGSZENTRUM

Institut für Technische Verbrennung | RWTH AACHEN UNIVERSITY

… of the setup and code

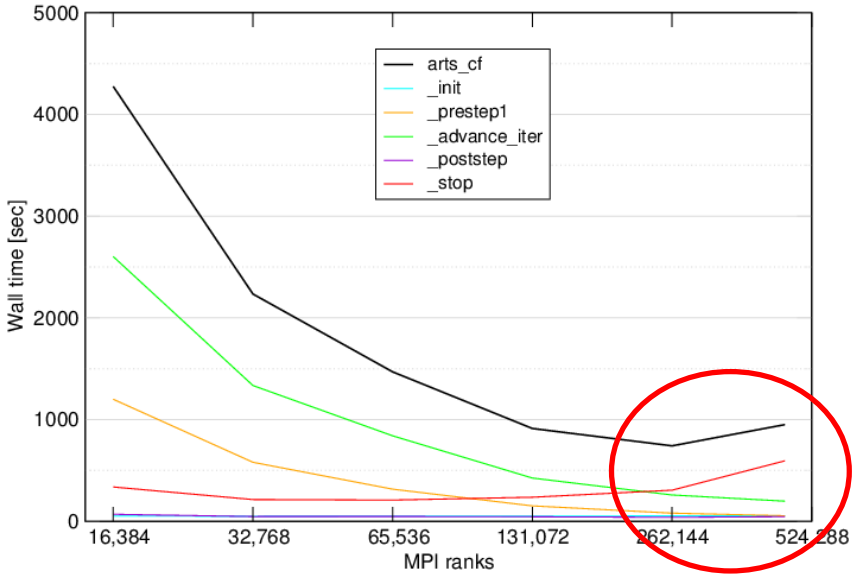
- High spatial resolution required
  - Large Reynolds numbers
- High temporal resolution required
  - Fast processes
  - droplet evolution or interest

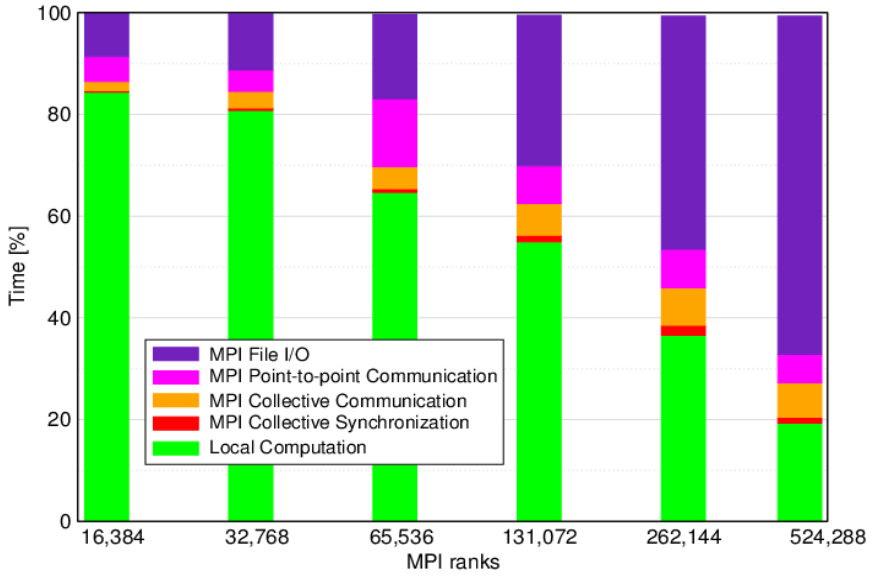
Current production case:

resolution: 4096 x 2048 x 2048
scalars / grid point: 68
dataset size of single time step : 8.5 TiB

Challenges

why not stick to the established workflow





For a reference case with a 1024^3 grid dumping data every 100 iteration:

- Excellent scaling of solver
- File writing dumping output is bottleneck at scale

dump simulation data with high temporal resolution not possible

Scalasca

scalable performance analysis

Toolset for scalable performance analysis of large-scale parallel applications

- capable of runtime summary profile and parallel event trace analyses
- for MPI, OpenMP, Pthreads and mixed MPI+threading
  - *successfully used with 1.75M threads and 1.28M processes*
- supporting most popular HPC computer systems
  - *Blue Gene/Q, Cray, K computer, Stampede, Tianhe, etc.*
- using **Score-P** community-developed instrumentation and measurement infrastructure, and **CUBE** analysis report explorer and utilities
  - *compatible with TAU & Vampir*
- available under New BSD open-source license
- http://www.scalasca.org (mailto: scalasca@fz-juelich.de)

Scalasca (CUBE)

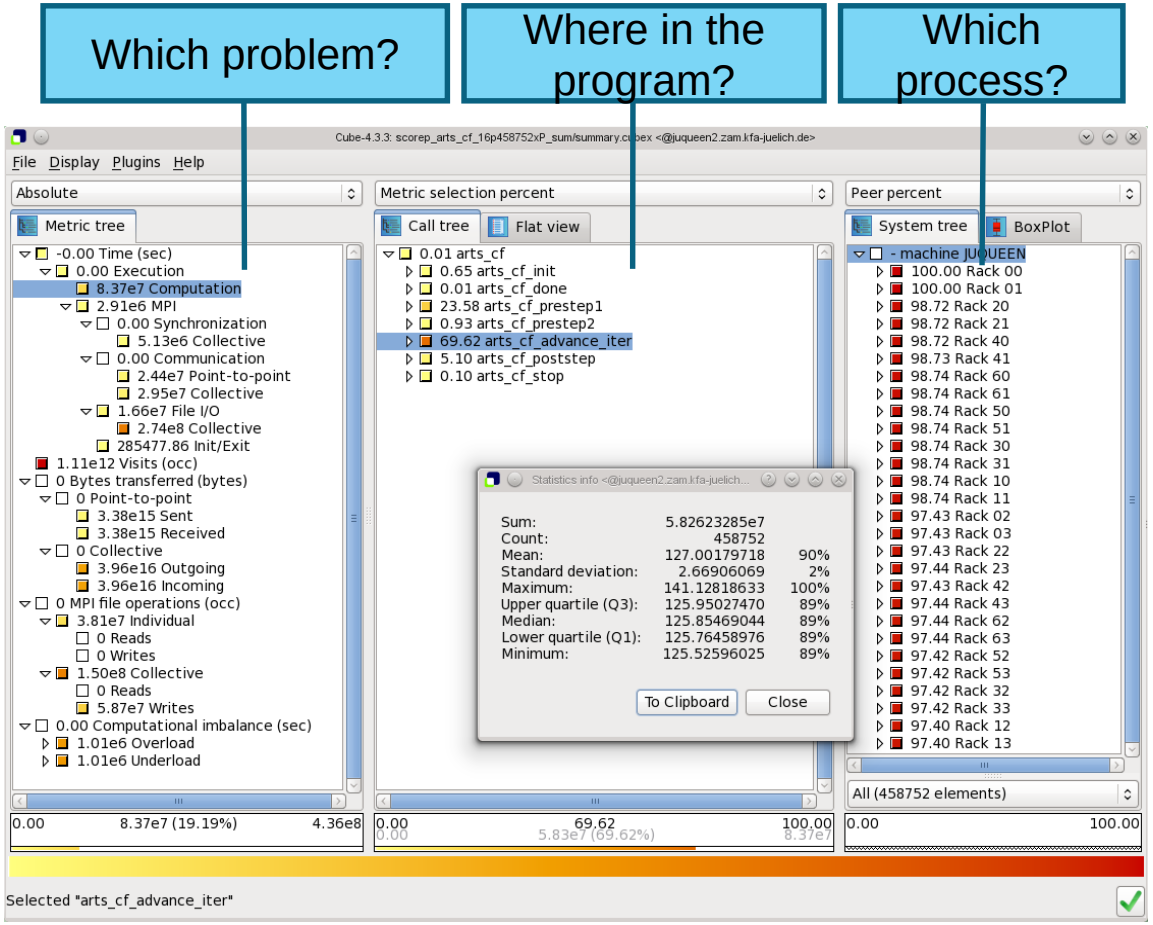
execution profile summary

Measurement of

- 458,752 MPI ranks
- (28 racks) on BG/Q
- 1 billion grid cells
- I/O every 100 iteration

19% of total CPU time is computation

- 70% of the compute time is in the WENO5 solver
- Variation by process from 125 to 141 sec., (fairly well balanced)



Hierarchies of metrics

Tree of execution call-paths (values for selected metric)

Distribution of MPI rank severity values

Scalasca (CUBE)

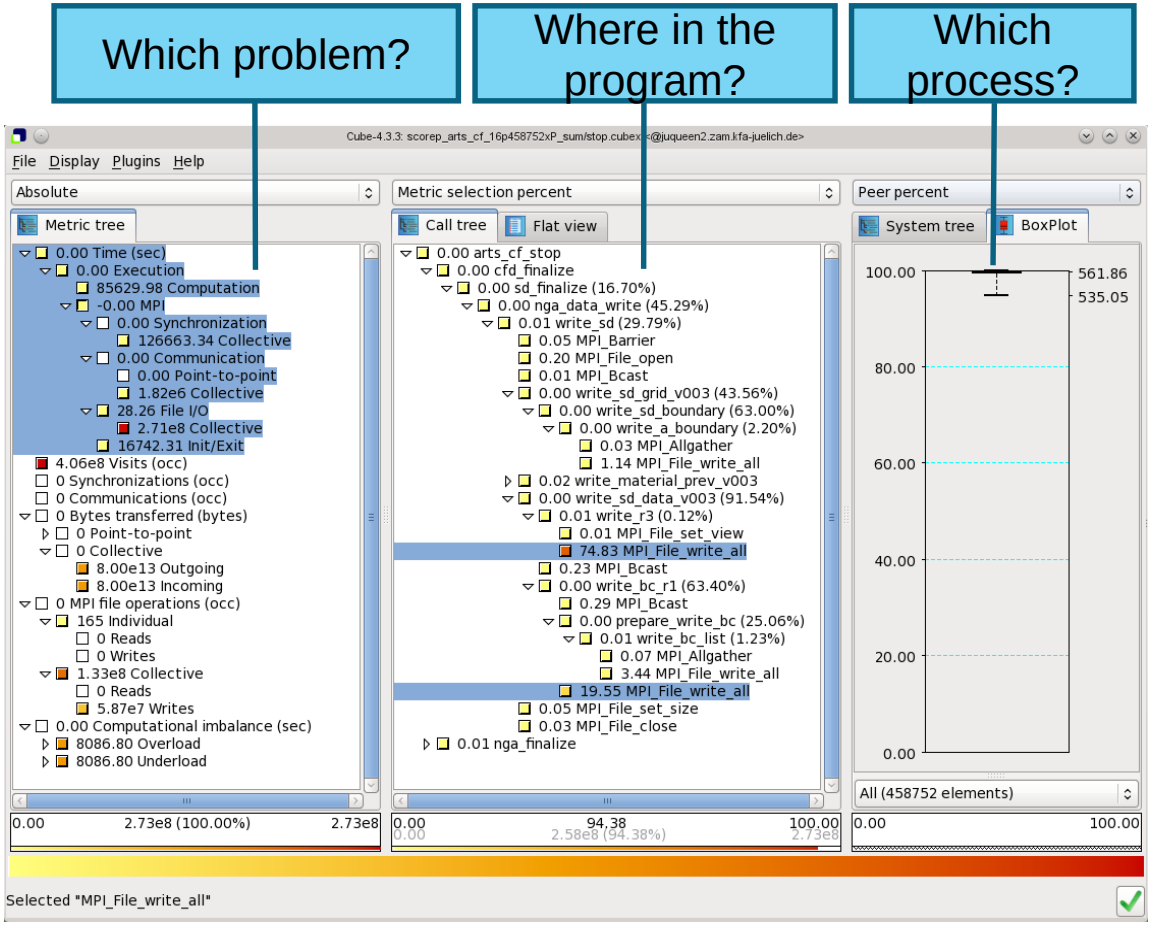
execution profile summary

Measurement of

- 458,752 MPI ranks
- (28 racks) on BG/Q
- 1 billion grid cells
- I/O every 100 iteration

81% of total CPU time is MPI

- 70% of the MPI time is writing to single shared file.
- 99% of I/O time is spent in calls to the MPI File I/O collective *MPI_File_write_all()*



Hierarchies of metrics

Tree of execution call-paths (values for selected metric)

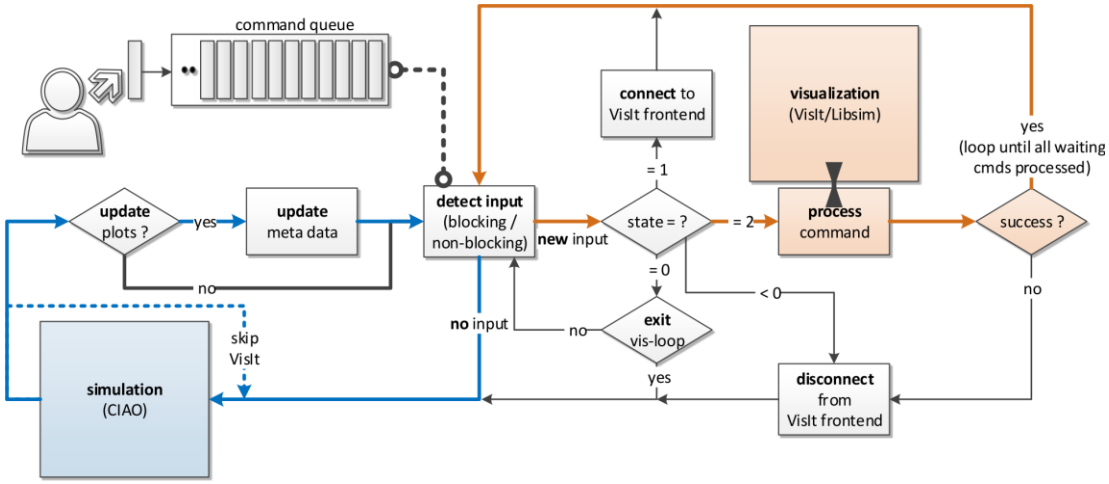
Distribution of MPI rank severity values

In-Situ Visualization

adding VisIt/Libsim to CIAO

Frequent dumping of simulation output
can be avoided **with appropriate in-situ visualization**

- VisIt/Libsim was successfully coupled to CIAO
  - for interactive visualization
  - for batch visualization



Coupling mechanism between simulation CIAO and visualization VisIt/Libsim.

In-Situ Visualization

challenges on BlueGene/G JUQUEEN

… major challenge on BlueGene/Q

- 458,752 cores
- 28,672 nodes
- 448 TiB main memory
- node:
  - 16 cores
  - 16 GiB memory

Limited memory per core

In-Situ Visualization

challenges on BlueGene/G JUQUEEN

… major challenge on BlueGene/Q

- VisIt/Libsim statically linked
  - executable size: 167 MiB
- MPI rank 0 requires additional memory
  - Interactve mode: 440 MiB
  - Batch mode: 100 MiB

case	grid		in-situ visualization		Score-P
	grid size	cells per rank	interactive	batch	
1	640^3	571	x	x	
2	1024^3	2340		x	x
3	2560^3	36571		x	

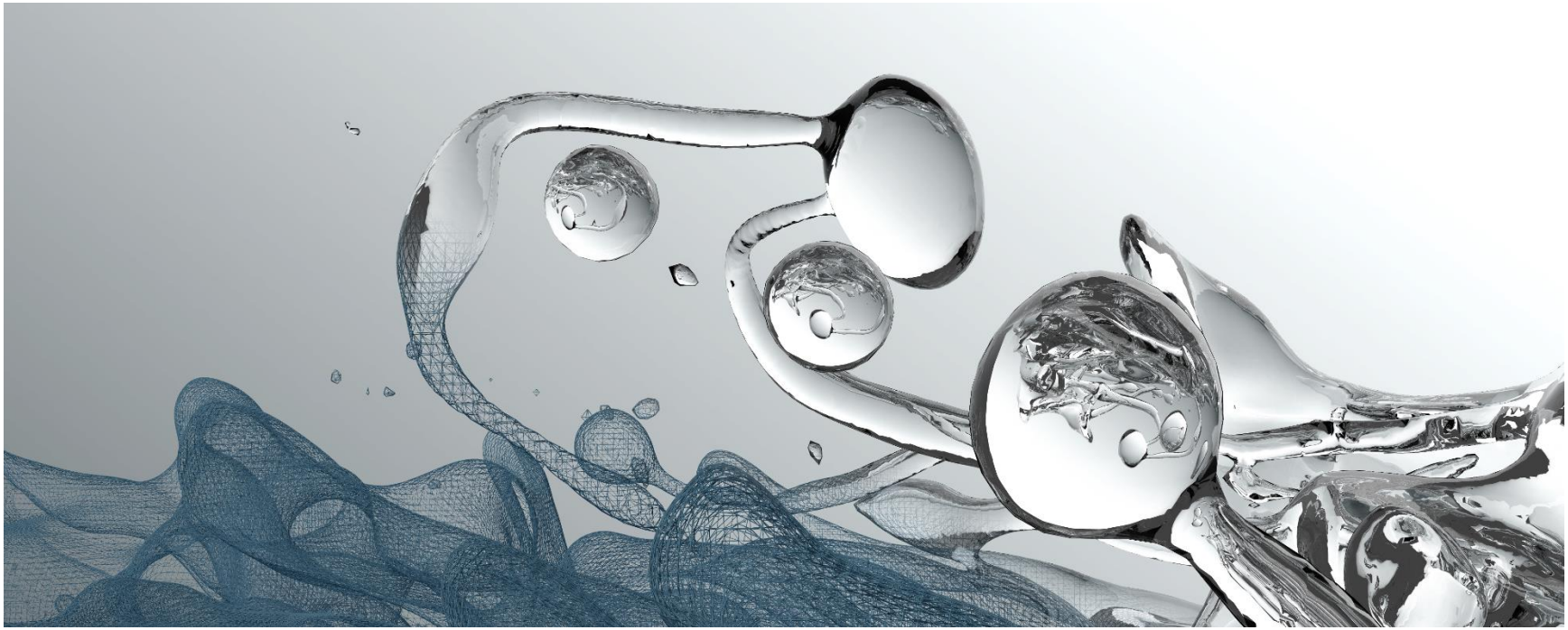
16 MPI ranks per core not feasible -> hybrid parallelization
Reduction of memory overhead on rank 0 desirable

Summary & Conclusion

- **Simulations of spray injection & droplet formation** is of high importance for the development of modern combustion engines.
- With the need for **high spatial and temporal resolution** the time for I/O increases rapidly.
- **In-situ visualization using VisIt/Libsim** was added to CIAO to reduce the I/O time, while adding new possibilities for the user.

- CIAO + VisIt/Libsim runs **successfully on the full BlueGene/Q JUQUEEN**
- To overcome the **memory limitations** on MPI rank 0 **hybrid parallelization** is needed in CIAO and/or the **memory overhead** of the visualization has to be reduced.

Thank you for your attention
Questions ?



rendered with Blender from a DNS of a diesel injection spray of ITV, RWTH Aachen University