PERFORMANCE ANALYSIS AND OPTIMIZATION OF CFD APPLICATIONS

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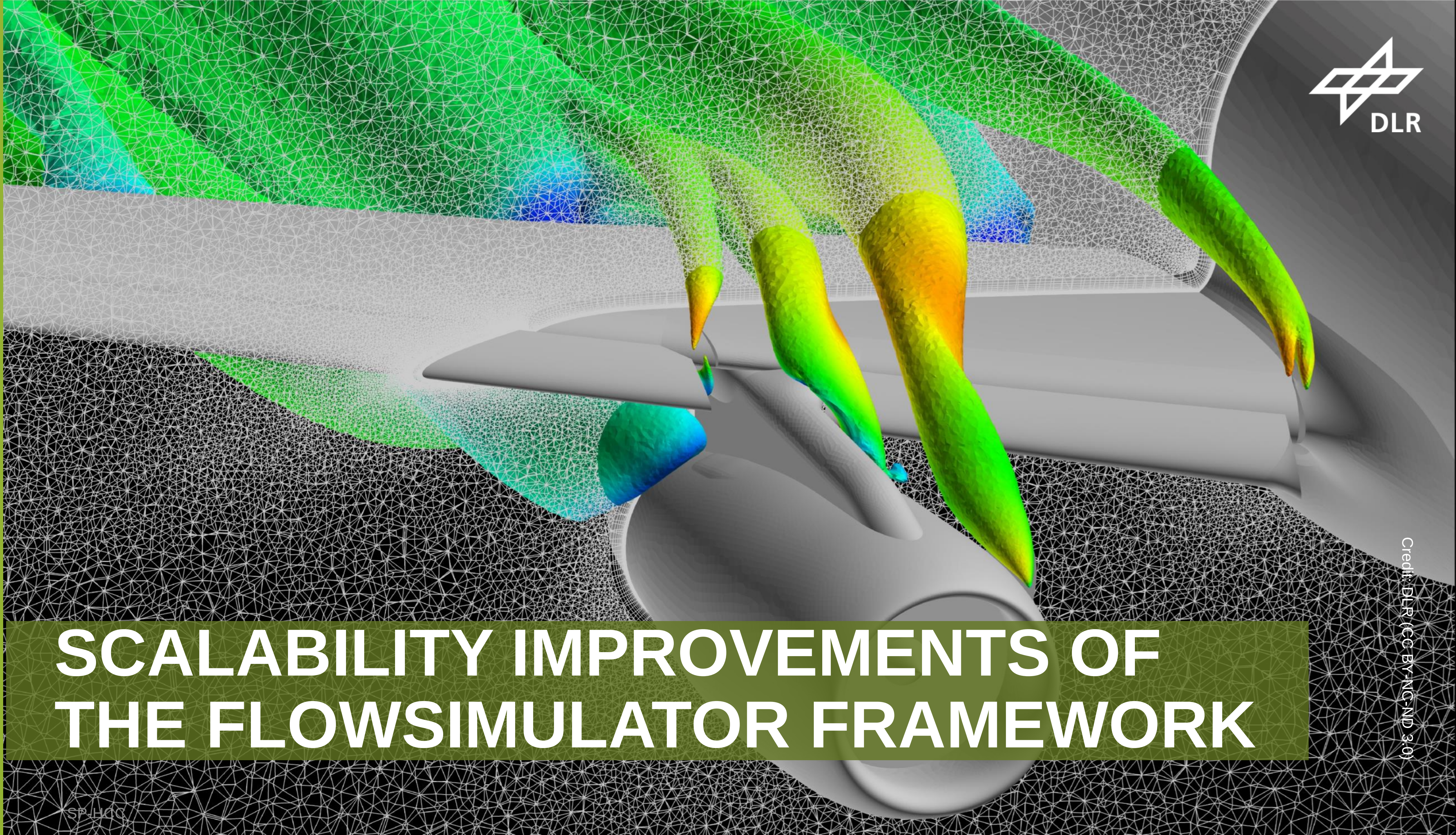
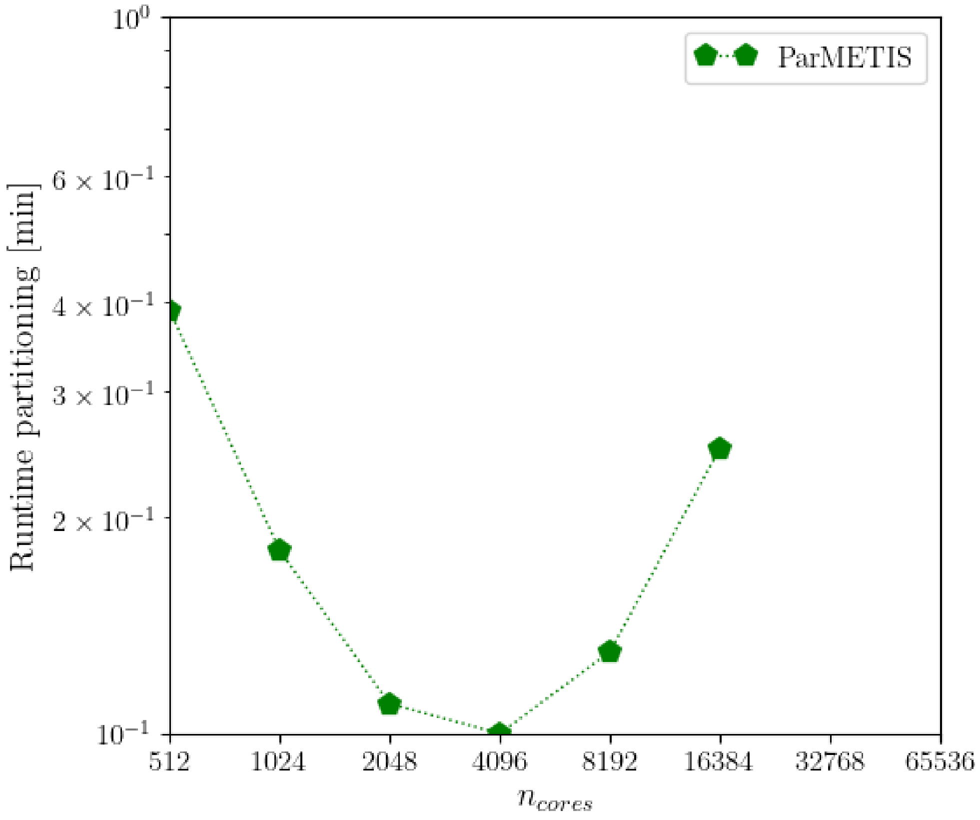
Agenda

- Scalability improvements of the FlowSimulator framework
- Investigation of HPC architectures using Amazon Web Services (AWS)
- Performance modelling of the CFD solver TRACE
- HPC operation



SCALABILITY IMPROVEMENTS OF THE FLOWSIMULATOR FRAMEWORK

Hierarchical Partitioning



- Partitioning runtime (pure MPI)
- Mesh with 723M cells, 629M nodes
- Problem: In FlowSimulator partitioning does not work anymore from a certain number of processes on.

Hierarchical Partitioning

- Partitioning data on multiple hardware hierarchy levels
- Can be done in two directions:
  - First partition data among compute nodes, then on lower hierarchy level within compute nodes, …
    - Benefit: reduced communication time, domain decomposition for less processes at once
    - Drawback: higher imbalance factor
  - First partition data among all processes, then redistribute partitions so that communication is minimized in higher hierarchy level, …
    - Benefit: reduced communication time, better imbalance factor
    - Drawback: potentially computation of large number of partitions at the same time

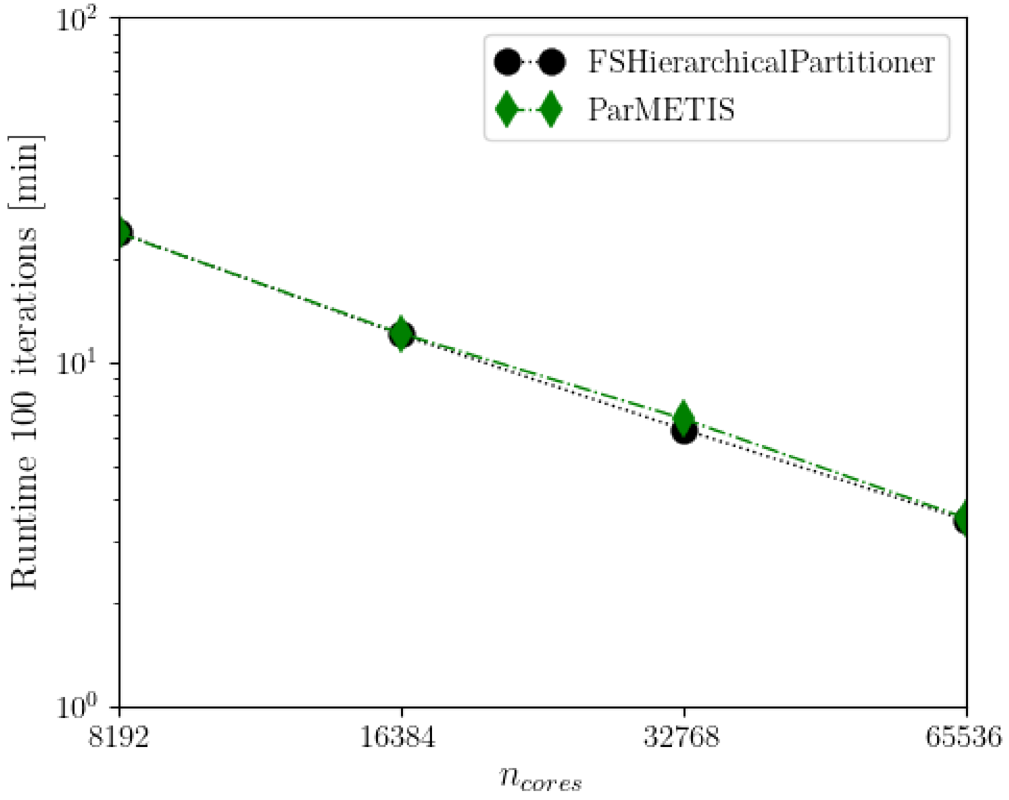
Hierarchical Partitioning Plugin for FlowSimulator

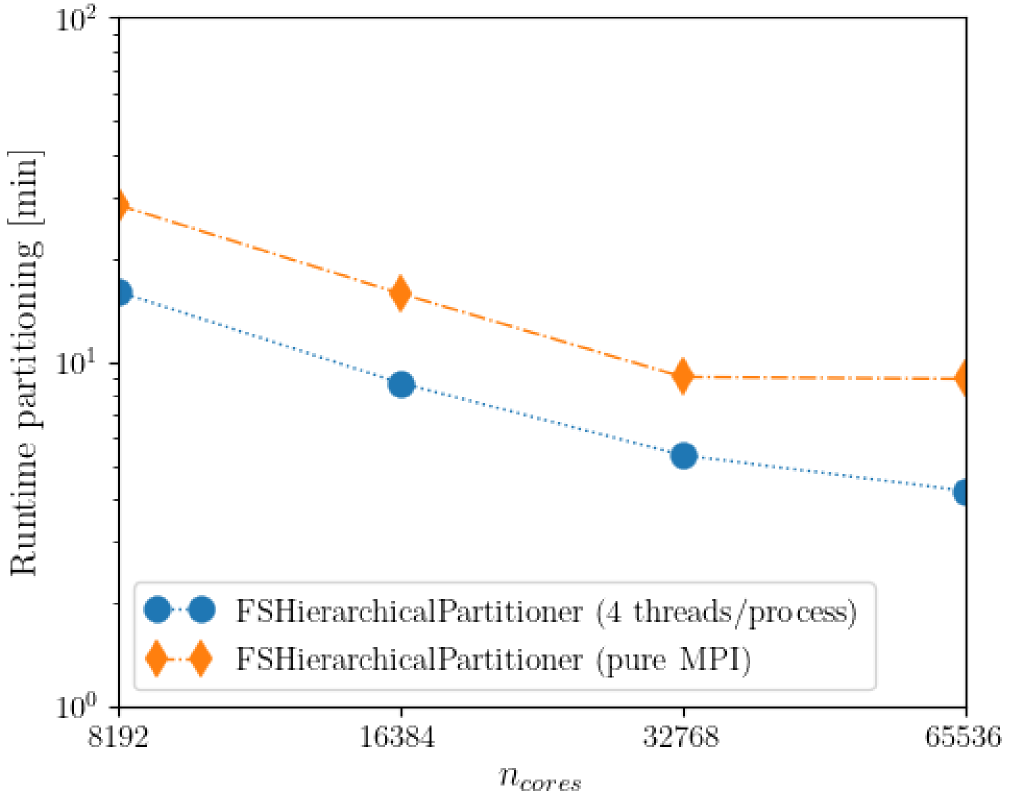
- Top down approach implemented as 2-level hierarchical partitioners
- To compute partitioning on each hierarchy level, an external graph partitioner is called (ParMETIS or Zoltan)
- To review the influence of the partitioning, CODA strong scaling benchmarks with large mesh (1.23B cells, 973M nodes) were done by taking the timings
- The partitioning were computed with ParMETIS because Zoltan does not work well for large meshes

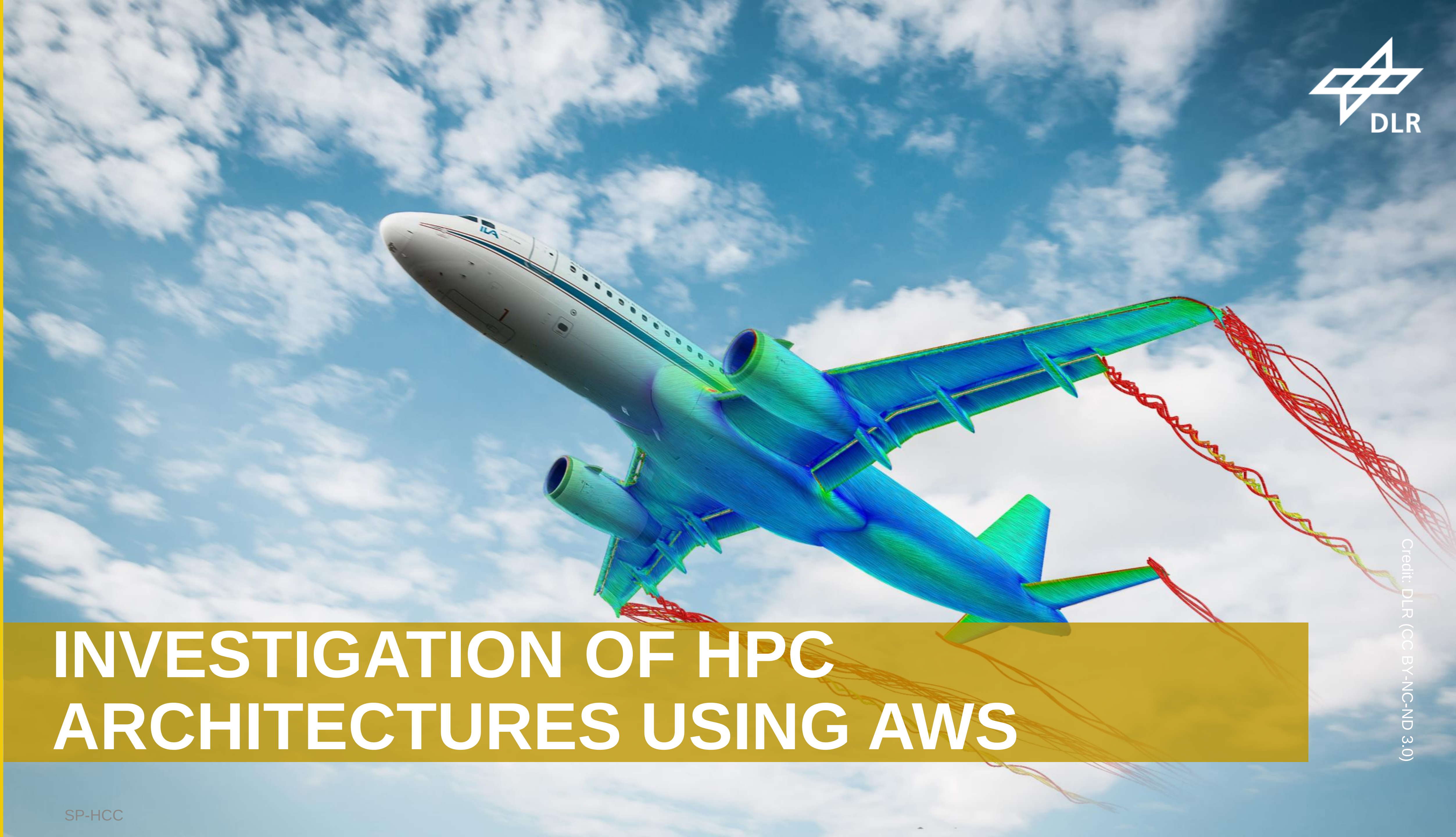
Results

Partitioning runtimes

- CODA runtimes (4 cores/process)







INVESTIGATION OF HPC ARCHITECTURES USING AWS

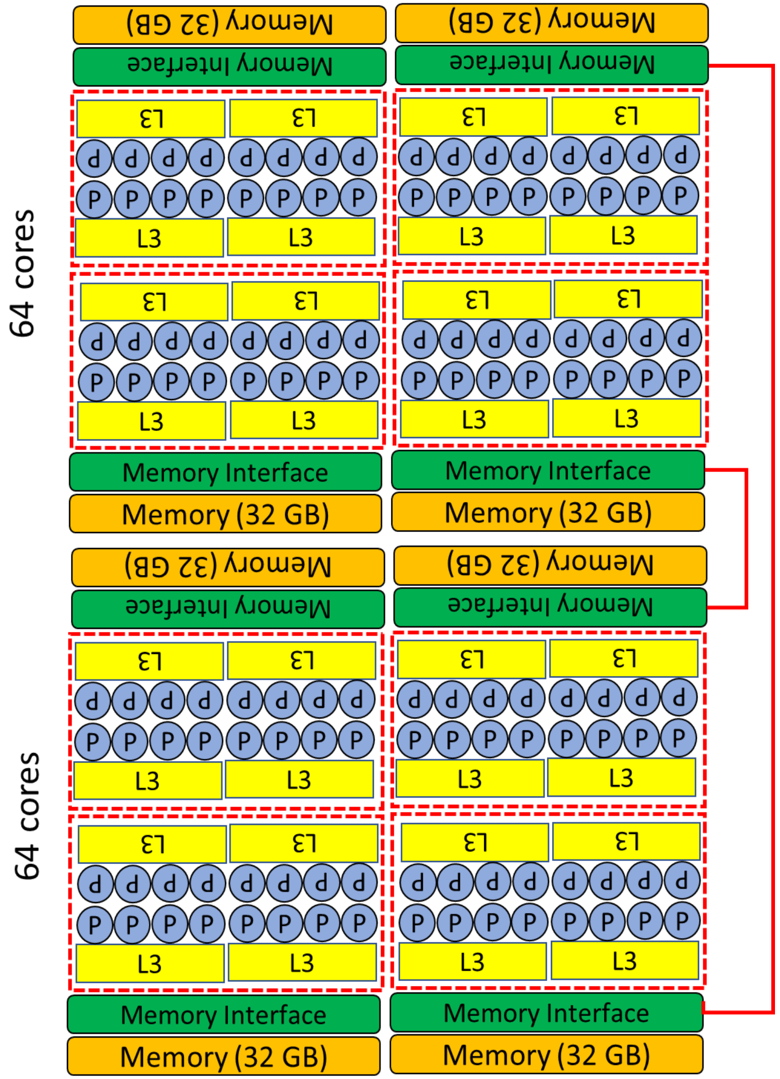
Architecture of Tested Nodes

DLR CARO	AMD EPYC Rome (Zen2) [100 Gbps Infiniband]
hpc7a	AMD EPYC Genoa (Zen4) [300 Gbps EFA (Elastic Fabric Adapter)]
hpc6a	AMD EPYC Milan (Zen3) [100 Gbps EFA]
c7gn, hpc7g	ARM Graviton3 instances, same specs and perf. [200 Gbps EFA]
c6gn	ARM Graviton2 [100 Gbps EFA]

Reference: https://aws.amazon.com/ec2/instance-types/

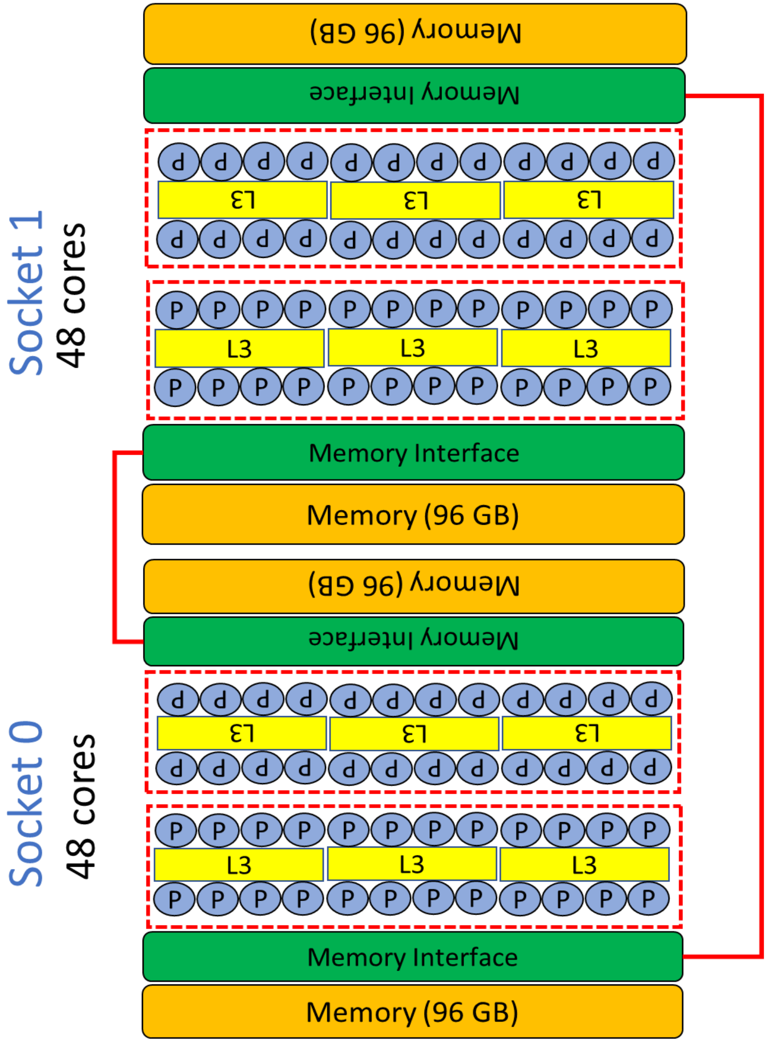
Zen Architectures

DLR CARO (AMD EPYC 7702)



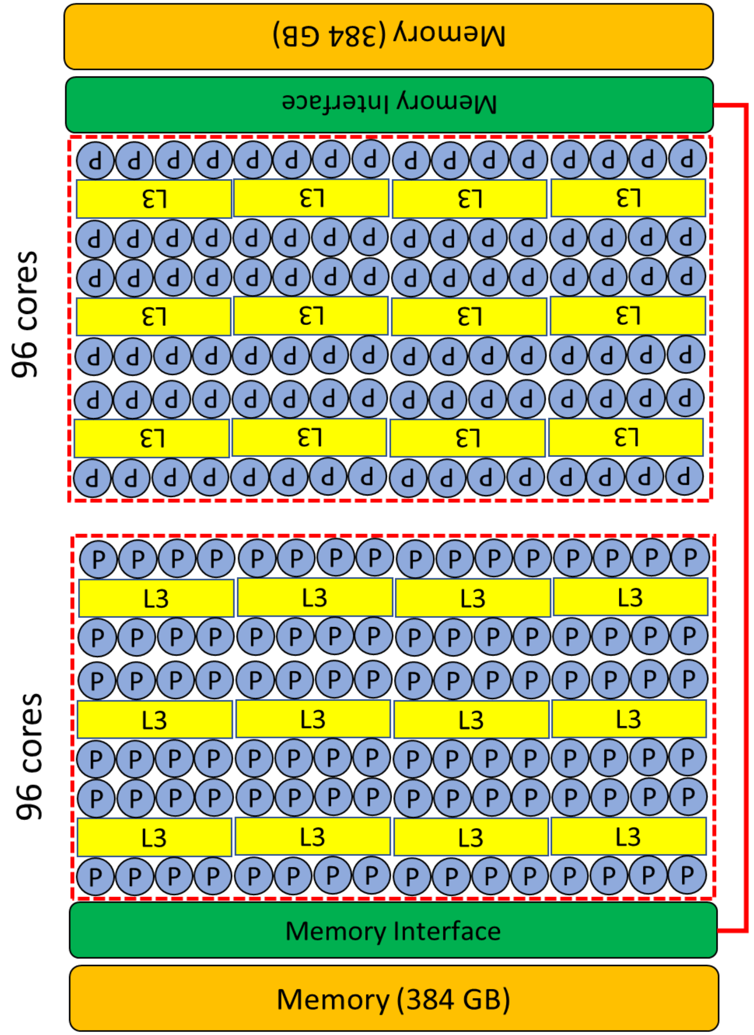
*L1 (32kB) and L2 (512 kB) *per core, L3 (16 MB)*

hpc6a.48xlarge (AMD EPYC 7R13)



*L1 (32kB) and L2 (512 kB) *per core, L3 (16 MB)*

hpc7a.96xlarge (AMD EPYC 9R14)



*L1 (32kB) and L2 (1 MB) *per core, L3 (32 MB)*

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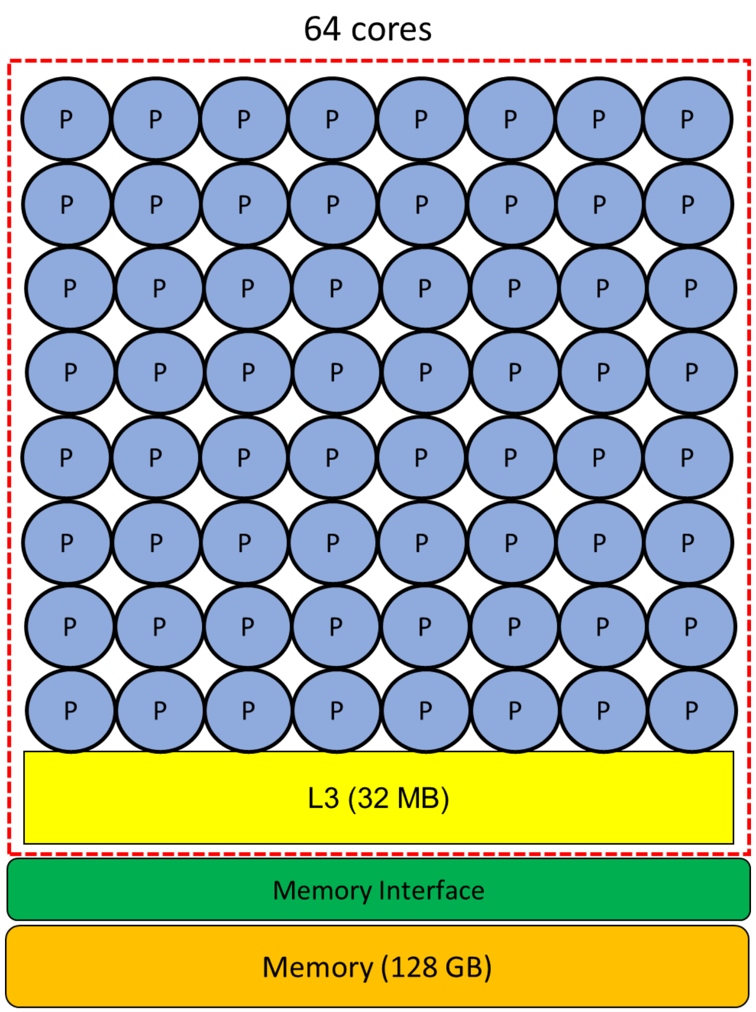
AWS Graviton Processor

- ARM 64bit architecture
- Graviton 3 is the successor of Graviton 2
- Graviton 3 (ARMv-8.4 ISA) vs Graviton 2 (ARMv-8.2 ISA)
- UMA – Uniform Memory Access system
- Single socket system with 64 cores
- 1 Node = 1 Socket
- Graviton3 – 8 memory channels
- L1 Cache - 64 kB (per core)
- L2 Cache - 1 MB (per core)
- L3 Cache - 32 MB (shared between 64 cores)
- Memory - 128 GB for Socket
- Graviton 3 (2.6 GHz) vs Graviton 2 (2.5Ghz)
- Graviton 3 has more core width than Graviton 2 - (higher IPC)
- Graviton 3 has DDR5 and faster memory channels than Graviton 2

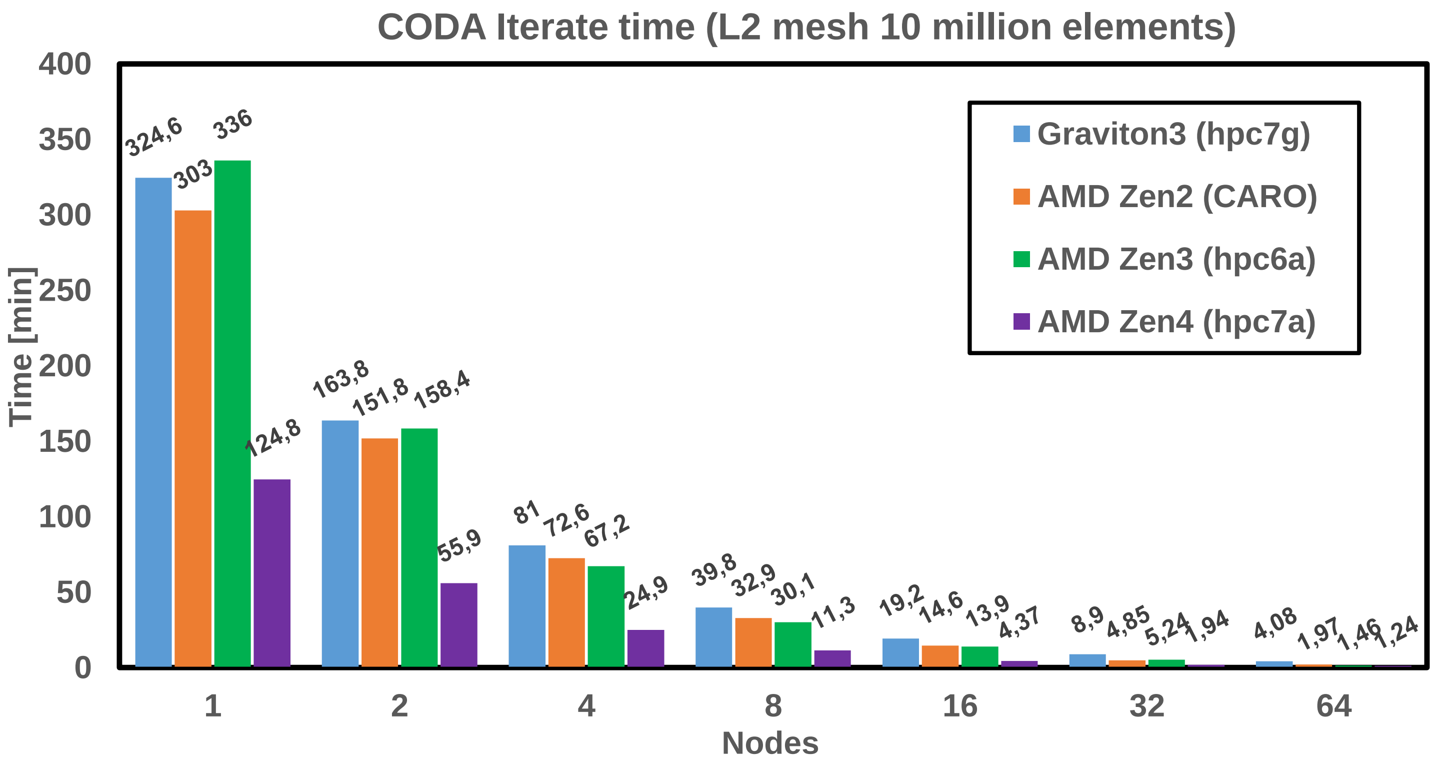
Graviton 3 and Graviton 2

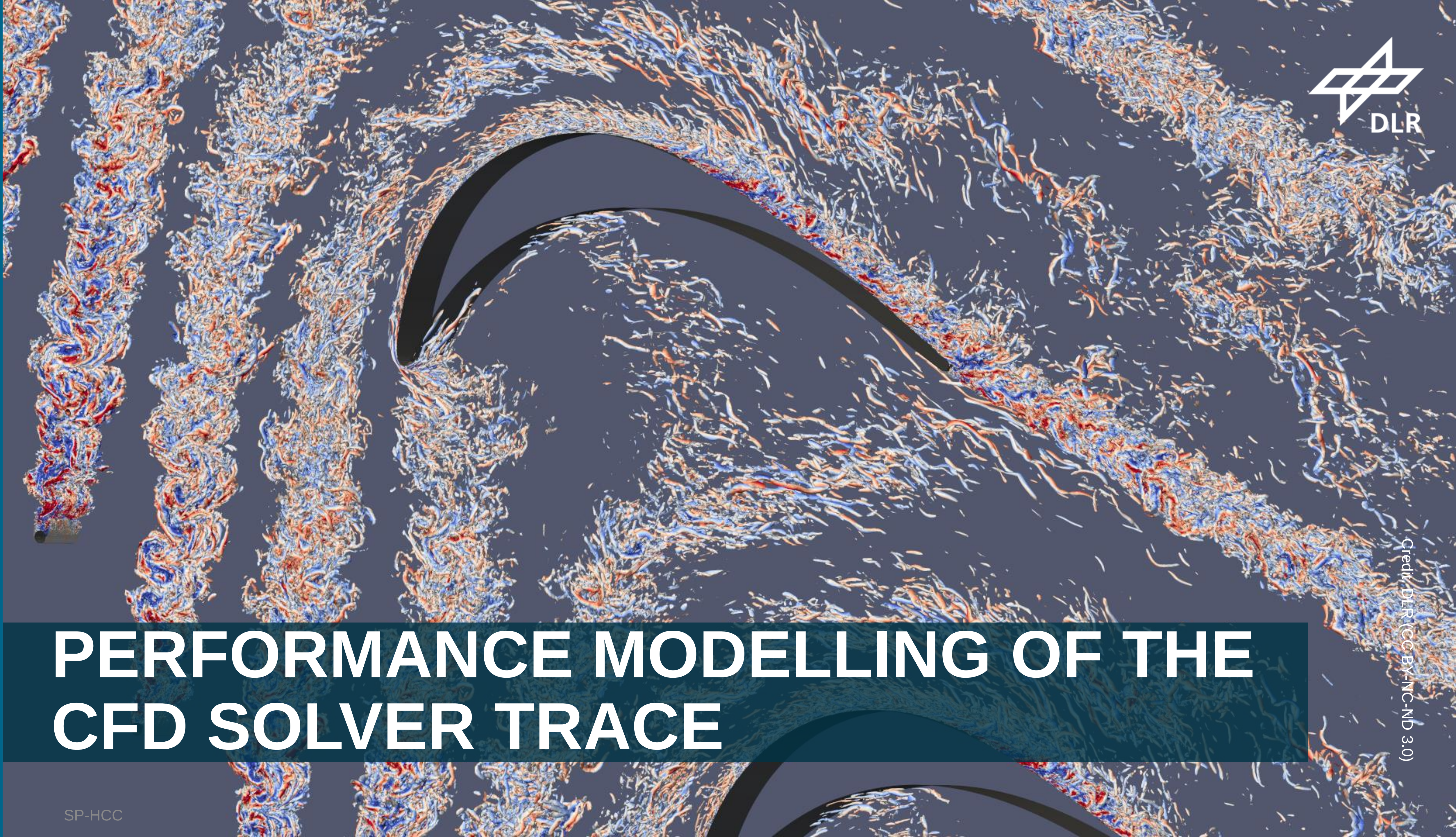


*L1 (64 kB) and L2 (1 MB) *per core*

CODA Iterate time comparison

• Graviton3 (hpc7g)	- 16 MPI tasks x 4 OMP threads per task (64 cores/node)
• CARO (Zen2)	- 32 MPI tasks x 4 OMP threads per task (128 cores/node)
• hpc6a (Zen3)	- 12 MPI tasks x 8 OMP threads per task (96 cores/node)
• hpc7a (Zen4)	- 24 MPI tasks x 8 OMP threads per task (192 cores/node)





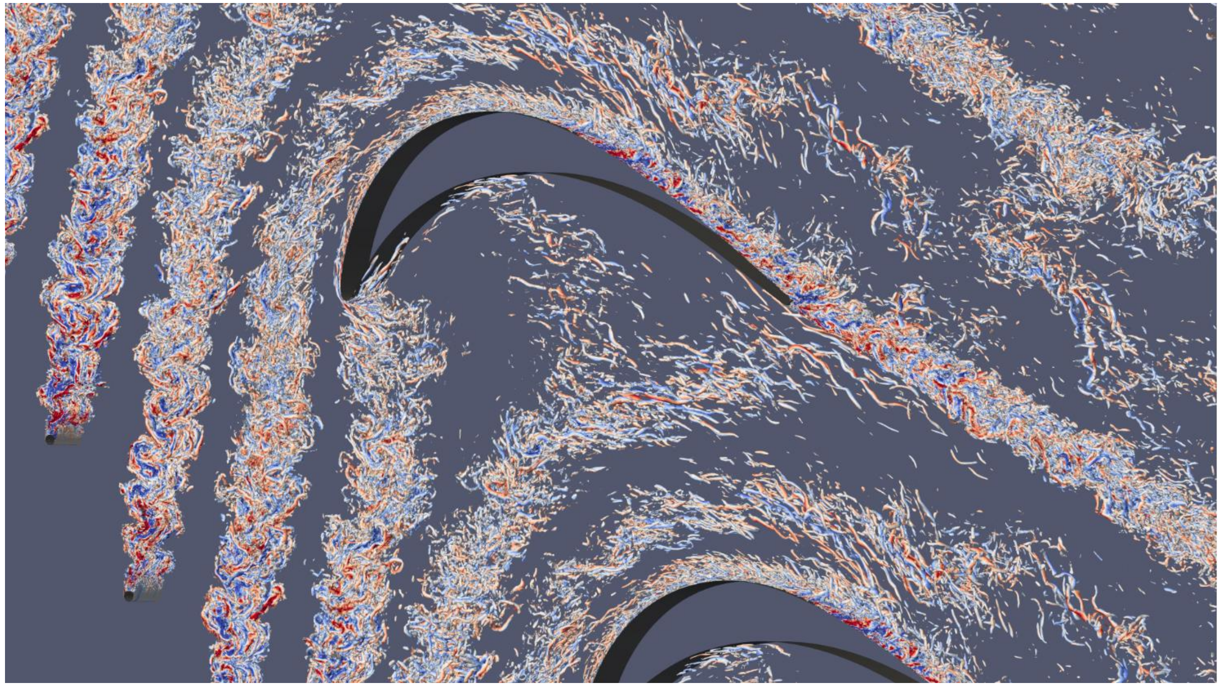
PERFORMANCE MODELLING OF THE CFD SOLVER TRACE

TRACE

Turbomachinery Research Aerodynamic Computational Environment

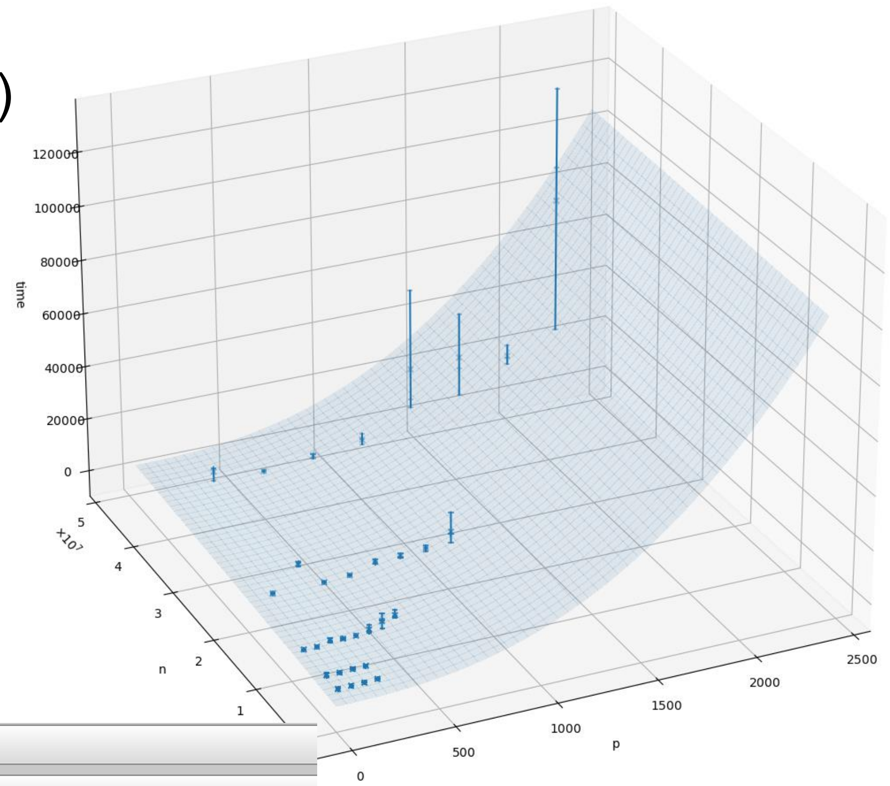
- DLR‘s standard CFD solver for turbomachinery flows
- Also used in industrial design processes by MTU Aero Engines AG and Siemens Energy AG

- Steady and unsteady RANS solver on structured and unstructured grids
- Hybrid parallelization with MPI and OpenMP



Extra-P

- Fix model parameters (#procs, #cells, polynomial degree, …)
- Run repeated measurements
  → experiment directory with Cube profiles
- Automatically generate performance model for every node in the call tree using Extra-P
  - Metrics include time, #calls, MPI bytes sent, …



Model: Default Model

Metric: time

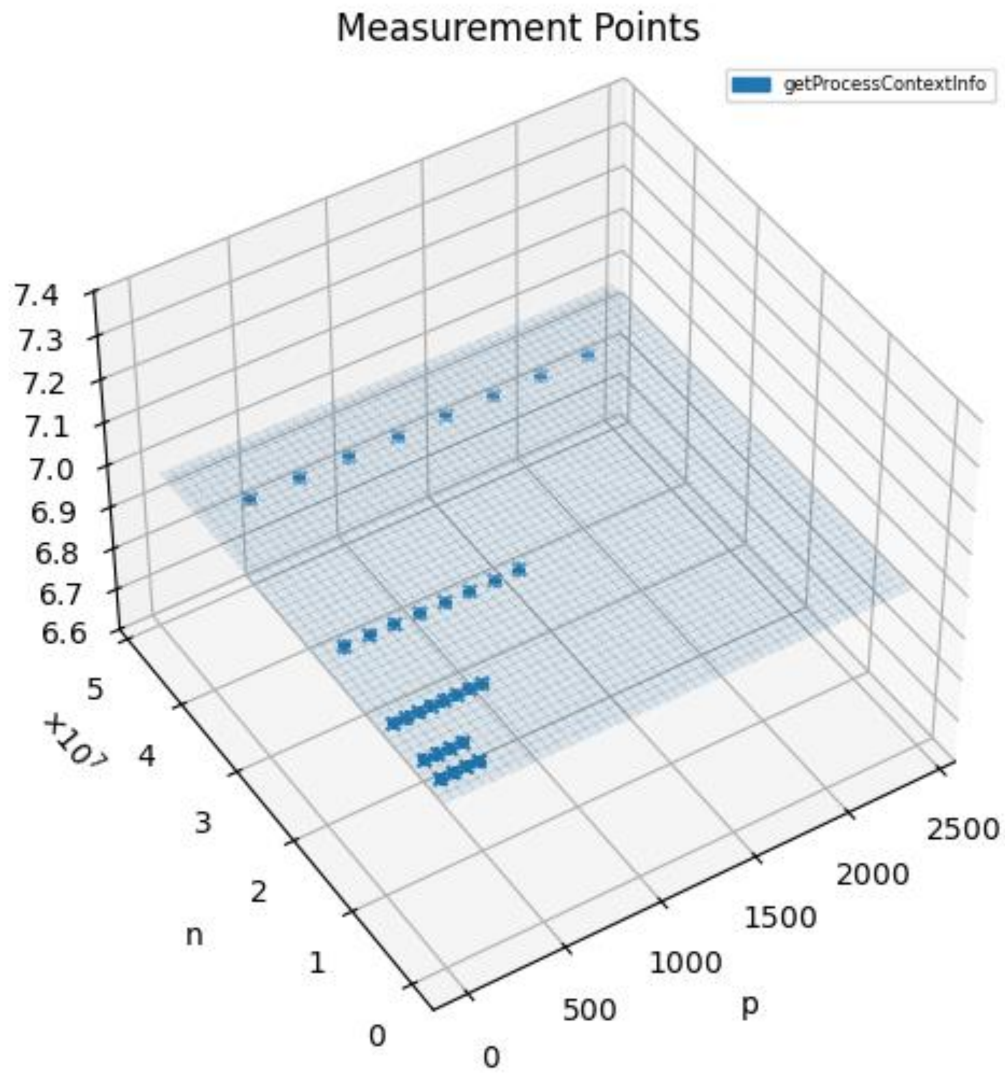
Se	Callpath	An	Value	RSS	Adj. R^2	SMAPE	RE
	TRACE		$0.351 + 5.395\times10^{-06} * p^{3/2} * \log_2(p)$	4.428	0.924	36.819	0.532
	main		$0.160 - 2.514\times10^{-04} * n^{2/3} + 3.427\times10^{-05} * \log_2(p) * n^{2/3}$	78.718	0.893	66.985	1.080
	traceInitEnvironment		$155.225 - 0.013 * n^{1/2} * \log_2(n) + 5.827\times10^{-06} * p^{3/4} * \log_2(p)^2 *$ …	1.050…	0.954	56.301	0.694
	allocateSolverStructures		$2752.430 - 0.208 * n^{2/3} + 2.986\times10^{-03} * p^{3/4} * n^{2/3}$	1.002…	0.941	74.168	1.147
	commProcessIsRootGroupMaster		$2.924\times10^{-03} + 3.502\times10^{-06} * p * \log_2(p) + 2.944\times10^{-10} * n^{1/2} *$ lo…	0.019	0.367	75.980	1.275
	getProcessContextInfo		$5.084\times10^{-05} + 9.093\times10^{-13} * n$	2.017…	0.353	14.844	0.147
	passLogMessage		0.088	0.612	1	109.9…	0.856
	MPI_Comm_rank		$-0.132 - 0.024 * p^{1/2} + 5.974\times10^{-04} * p^{1/2} * n^{1/4}$	0.644	0.808	116.3…	10.161
	MPI_Allreduce		$-434.672 + 3.593\times10^{-04} * p^{5/2} + 1.491\times10^{-05} * n^{3/4} * \log_2(n)^2$	9.499…	0.891	41.482	0.424

Testcase

- 6 grids with number of cells ranging from 2.5e6 to 8.1e7
  → strong scaling in p-direction

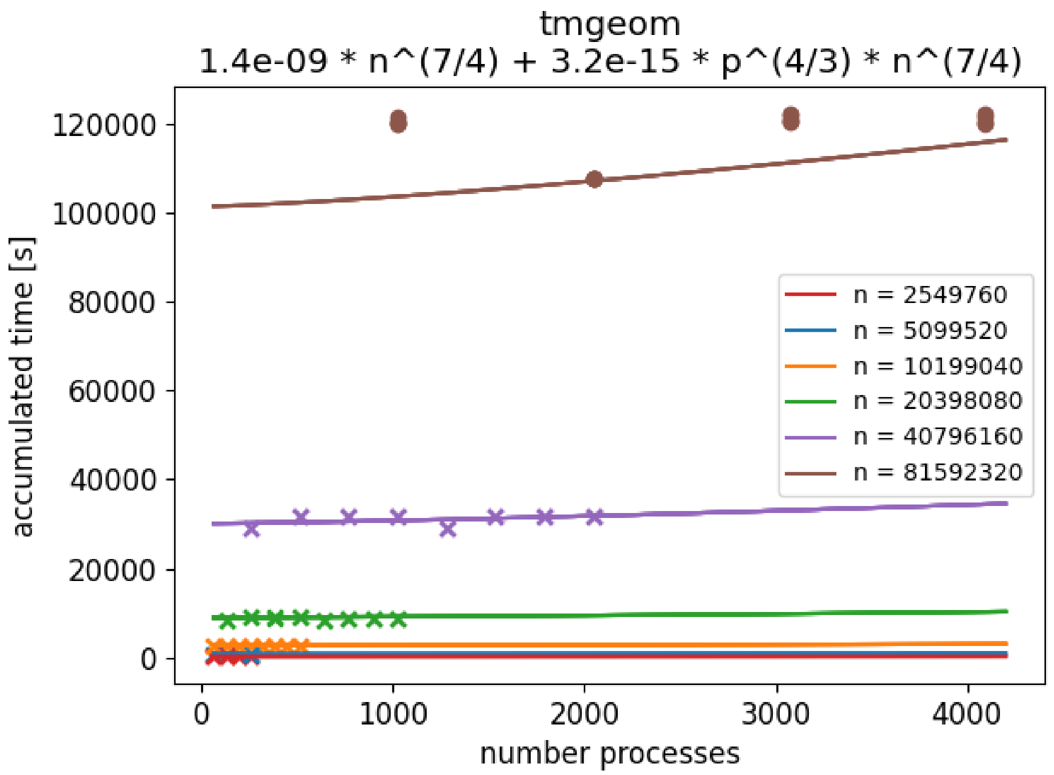
# cells (n)	# processes (p) Low	High	# partitions
2.5e6	64	256	4
5.1e6	64	256	4
10.2e6	64	512	8
20.3e6	128	1024	8
40.8e6	256	2048	8
81.6e6	1024	4096	4

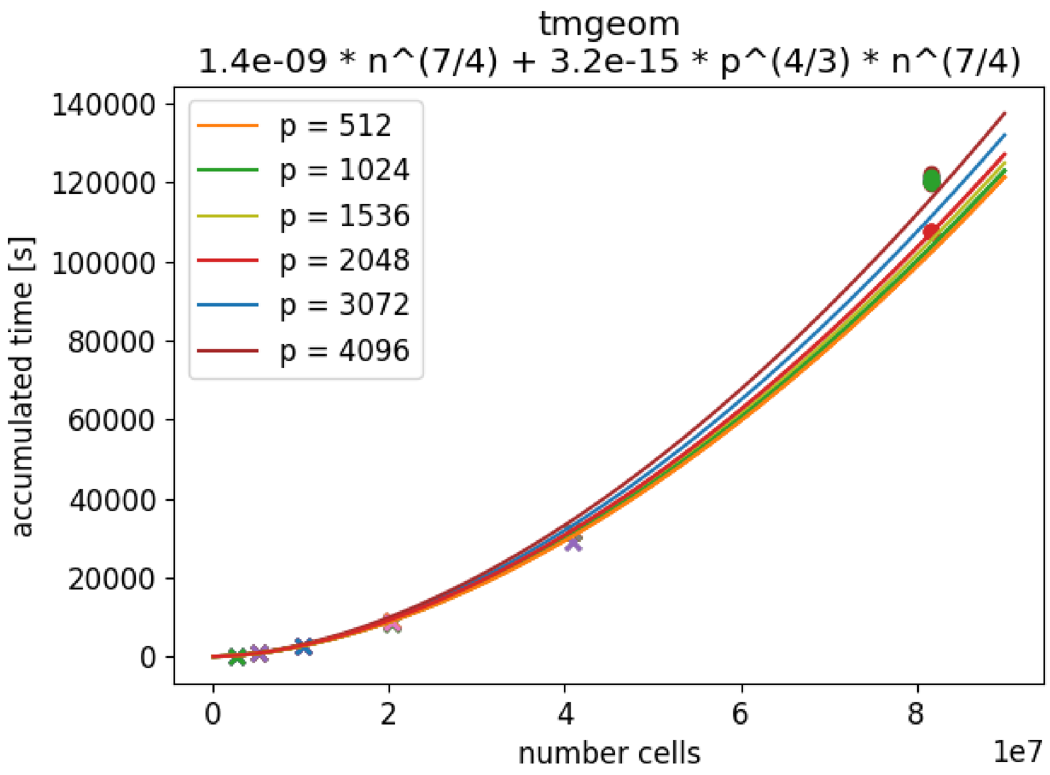
- Last line used as validation data
- Variables:
  - n: number of cells
  - p: number of processes
- Investigated routines part of not optimized setup



Results: Computation

- For every cell (n) lookup distance to wall in kd-tree (ideally log(n))
- Satisfying model

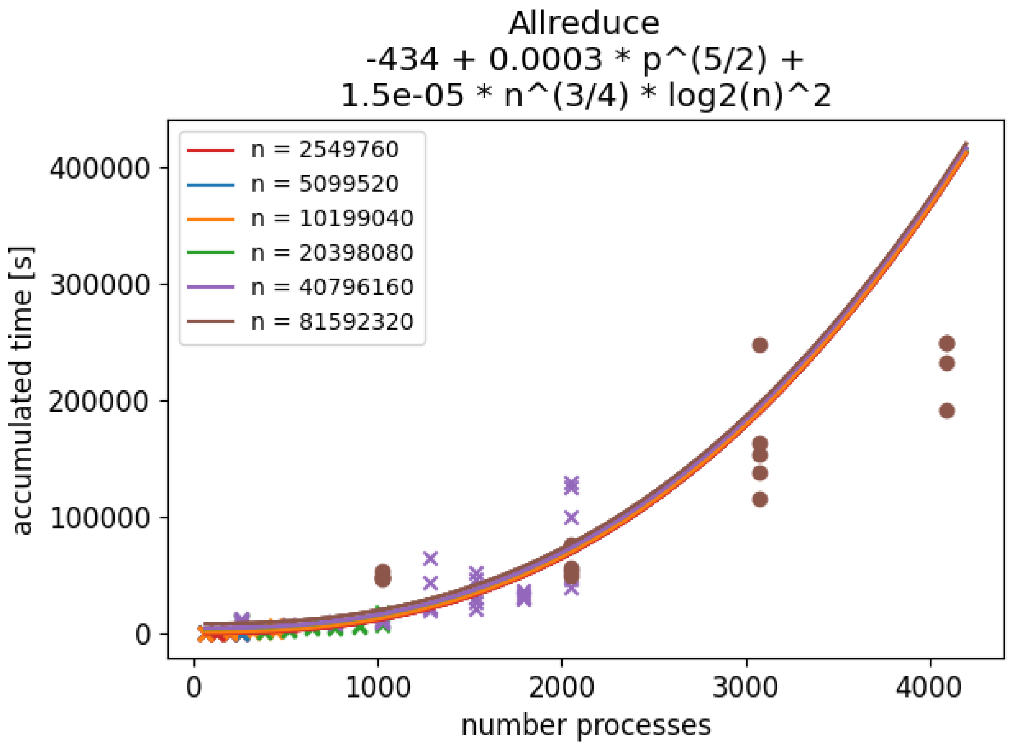


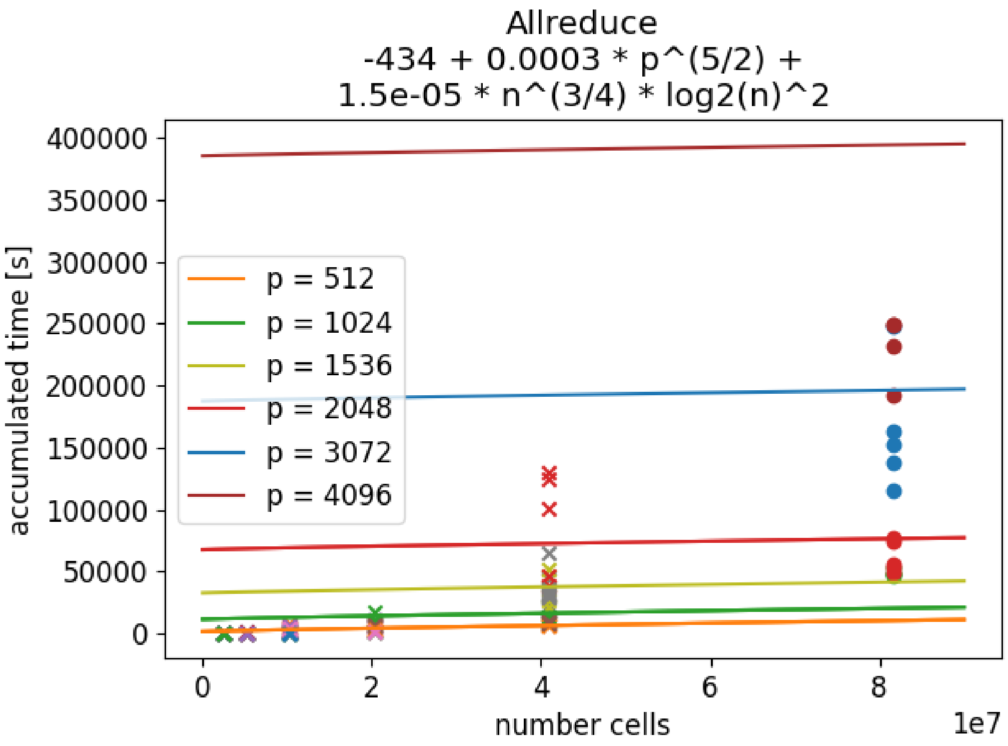


Results: Communication

- Deeper look in p^(5/2) runtime necessary
- Model satisfying only in trend, not in quantitative values

- Problems:
  - Spread of measurement points
  - Setup of testcase





HPC OPERATION

HPC Systems operated by DLR-SP

HPC cluster CARA, Dresden

Credit: DLR (CC BY-NC-ND 3.0)

- 2,168 CPU-nodes with 2 AMD EPYC 7601 (2x 32 cores)
- 664 CPU-nodes with 2 AMD EPYC 7702 (2x 64 cores)
- 10 GPU-nodes with 4 Nvidia A100 and 2 AMD EPYC 7702
- 17 PB Luste file system (0,5 PB SSD / 16,5 PB HDD)
- Operational since 2020/2023 → Replacement 2025

HPC cluster CARO, Göttingen

Credit: DLR (CC BY-NC-ND 3.0)

- 1,364 CPU-nodes with 2 AMD EPYC 7702 CPUs
- 8.4 PB Lustre file system (HDD with SSD cache)
- Operational since 2022 → Replacement 2027/28

HPC Operation

- Continuous application monitoring
  - Identify applications with inefficient resource usage
  - Identify candidates for detailed performance analysis
  - Verify performance optimizations
  - Track performance degradation

- Input for next HPC procurements
  - Information about (performance) characteristics of our application mix
  - Investigation of HPC architectures
  - Performance modelling to estimate performance on future systems

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