OpenFOAM Scaling on Cray Supercomputers

Dr. Stephen Sachs | GOFUN 2017

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Supercomputing Leadership

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Supercomputing Leadership

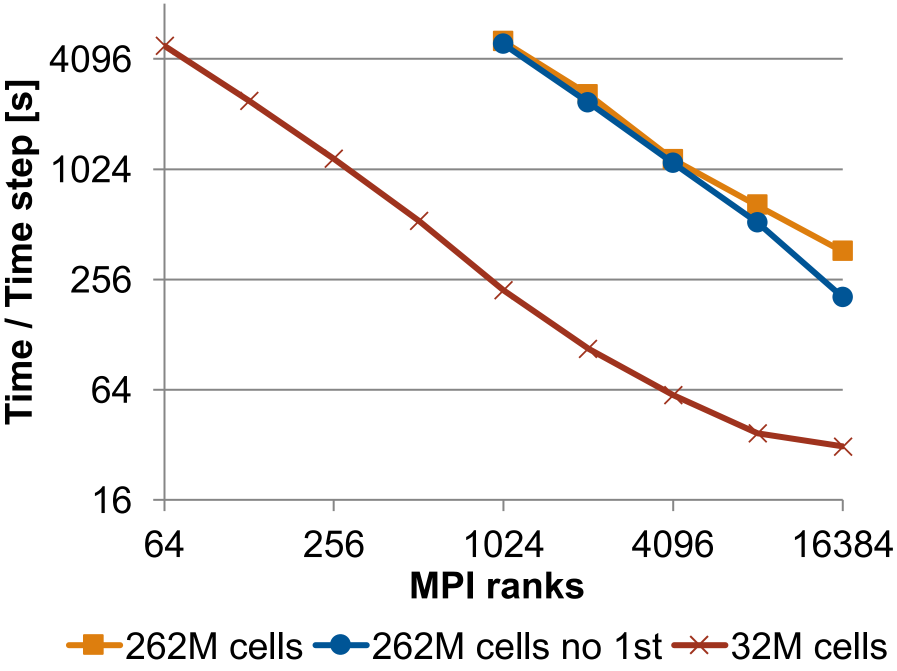
OpenFOAM a HPC code?

- **Portability to HPC architectures – Yes**
  - Support for multiple compilers
  - Support for Intel MIC, GPU
- **MPI parallelism – Yes**
  - Scalability limit could be improved
- **Hybrid parallelism – Partial**
  - Multiple attempts
  - Not in main release
- **High Performance I/O – No**
  - Design follows structure contradicting HPC parallel file system

There is potential | Old slide from 2012

- Inflated cavity tutorial
- AMD Opteron 6276
- OpenFOAM/2.2.0
- icoFoam

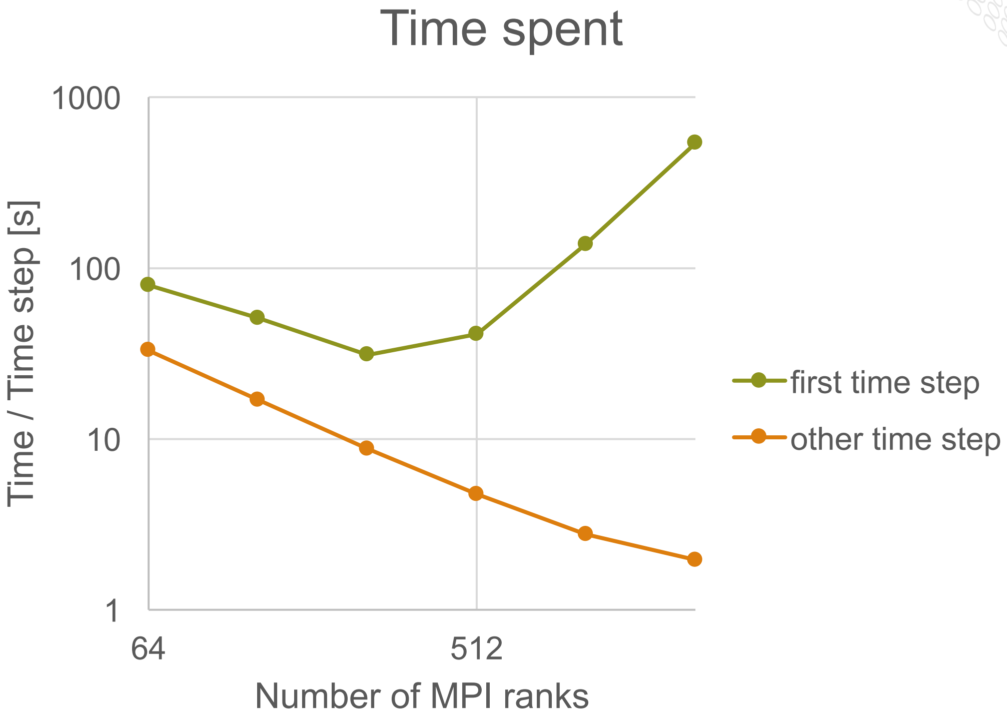
1.0 PFLOP/s
3,552 nodes
AMD Interlagos 32 cores/node



HPC Programmers Wish List for OpenFOAM

Some wishes have been granted | Startup phase

- Communication pattern in initialization
- Serial I/O reading one file per MPI rank
- First time step often skipped in benchmarks



Comparison at Scale

Laptop

- 4 cores
- 2 Mem Channels
- 1 Disk
- 1 Metadata Target

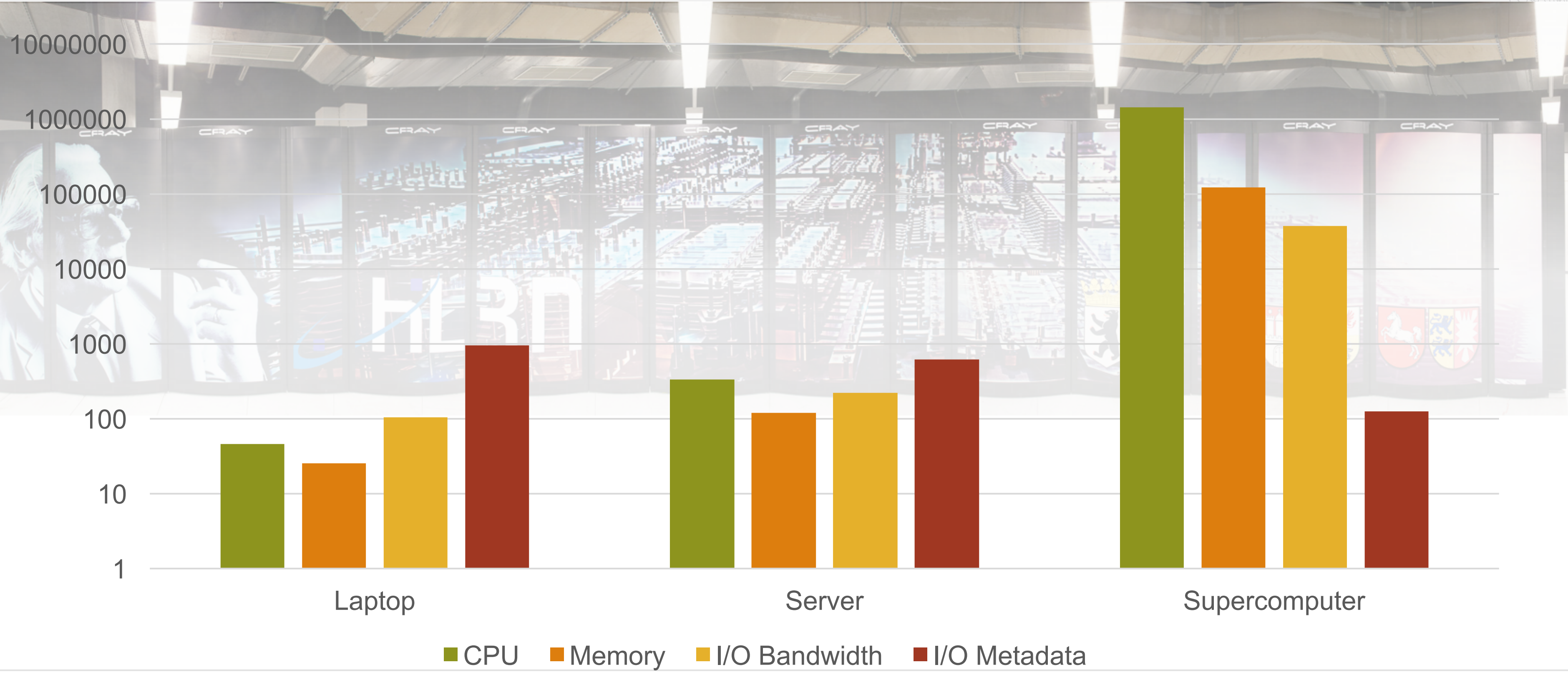
Server

- 20 cores
- 8 Mem Channels
- 6 Disks
- 1 Metadata Target

Comparison at Scale

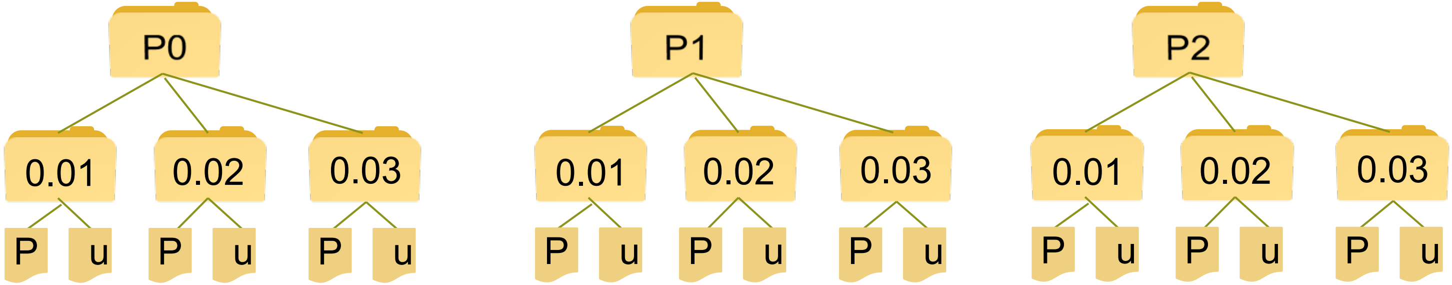
- 44,928 cores
- 14,976 Mem Channels
- 1480 Disks
- 1 Metadata Server

Comparison at Scale



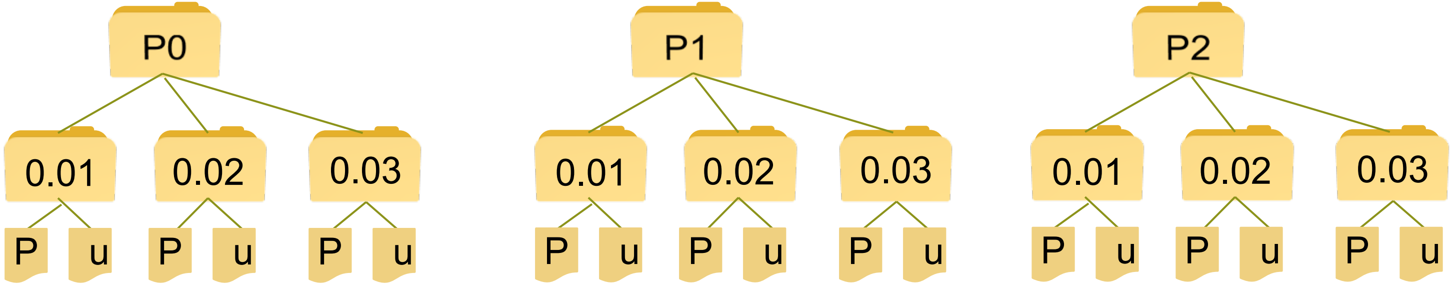
Metadata Operations

- Every time a file is opened or checked
  - Files in the respective directory and subdirectories are checked
- Workstation
  - 1-8 MPI ranks are doing 60-480 metadata calls per second – OK



Metadata Operations

- Every time a file is opened or checked
  - Files in the respective directory and subdirectories are checked
- Workstation
  - 1-8 MPI ranks are doing 60-480 metadata calls per second – OK
- Supercomputer
  - 1.000-10.000 MPI ranks are doing 60.000-600.000 metadata calls per second - Problem



What is in our Toolbox?

Optimization at Scale

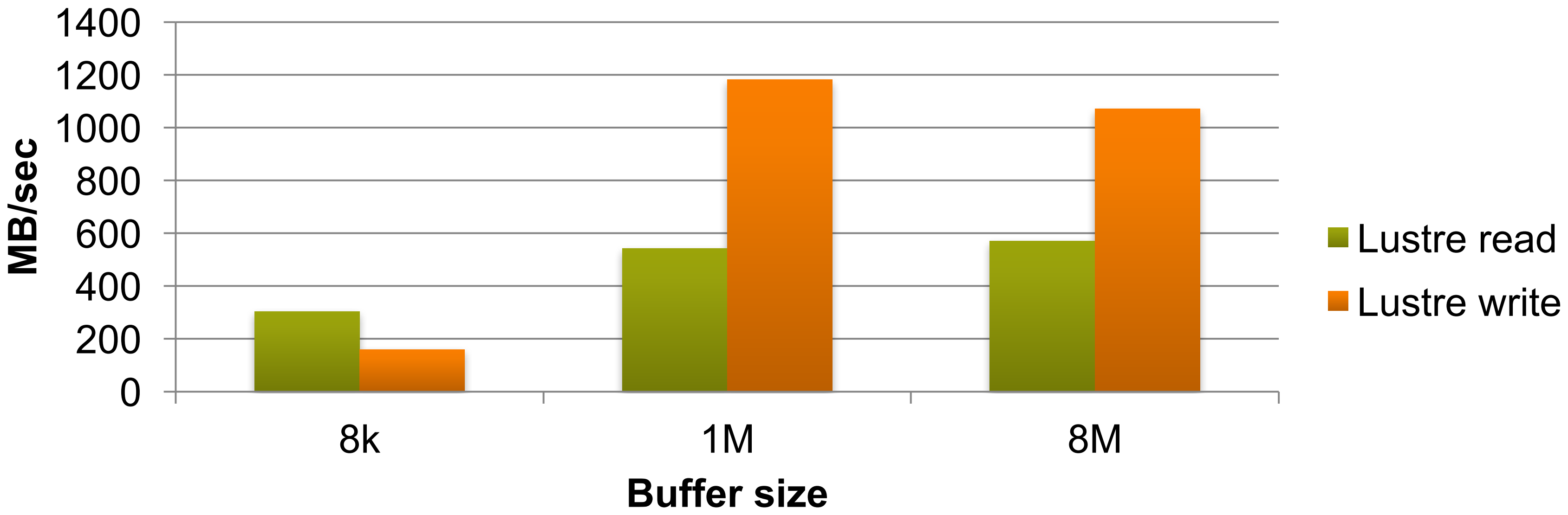
- **Inspect solvers at scale**
  - In case of strong scaling issues
  - GAMG runs faster than PCG, but scales worse
- **Do not check for file changes**
  - Disable runTimeModifiable
  - Accessing metadata can be a source for congestion
- **More MPI messages on the Eager 0 path**
  - Valid for MPICH derivatives
  - Saves one copy for most messages

Optimization at Scale (cont.)

- **Use Huge pages**
  - Larger memory pages can increase memory performance
- **Underpopulate compute Nodes**
  - OpenFOAM is memory bandwidth sensitive
- **Decomposition is key**
  - Scalability limit due to load imbalance
- **Hardware Collection Engine**
  - Offload MPI work to NIC

Optimization at Scale (cont.)

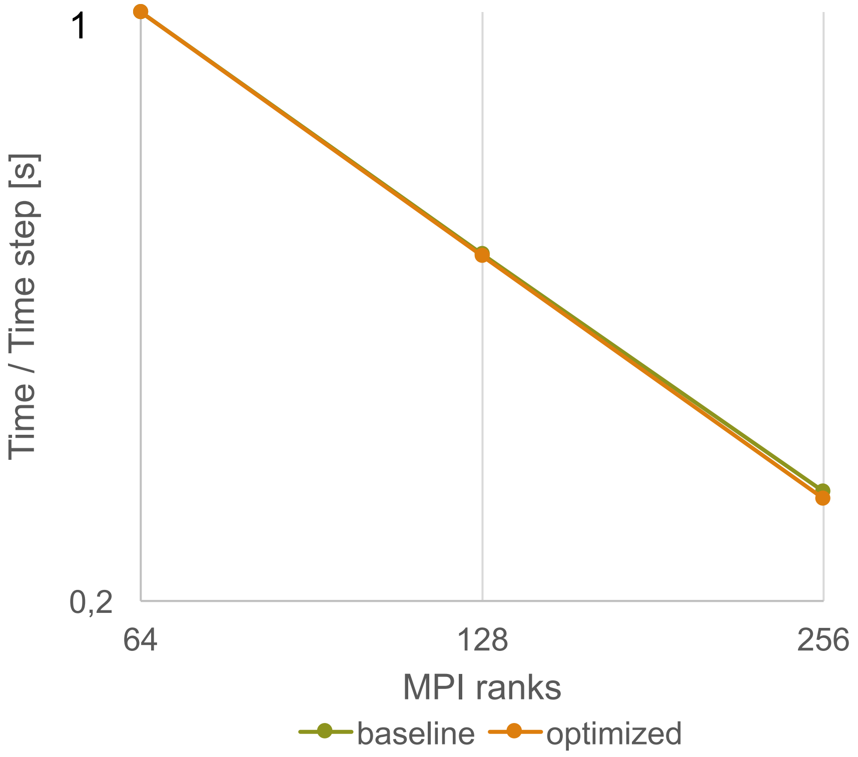
- Standard buffer size does not take advantage of high bandwidth file system



Scalability Results

- OpenFOAM/2.2.2
- ~100M cells
- GAMG solver
- Intel E5-2698 v3 @ 2.30GHz

- 3 weeks of work...



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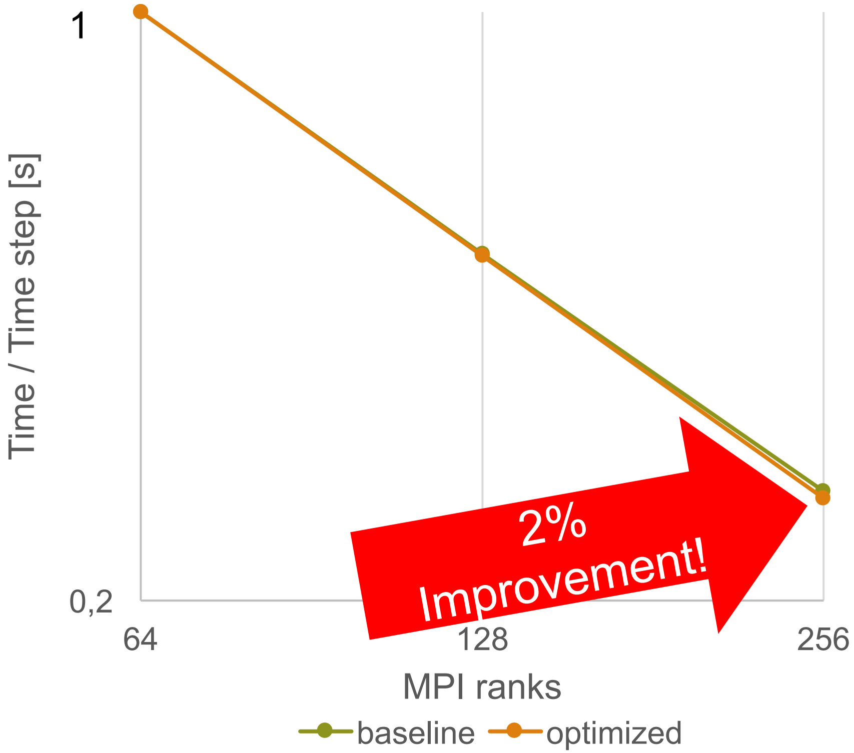

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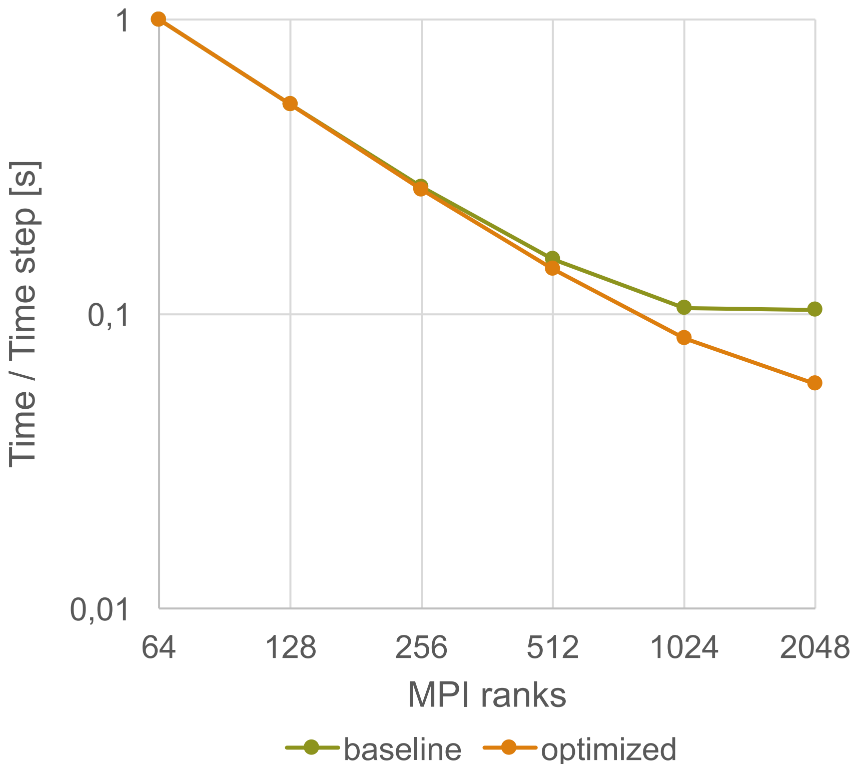

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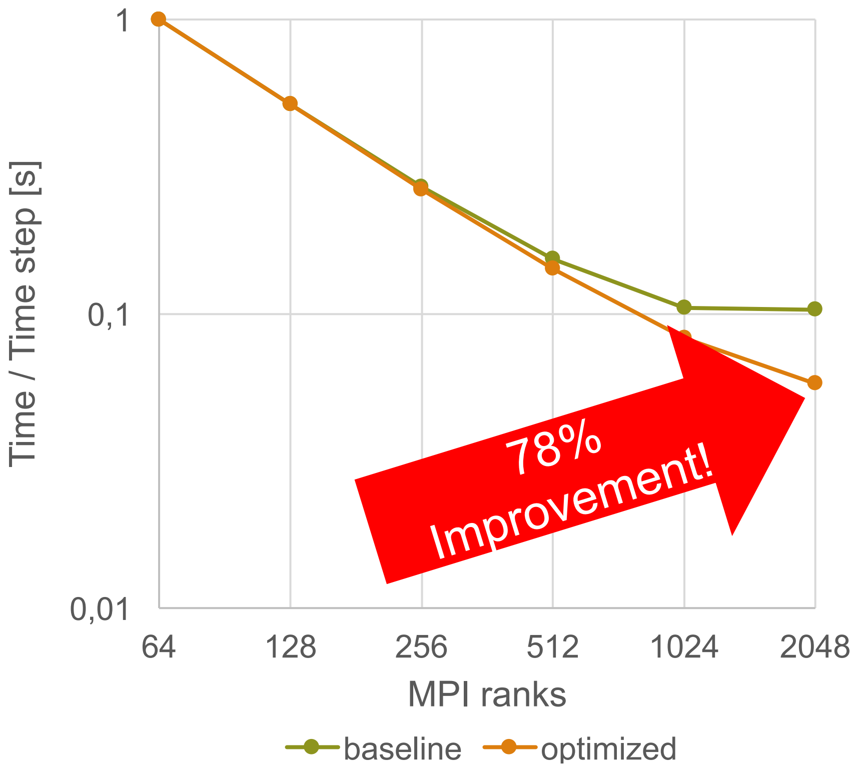
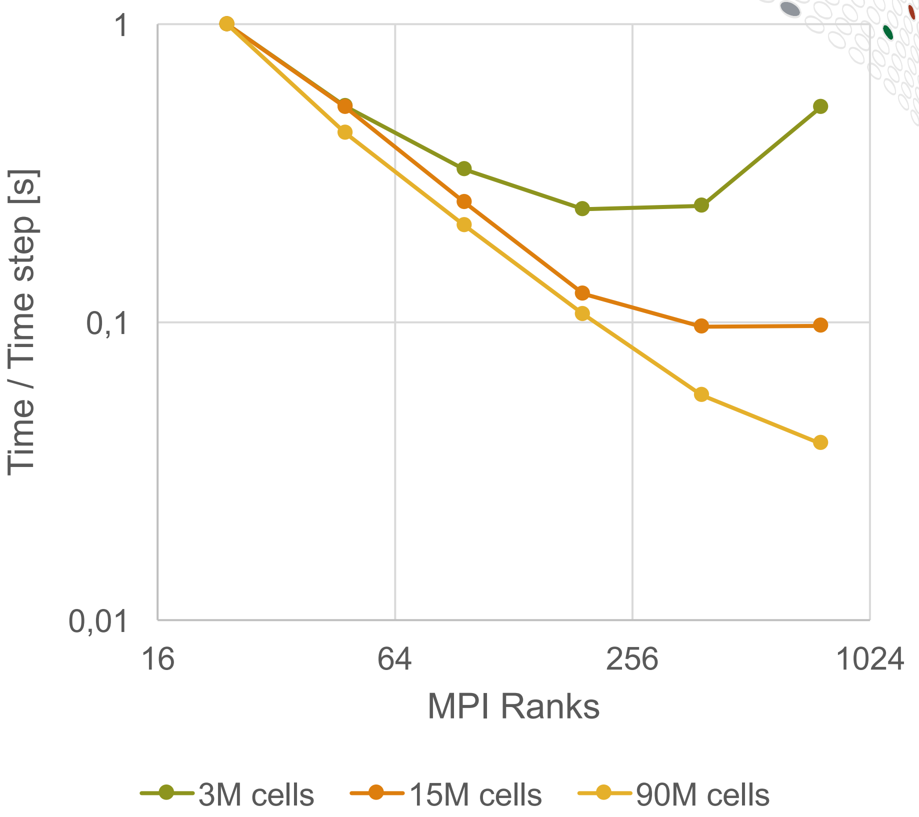
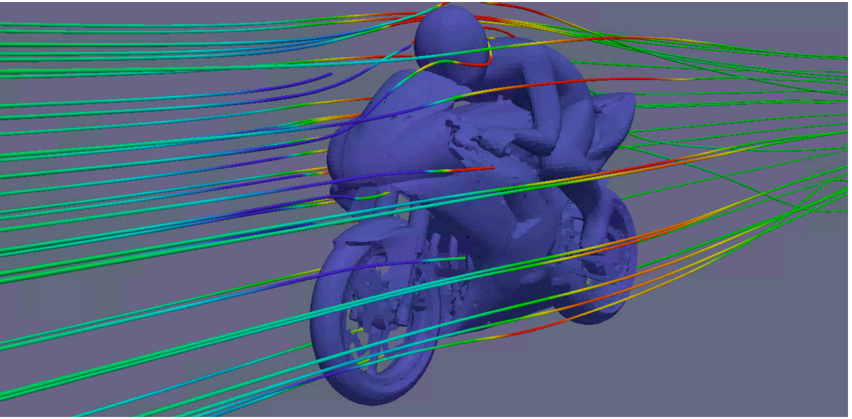


Scalability Limit

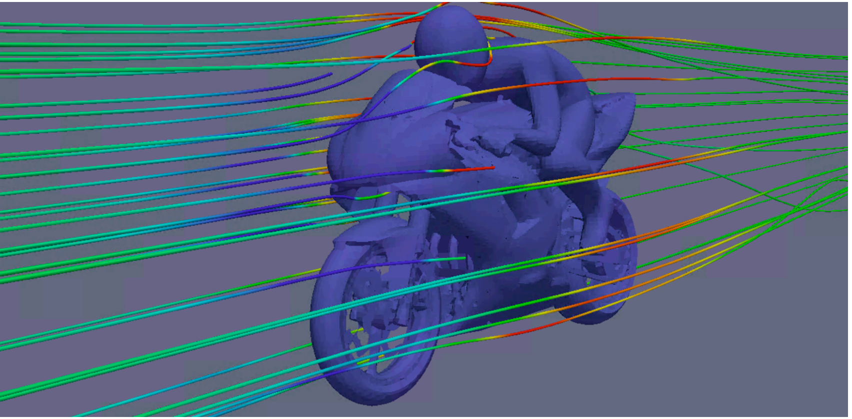
- Inflated motorBike
- Intel E5-2680v3 @ 2.5GHz
- OpenFOAM/2.3.1

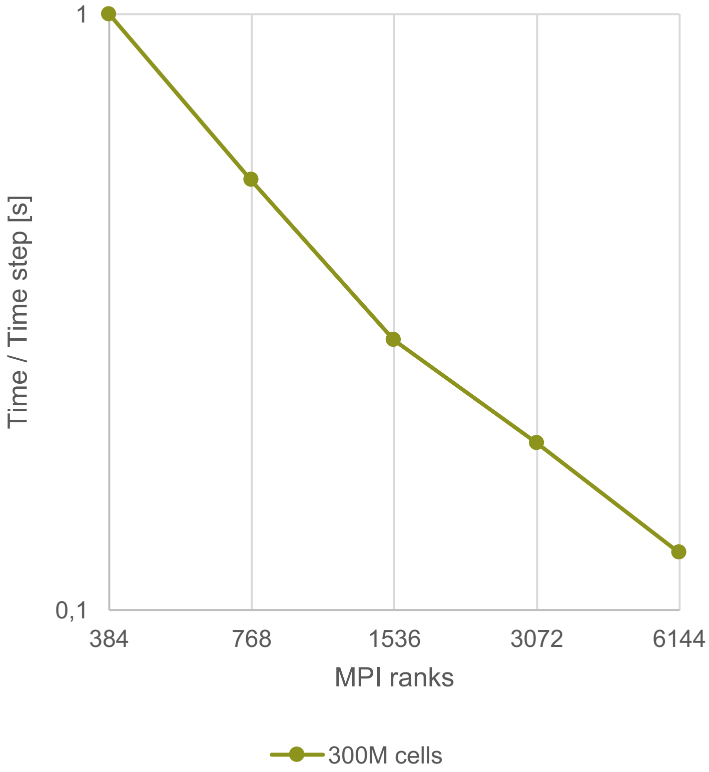




Scalability Limit

- Inflated motorBike
- Intel E5-2680v3 @ 2.5GHz
- OpenFOAM/v1612+





Recap | Where do we want to go?

- **Multi and many core architectures**
  - A lot more cores to feed
  - Need for further scaling and/or hybrid approach
- **Wider SIMD/Vector instructions**
  - Suboptimal vectorization will hurt you more
- **Find optimal solution for I/O design**
  - This may be solved from vendor side

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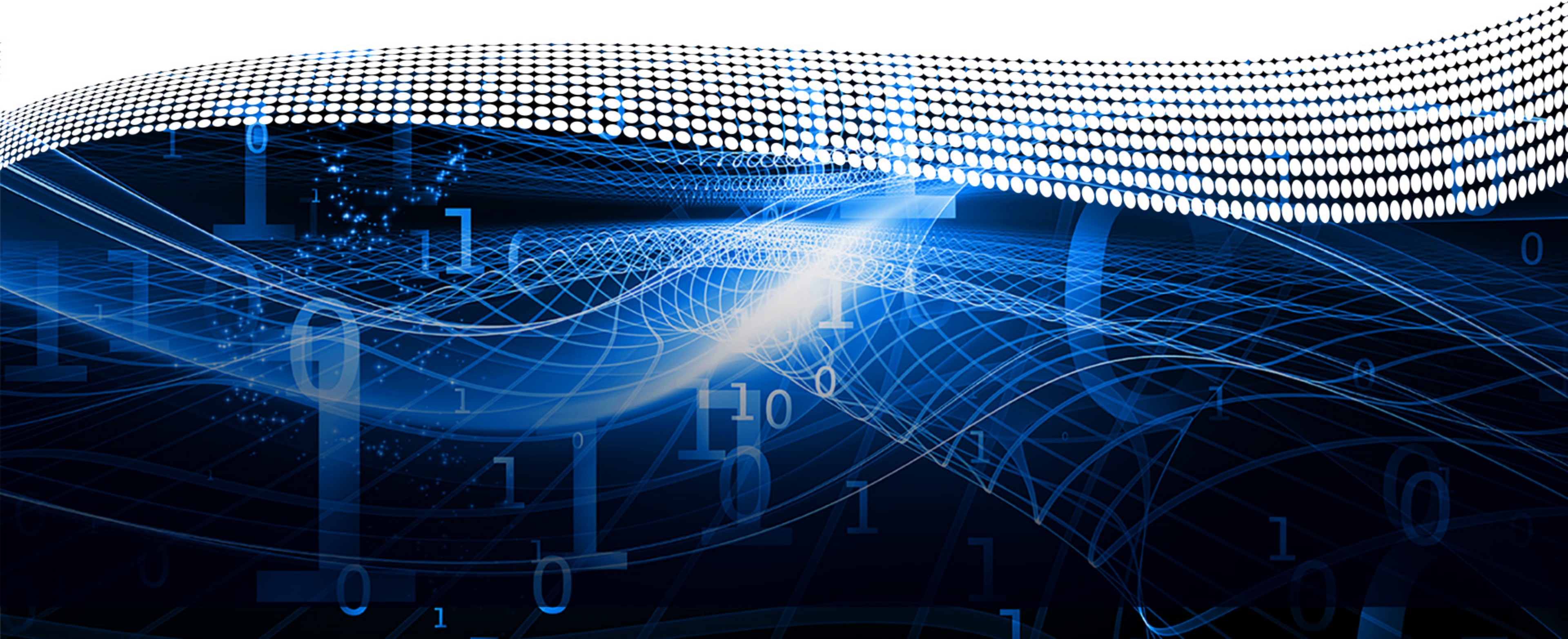

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