Simulation Techniques & Scientific Computing

UNIVERSITÄT SIEGEN

Results of Ateles and Musubi Code Analyses

Harald Klimach

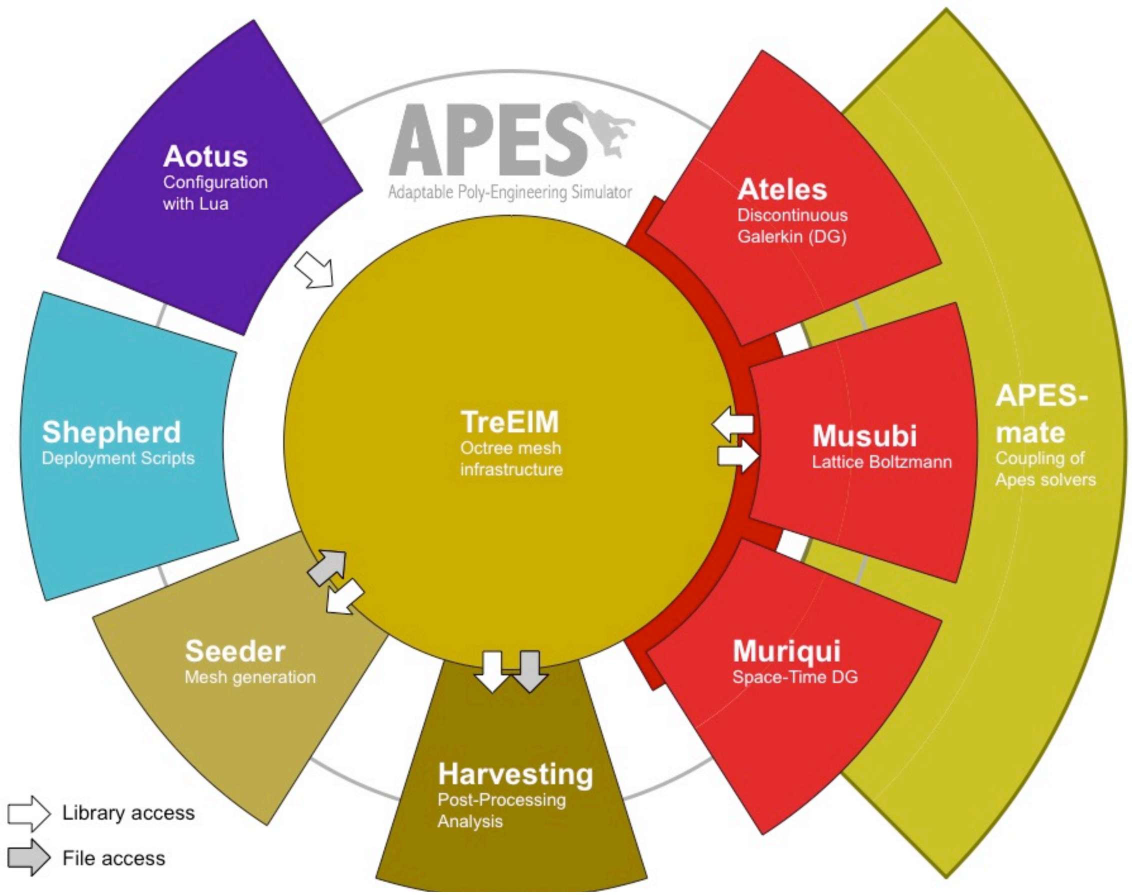
harald.klimach@uni-siegen.de

University of Siegen

Our Group

- Simulation Techniques and Scientific Computing at University of Siegen
- Head: Sabine Roller
- Part of the engineering department
- Looking into large scale simulations, mainly in the field of computational fluid dynamics

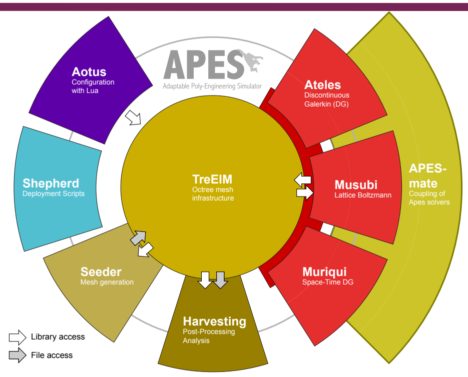
About our Software (APES)



About our Software

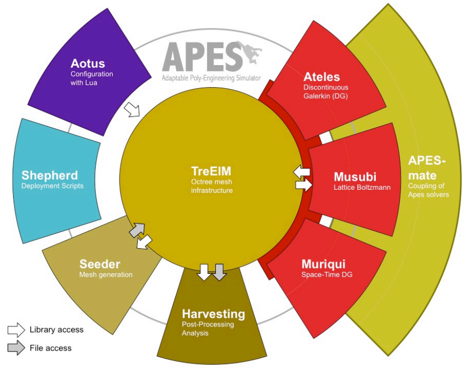
- Started development in 2011 at the German Research School for Simulation Sciences in Aachen
- Set out to overcome scalability limitations we encountered with previous tools
- Development in modern Fortran (mainly F95, but some F2003 features required)
- All in all somewhat more than 100,000 lines of code. Definitely smaller than 200k.

About TreElM



- Basis: octree mesh representation
- Partitioning by space-filling curve
  - Simplistic mesh representation on disk, easy to read on a distributed parallel system
  - Little amount of meta data (number of elements, definition of root node) can be read in by single process and broadcasted
  - All other data can be read independently
- Distributed parallel neighbor identification in locally refined meshes

Mesh Generation (Seeder)



- Creating Octree Meshes
  - With specific data format
  - Allow for special boundary treatment in
    - Lattice-Boltzmann (q-values)
    - Discontinuous Galerkin (penalty terms)
- Serial for up to 2 billion elements
- Parallel version for larger meshes

- Solver internal generation of simple meshes

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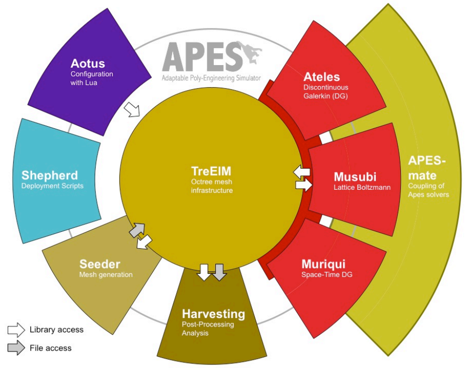
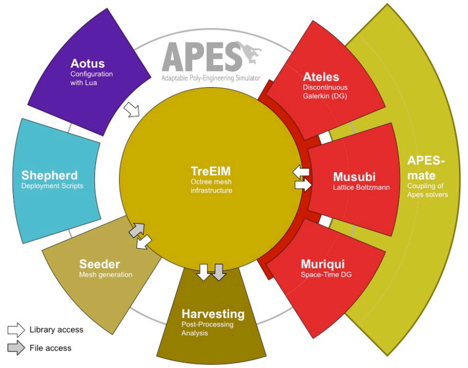
Post-Processing (Harvester)



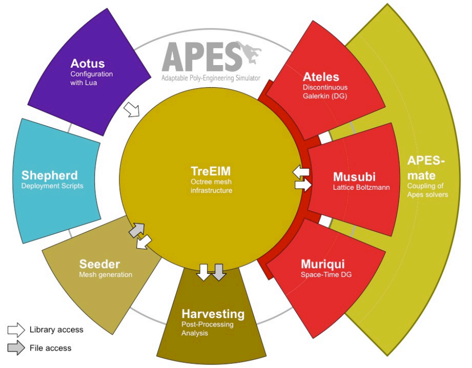
- Generating visualization files
  - (VTK)
- Out of binary dumps by the solver
- Solver writes binary data via MPI-IO to single file in solver-specific format
- Postprocessing separated to allow processing on different machines
- Allows extraction of parts and computation of derived quantities

Configuration (Aotus)



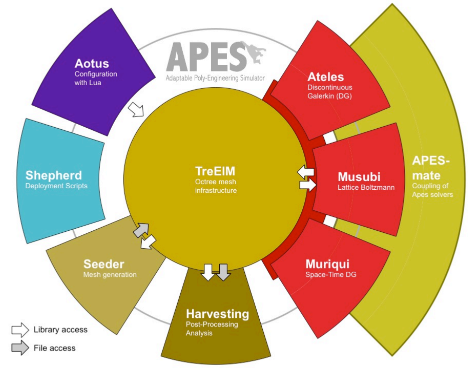
- Quite generic Lua binding
- Utilizes ISO-C interface
- Some abstractions to ease use as configuration for Fortran
- Allows for user-defined functions
- Parameter relations can be explicitly expressed in the configuration
- Read by single process and broadcasted

Musubi



- Lattice-Boltzmann Solver
  - Simple loop operation
  - Explicit scheme for incompressible flows
- Implements various Kernels
- Unstructured neighbor handling (from treelm), sparse matrix approach
- Allows for multi-species simulations
- Allows for locally refined simulations

Ateles



- Discontinuous Galerkin
  - High order (8 and higher)
  - Modal/nodal representations
- For compressible flows
- Also implements other hyperbolic systems, like Maxwell equations
- Cubical elements
- Geometry by penalization

On the Work by POP

- Code analyzed and improved by:
  - José Gracia
  - Christoph Niethammer
  - Stephan Walter
  - Anastasia Shamakina

- Many thanks to those kind colleagues at HLRS

Systems used?

- Ateles was analyzed on the Stuttgart system Hazel Hen

- Musubi was investigated on our local university cluster Horus
  - Tools were installed in cooperation between university computing center and POP staff
  - Was not involved in that as a user

Ateles Reports

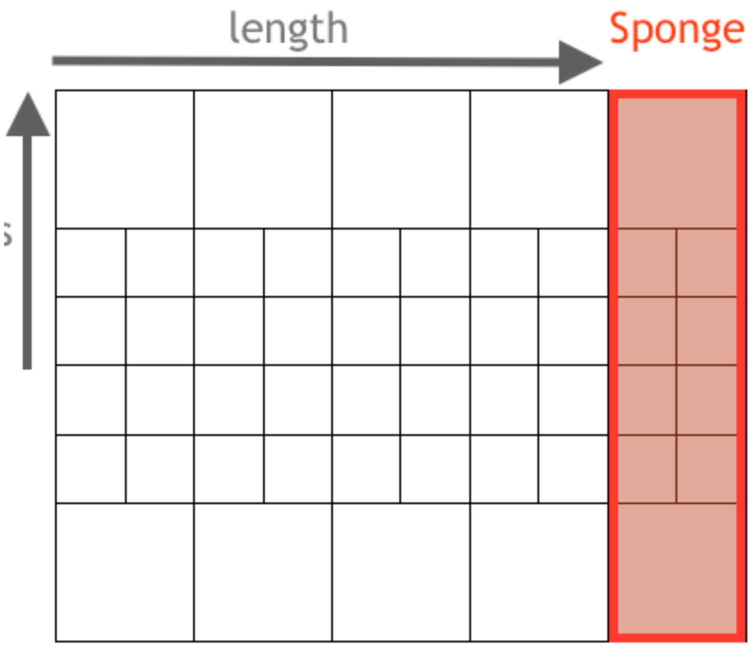
- There have been three reports on Ateles
  - The initial performance audit
  - A more detailed performance plan
  - A proof of concept implementing some suggestions

Ateles Setup

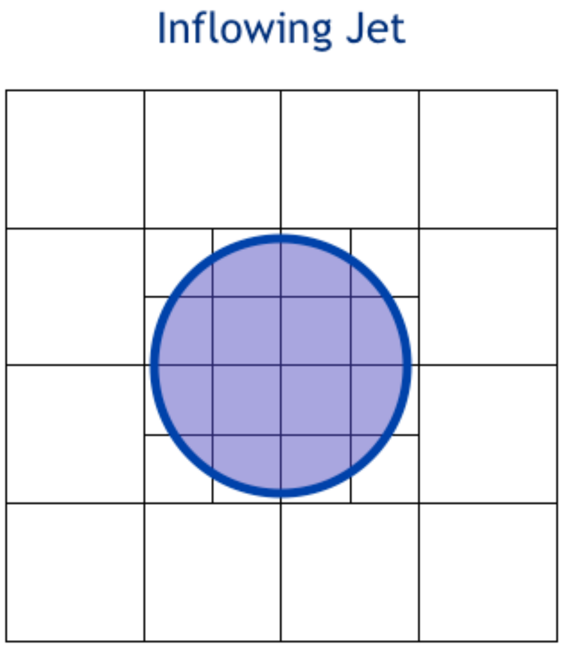
- POP asked for a realistic testcase
- The setup I provided them was the 3D Jet with local refinement, sponge and covolume
- This includes basically all relevant features

- Never looked into the performance of this ourselves before

Setup Illustration

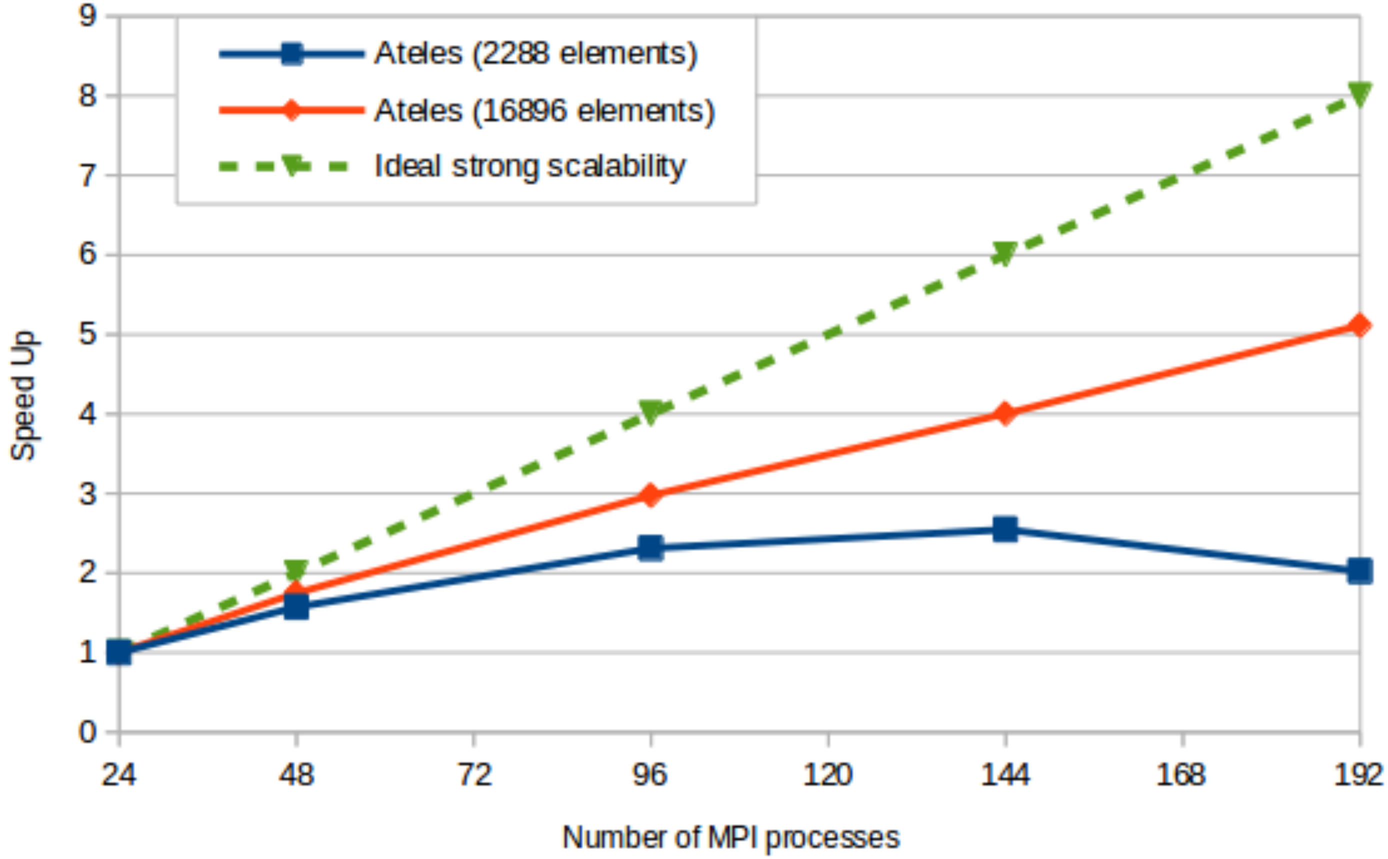


Cut in the xy-plane

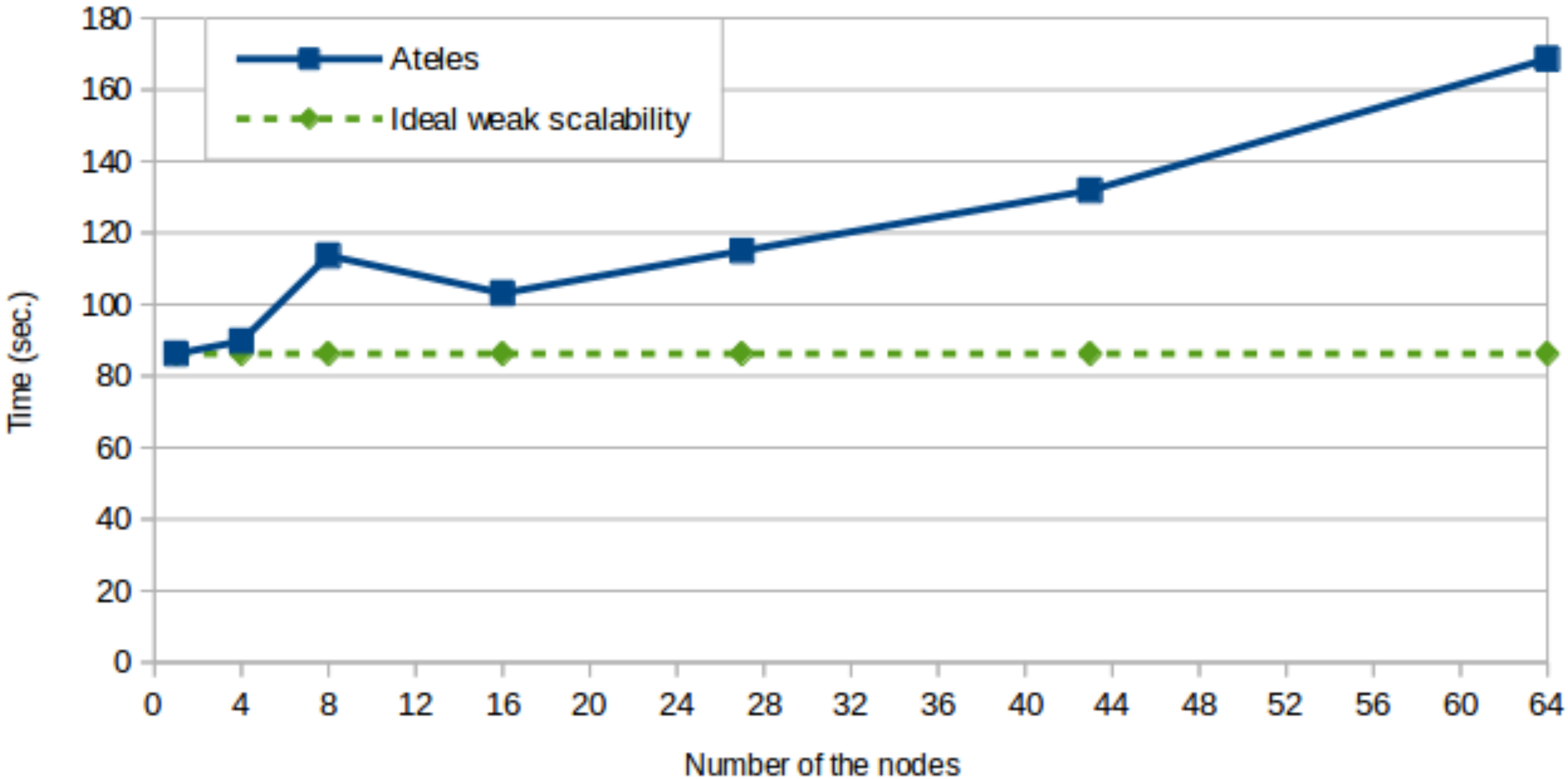


View from the left (yz-plane

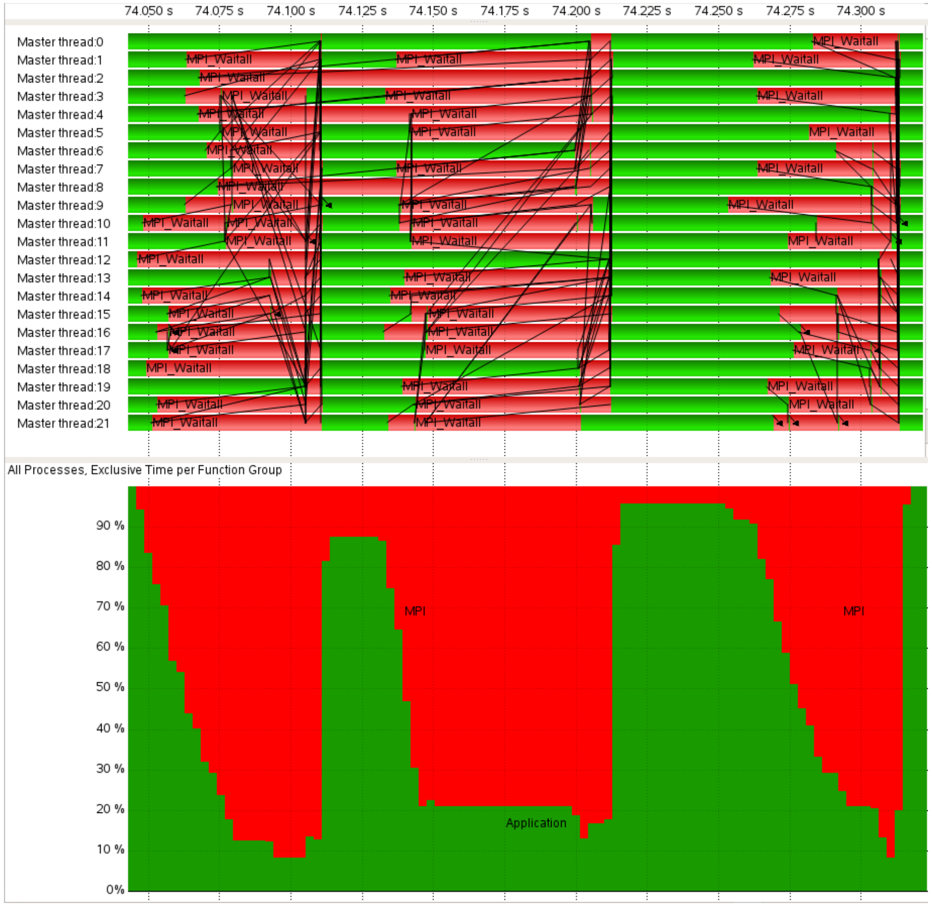
Bad Strong Scaling ...



Bad Weak Scaling



Reason: Large Load Imbalances



Code Analysis

- Load imbalances due to non-optimized code in covolume:
- Posofmodgcoeffqtens: Index lookup in the polynomials
  - Had been replaced in other parts of the code but not in covolume -> gone now completely
- Facevalleftbndans and facevalrightbndans: functions just returning 1 or -1, easily inlined
- Tem_isnan: check interval

Lua Functions...

- Flu_* and aot_* functions showed up as contributing factors to the load imbalance
  - Can be overcome by implementing the respective functions as predefined functions in Fortran itself.

Recommendations

- Avoid many small function calls.
  - Kind of done already by Peter

- Reduce the amount of duplicate computation, or specialise code a compiletime.
  - Harder to achieve, but probably due to no one looking into the covolume stuff for optimization so far
- Reduce load imbalance by improving static domain decomposition.

Performance Plan

- More detailed look into load imbalances
- Vampir traces
- And Scalasca analysis

Intermediate result

- Imbalances manifest at two points:
  - Allreduce after each timestep (actually controllable with check interval)
  - Waitall after each substep (neighbor exchange)
- Further investigation of the imbalances at the waitall as more severe.

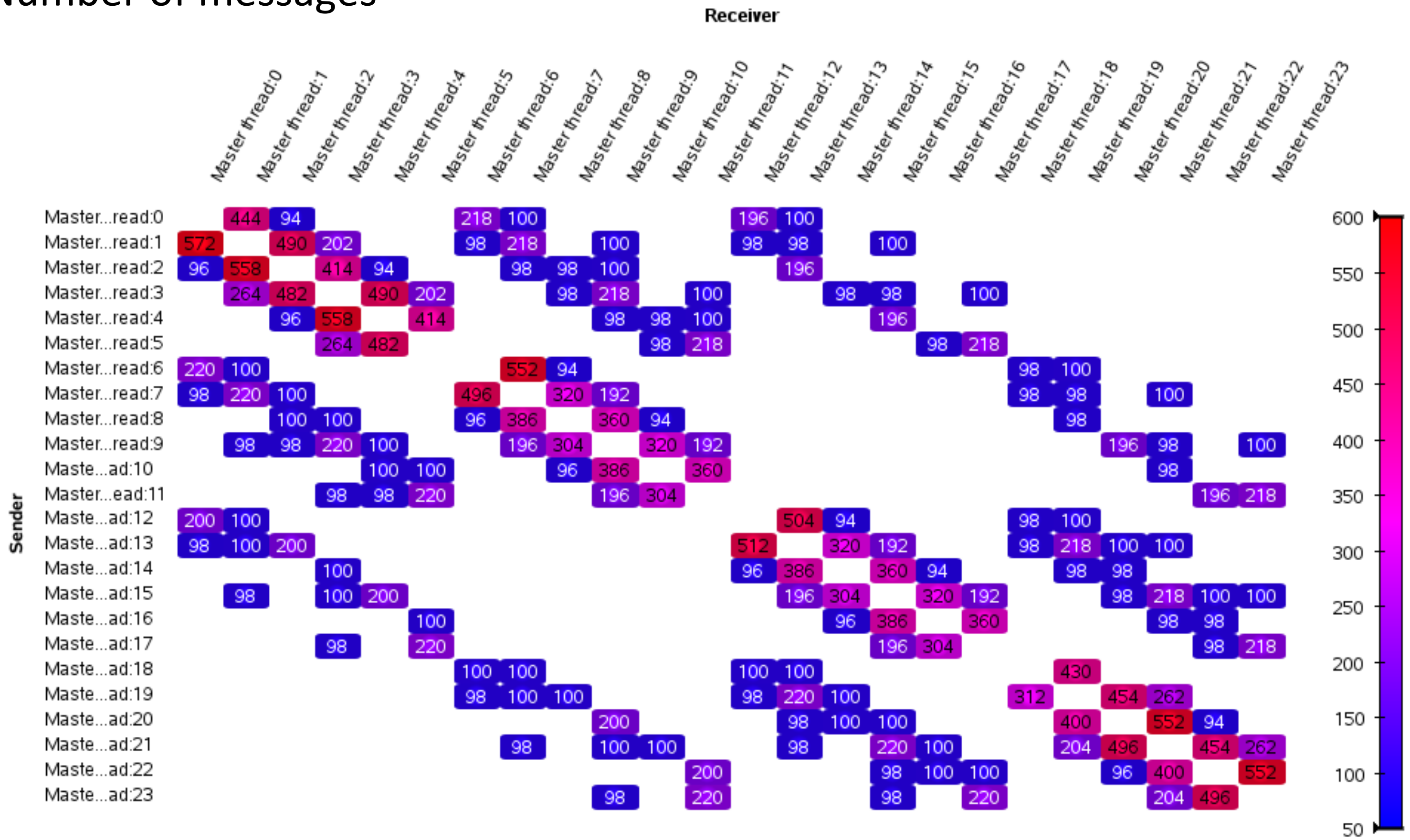
Observation

- Load imbalances mainly due to covolume interpolation at refinement boundaries
  - Note: These especially made use of many small function calls (low efficiency)

- The computational load imbalance clearly is of main interest.
- Nevertheless, also the communication has been investigated.

Communication Matrix

Number of messages



Surprise: 0-sized messages

Proof of Concept

- Look into serial performance and implementation of some of the suggestions from the Audit
- Improving code vectorization
- Brief evaluation on SX-ACE

Main Factors

- Inlining posofmodgqtens reduced the number of function calls by nearly 97 %
- Reduces the execution time on Hazel Hen to 94 % of the original, not inlined, code version
- Replace divisions by multiplications, further reduction to 72 % of the inlined version.

SX-ACE

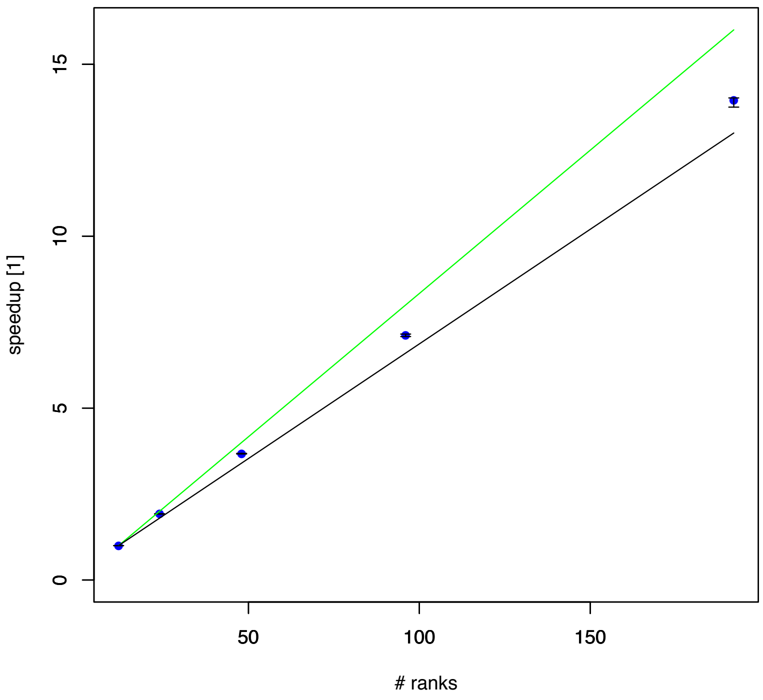
- Bad vectorization because sxmpif03 often vectorizes over nScalars
- In the meantime improved for various code paths

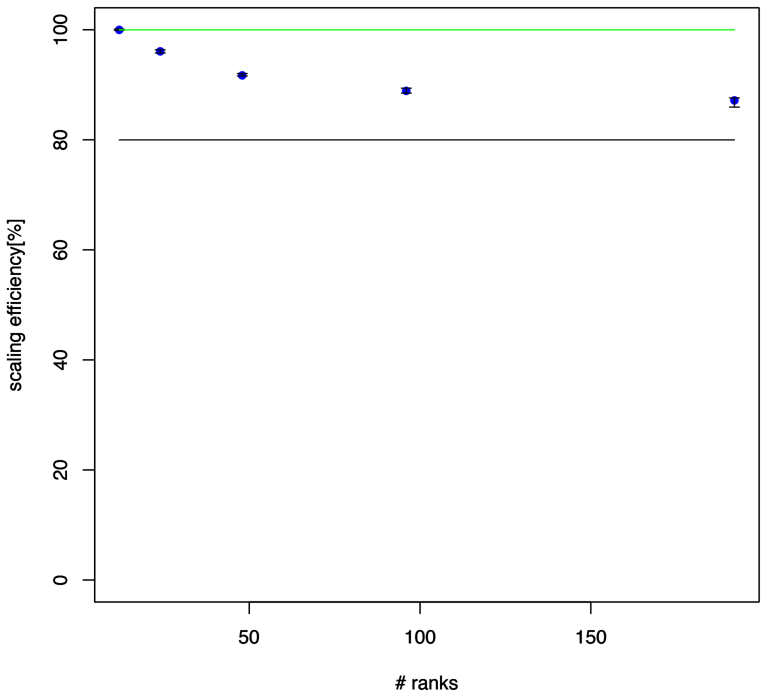
- Strong memory-conflicts for orders of powers of two (should be avoided, padding may need to be introduced)!

Musubi

- Testcase was flow around a sphere
  - With involved boundaries (q-values, inflow and outflow)
  - No local refinements
  - Excluded I/O (only reading of mesh in the initialization)
- Run on Horus
  - Intel Xeon X5600 6-core CPU, 2 sockets per node
  - Infiniband Interconnect

Main Focus: Scalability (Strong Scaling)



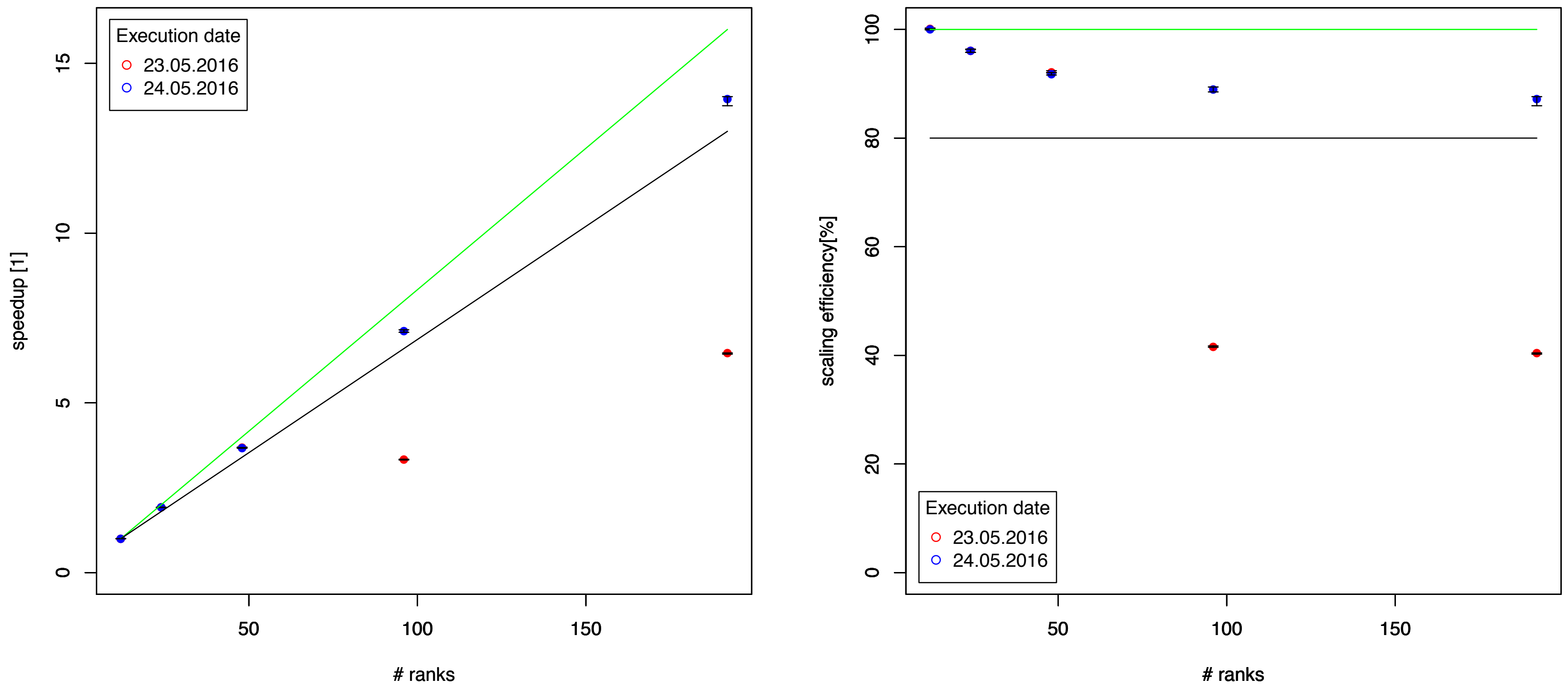


Surprisingly Bad Scaling

- Still acceptable, but...
- Expected to see a better scaling, as we usually observe nearly perfect scalability with these kind of testcases

- Turns out, the boundary conditions cause a larger load-imbalance than expected

Machine Seems to Have Bad Days...



Observations from the Machine (Horus)

- Significant performance variability
  - Clock speed degeneration, probably due to *ondemand* performance governor, mainly in MPI IO and MPI_Ssend
  - Day to day variation of overall instructions per second
  - Noise on the interconnect

Recommendations for Musubi

- Imbalances by bondaries should be taken care
  - We have dynamic load-balancing now
- Using non-temporal stores
  - Implemented now, improved performance by around 50%
- Avoid indirection
  - Can't do that
- Overlap communication and computation
  - Requires major effort

Feedback

- The audits by POP were very helpfull to us and revealed various issues, we weren't even aware of before
- Initial communication could have been a little more active (things like the inlining of small functions could have been easily resolved early on)
- Would be happy to have code modifications on a branch or somewhere

The Reports are Great

- I love the neat and well explained reports
- I can give them to the developers along with lessons learned
- Direct recommendations on Do's and Don'ts for everbody

- Again some earlier communication with preliminary results is even more productive.

Thank you!