Enabling Performance Engineering in Hesse and Rhineland-Palatinate

Manuel Baumgartner, Christian Bischof, André Brinkmann, Alexandru Calotoiu, Nicolas Gauger, Matthias Kretz, Volker Lindenstruth, Max Sagebaum, Dörte Carla Sternel, Felix Wolf

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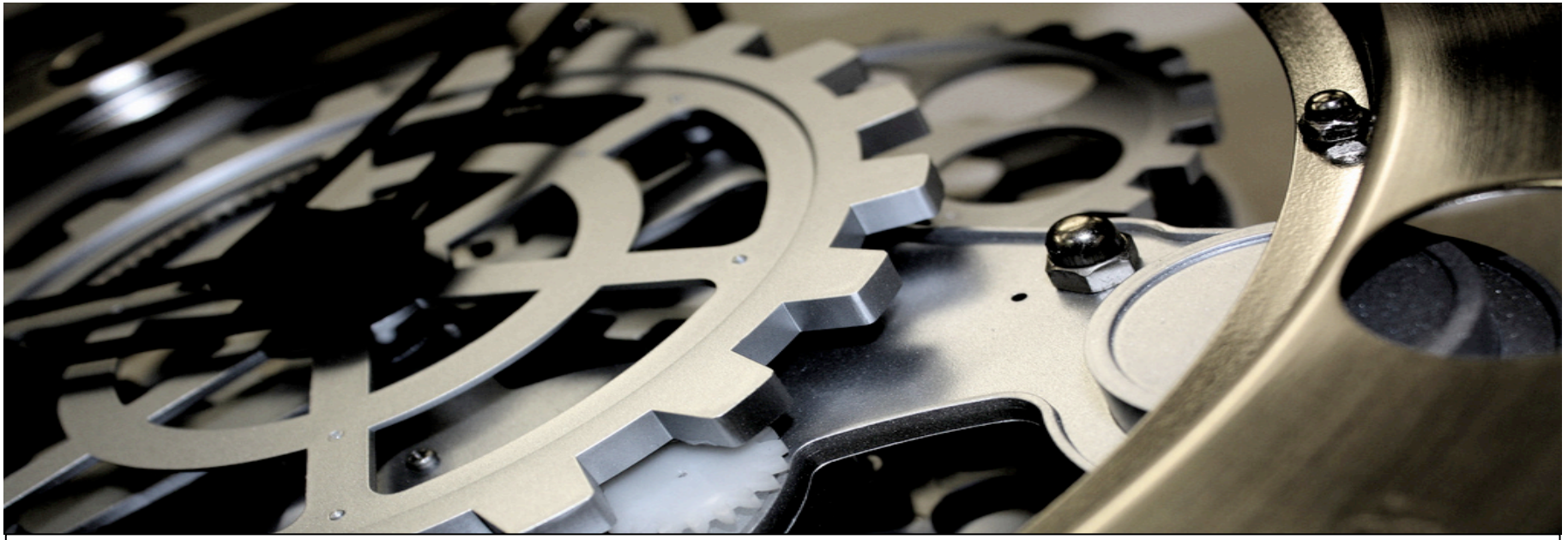

TECHNISCHE UNIVERSITÄT DARMSTADT

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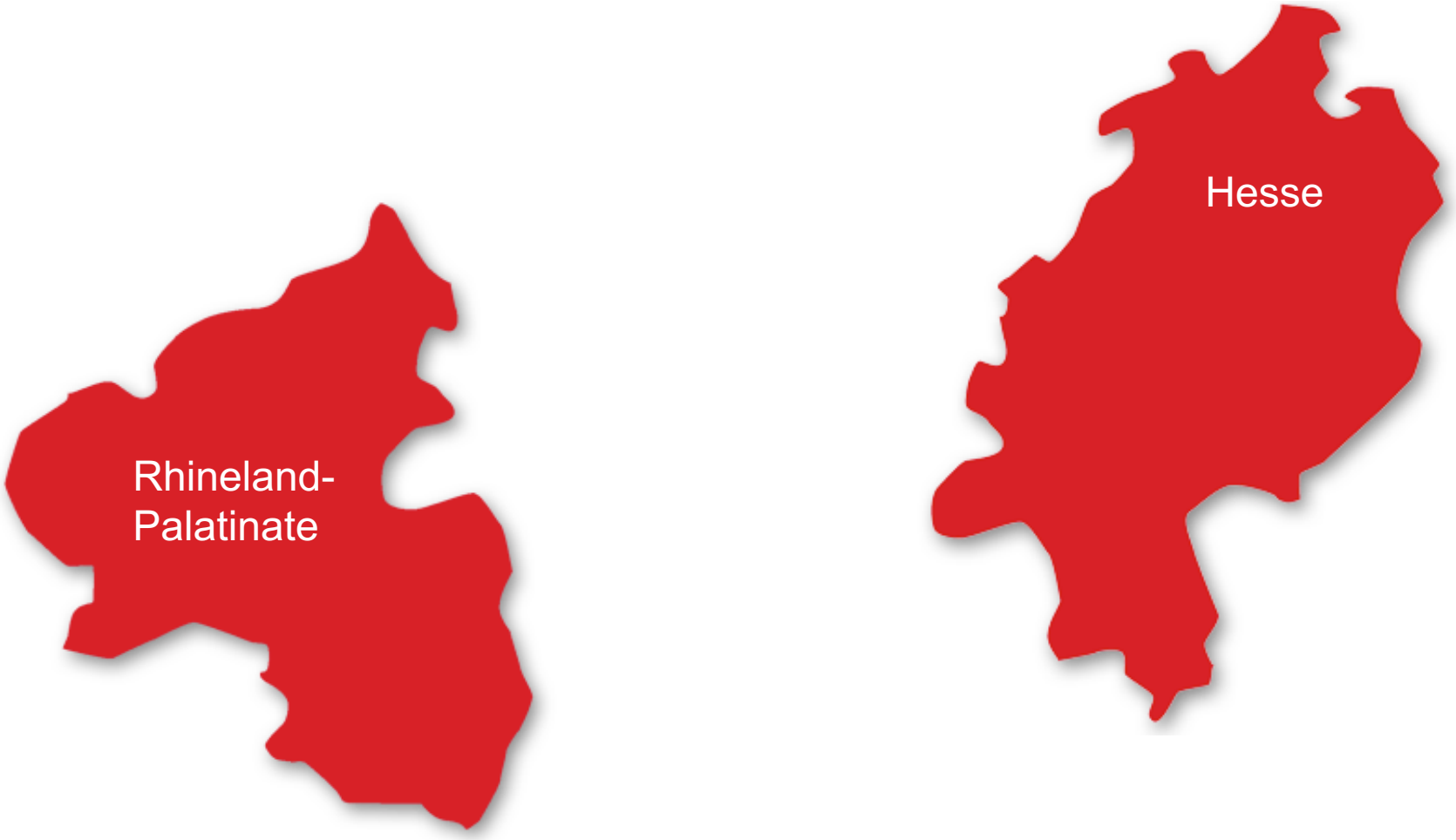
TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Enabling performance engineering

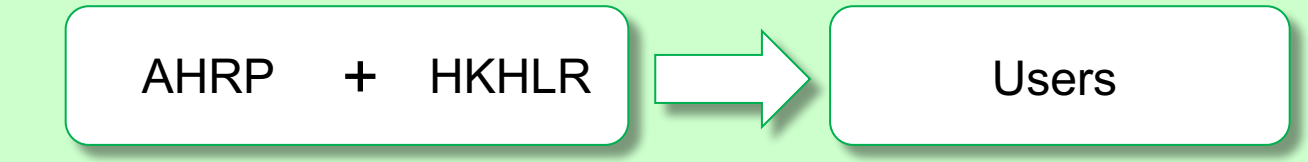


Enabling performance engineering

AHRP
Allianz für Hochleistungsrechnen Rheinland-Pfalz

Objective: Expand and deepen HPC support in areas where existing scientific expertise coincides with critical user needs.

Approach:



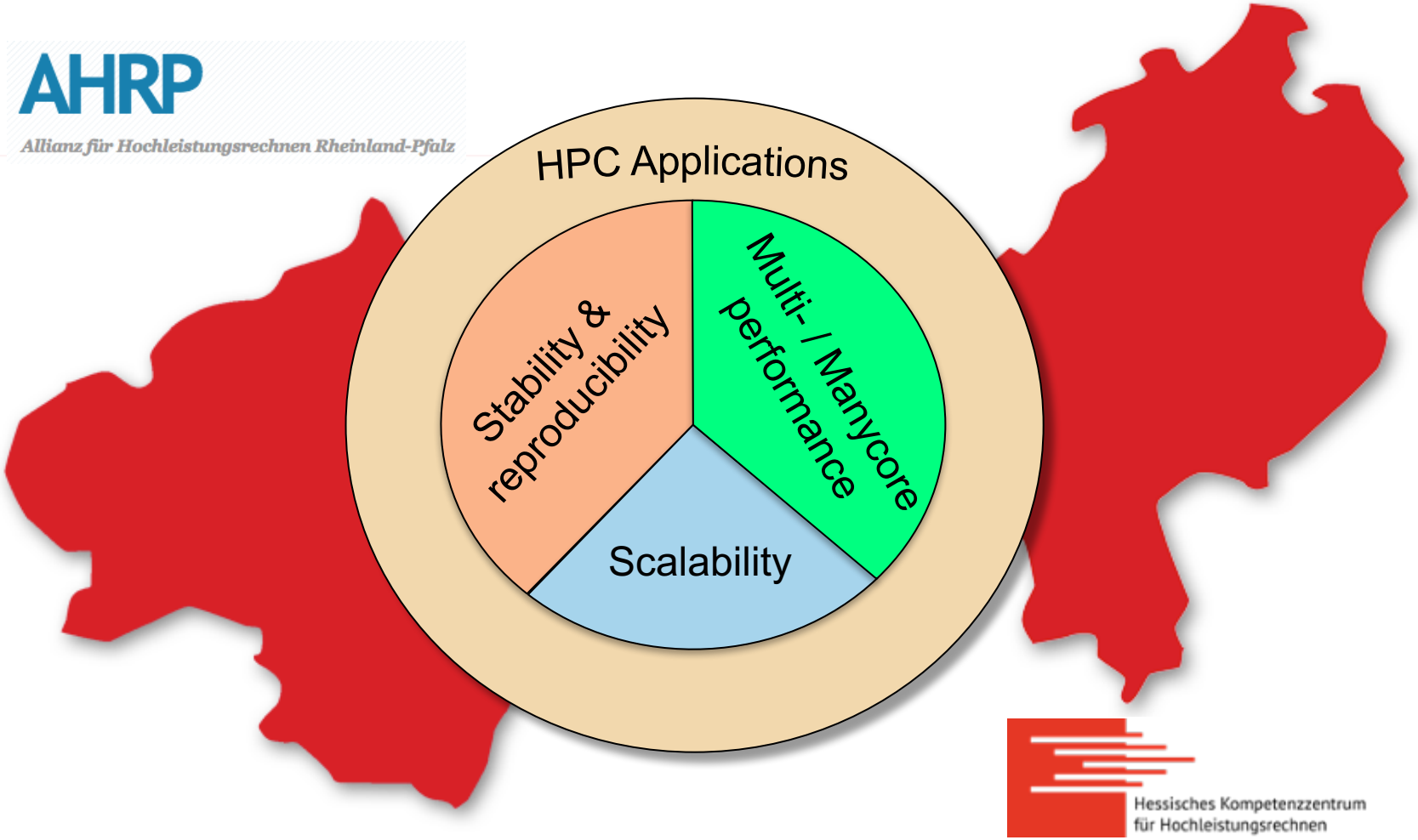
Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Enabling performance engineering

Principal Investigators

Christian Bischof (coordinator) – Technische Universität Darmstadt
André Brinkmann – Johannes Gutenberg Universität Mainz
Nicolas Gauger – Technische Universität Kaiserslautern
Volker Lindenstruth – Goethe-Universität Frankfurt am Main
Dörte Carla Sternel – Hessisches Kompetenzzentrum für Hochleistungsrechnen
Felix Wolf – Technische Universität Darmstadt

Enabling performance engineering



HPC support structures

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Hessisches Kompetenzzentrum
für Hochleistungsrechnen

EPE Activities

- 1st EPE workshop, Mainz, May 2017
- 8th HiPerCH workshop, Marburg, September 2017
- Expert workshop on scalability analysis, Darmstadt, November 2017
- User meeting on scalability analysis, Darmstadt, February 2018
- Totalview tutorial, Kaiserslautern, March 2018
- Minisymposium at WCCM 18, July 2018
- FEPA-Workshop Erlangen, July 2018
- 10th HiPerCH workshop, Darmstadt: September 2018

Courses

- Introduction to Bash
- Introduction to Mogon

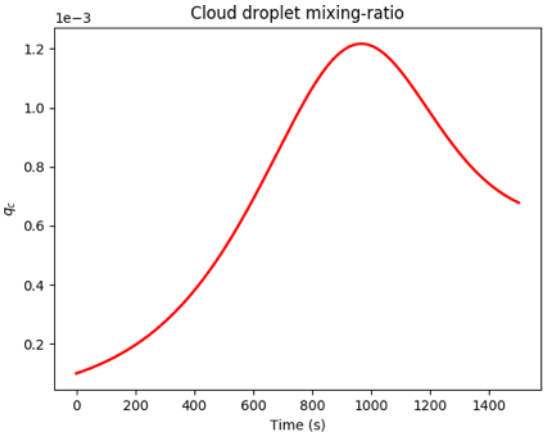
User Engagement

- HPC-Cafe
- Bachelor & Master Theses

Algorithmic reproducibility

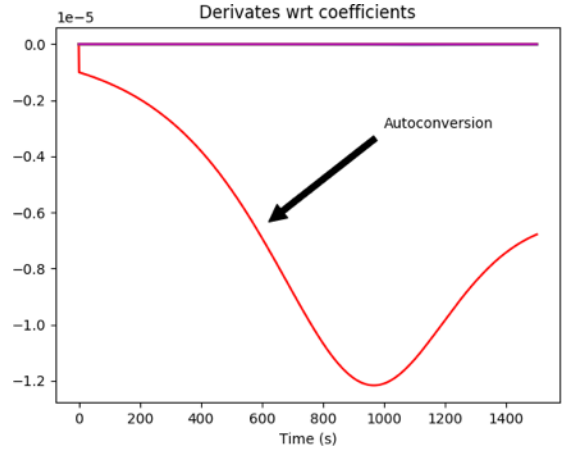
What affects the predictability of weather?

- Sensitivity of numerical models
- Collaboration with **TRR 165** “Waves to weather”



Status

- Applied algorithmic differentiation to cloud scheme
  - Warm cloud scheme of COSMO
- Identified coefficients and parameters with large derivatives



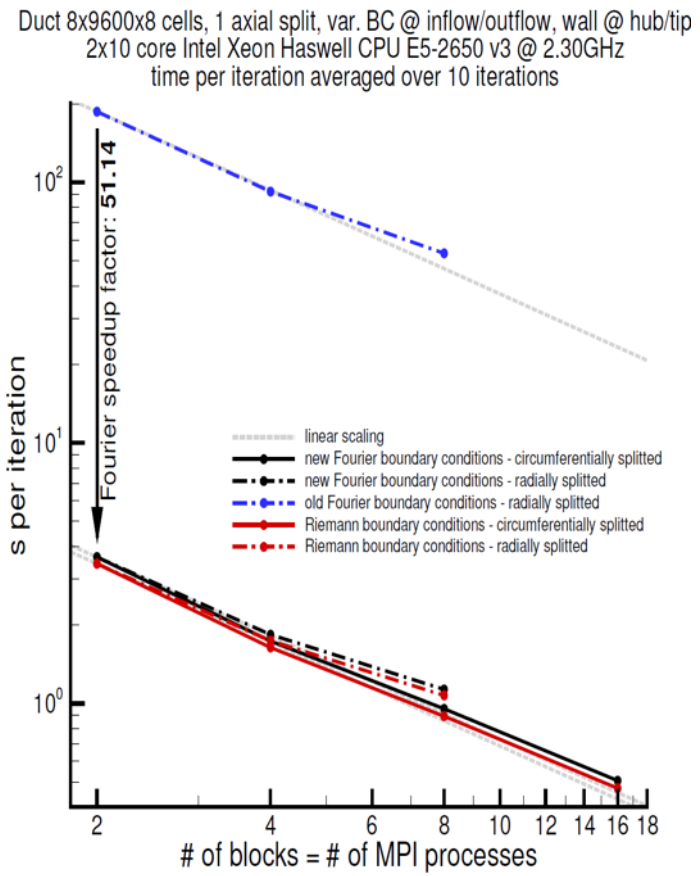
Algorithmic stability & performance

Help measure stability of algorithms

- Provide tools to analyze the Lipschitz constants / condition numbers of each code part

Status

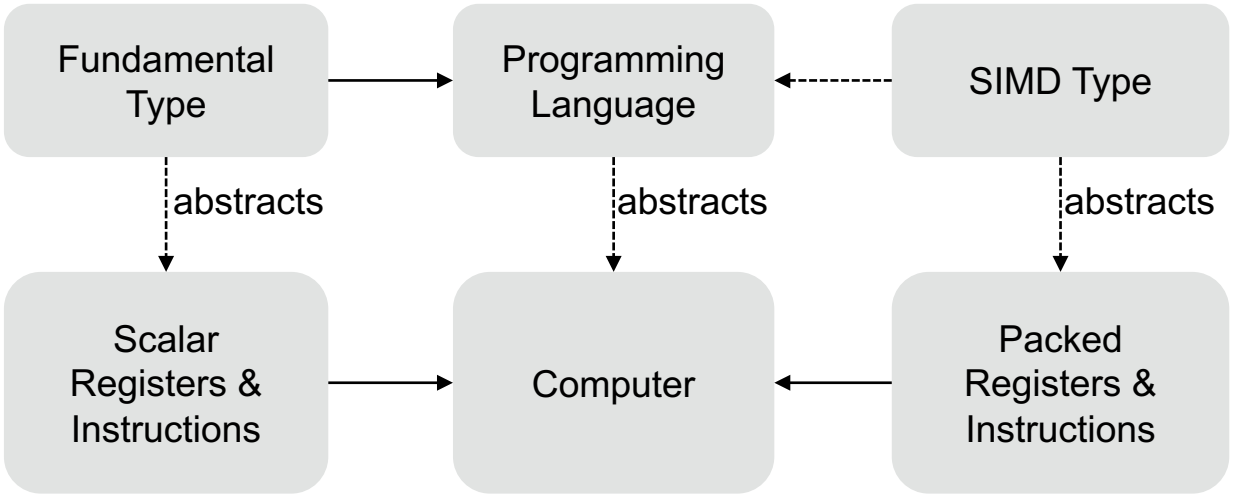
- CFD suite TRACE – Replacement of hand-made FFT implementation through library
  - Stability proven
  - **Greatly improved maintainability**
  - **Speedup of 51!** (according to DLR)
- Ongoing: exchange of hand-made linear solver in industrial mold-filling simulation



Multi- and manycore performance

C++ extension for explicit data parallelism

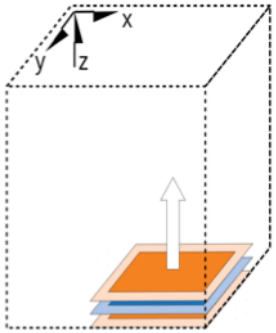
- Allows numerical algorithm developers to exploit hardware parallelism in a portable way and with minimal effort
- Vc library provides portable, zero-overhead C++ types for explicitly data-parallel programming



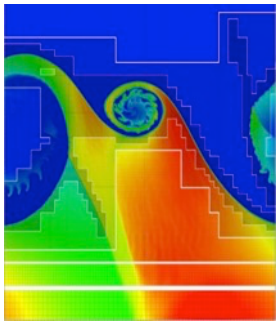
Multi- and manycore performance (2)

Status application

- Collaboration with Prof. Rezolla @ Goethe-Universität Frankfurt
  - Relativistic hydrodynamics simulation, encompassing turbulence, accretion and neutron star collision
- Coupled wit the AMRex framework
- **3x CPU speedup** with Vc library
- GPU port in progress



2.5D Blocking

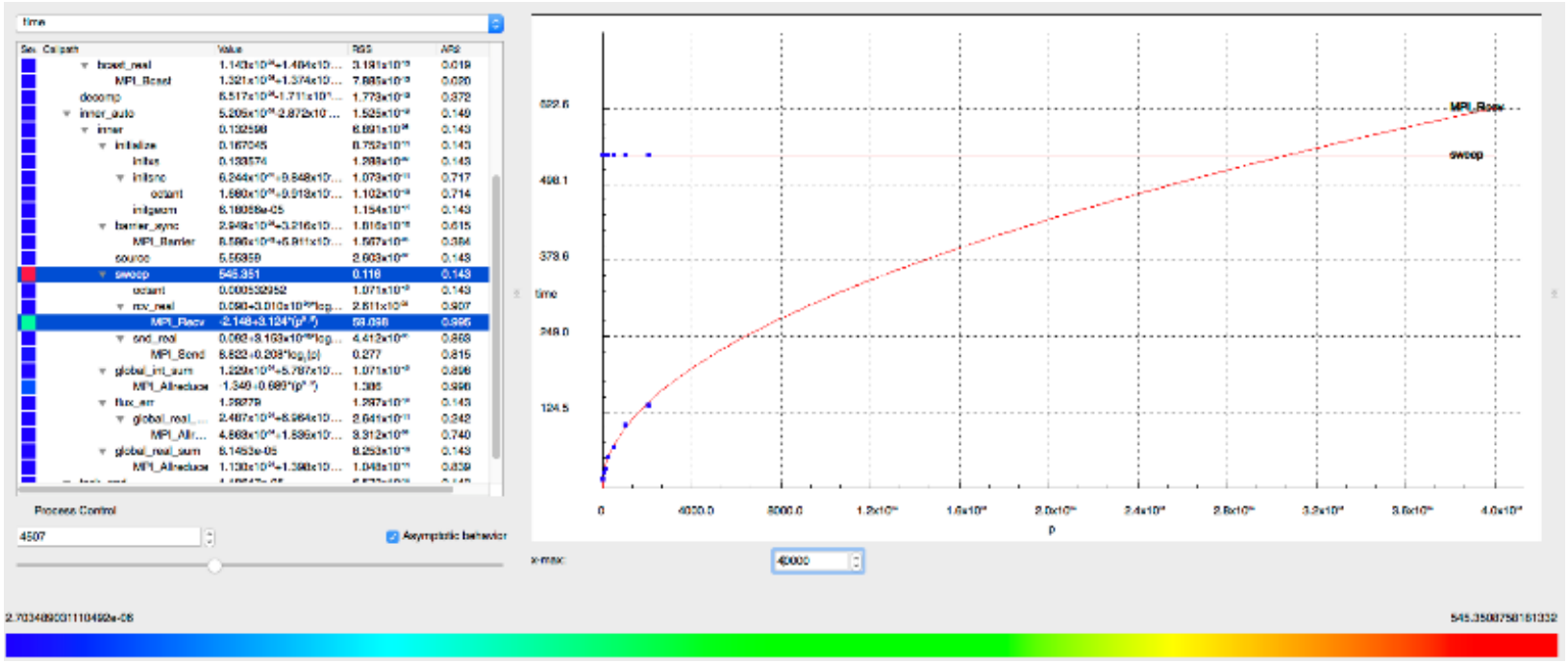

Elias R. Most
(dev of CPU code)

Status standardization

- ISO TS 19570:2018, containing SIMD types, awaiting publication
- Independent implementation exists in libc++ (Clang)
- Contributed implementation to libstdc++ (GCC)

Scalability

Help developers identify and resolve scalability limitations in their codes using **Extra-P**

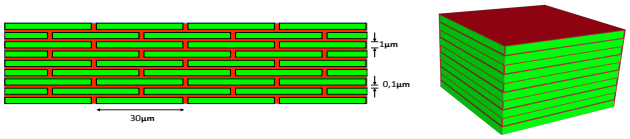


http://www.scalasca.org/software/extra-p/download.html

Scalability (2)

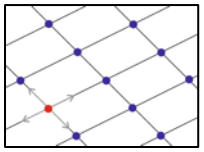
UG4 @ GCSC, Frankfurt

- Grid-based solution of PDEs
- Effects of problem size and #processes on performance



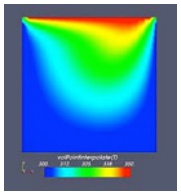
LLL Algorithm @ SC, Darmstadt

- Lattice-based cryptographic algorithm
- Higher complexity desirable !
- Empirical complexity lower than expected



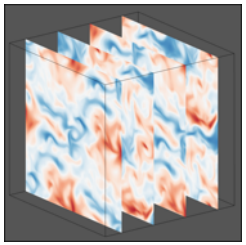
OpenFoam @ MMA, Darmstadt

- Open-source CFD package
- Many different solvers
- Derived hardware requirements for icoFoam



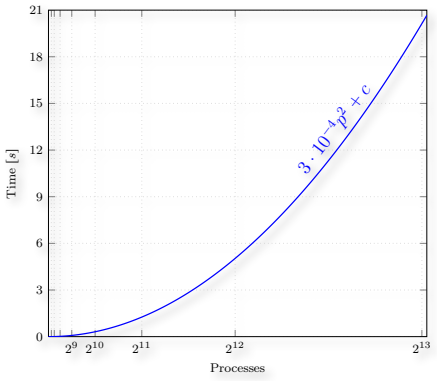
FASTEST @ SC, TU Darmstadt

- Flows in complex 3D configurations
- Modeled strong scaling behavior
- Reproducibility of performance

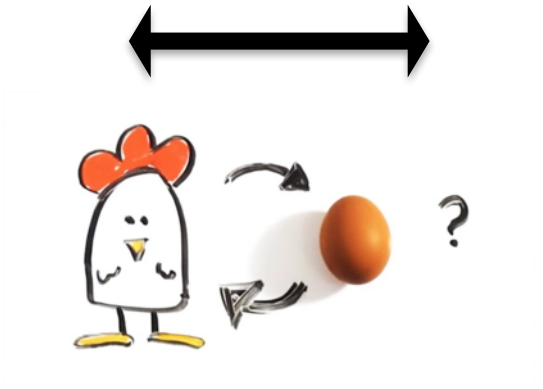


Service: automated scalability proof for compute time applications

Required for access to large-scale cluster



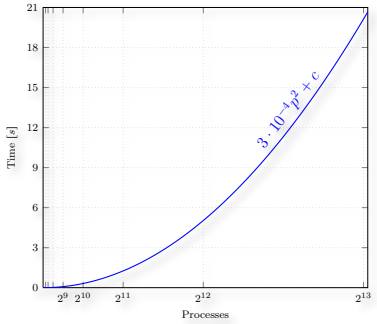
Scalability proof



Access to HPC resources

Service: automated scalability proof for compute time applications (2)

Application



Scalability proof

Status

- Prototype available for Lichtenberg cluster users at TU Darmstadt
- Integration with Workflow Manager JUBE (FZJ) in progress

Summary

- New performance engineering services offer
  - Speedup
  - Productivity improvements
  - Increased maintainability
  - Easier ways of preparing compute time grant proposals
- Teaching activities bring knowledge to users
- Individual user support allows complex application tuning

Project publications

[1] Michael Burger, Christian Bischof, Alexandru Calotoiu, Felix Wolf, Thomas Wunderer, Johannes Buchmann: Exploring the Performance Envelope of the LLL Algorithm. In *CSE 2018 - 21st IEEE International Conference of Computational Science and Engineering, Romania*, IEEE Computer Society, October 2018, (to appear).

[2] Alexandru Calotoiu, Alexander Graf, Torsten Hoefler, Daniel Lorenz, Sebastian Rinke, Felix Wolf: Lightweight Requirements for Exascale Co-design. In Proc. of the 2018 IEEE International Conference on Cluster Computing (CLUSTER), Belfast, UK

[3] Aamer Shah, Matthias S. Müller, Felix Wolf: Estimating the Impact of External Interference on Application Performance. In *Proc. of the 24th Euro-Par Conference, Turin, Italy*, volume 11014 of *Lecture Notes in Computer Science*, pages 46-58, Springer, August 2018.

[4] Alexander Hück, Christian Bischof, Max Sagebaum, Nicolas R. Gauger, Benjamin Jurgelucks, Eric Larour & Gilberto Perez: A usability case study of algorithmic differentiation tools on the ISSM ice sheet model, Optimization Methods and Software, 33:4-6, 844-867, 2018)

[5] Manuel Baumgartner & Peter Spichtinger: Towards a bulk approach to local interactions of hydrometeors, Atmos. Chem. Phys., 18, 2525-2546, 2018

[6] Kashif Ilyas, Alexandru Calotoiu, Felix Wolf: Off-Road Performance Modeling – How to Deal with Segmented Data. In Proc. of the 23rd Euro-Par Conference, Santiago de Compostela, Spain

[7] Patrick Reisert, Alexandru Calotoiu, Sergei Shudler, Felix Wolf: Following the Blind Seer – Creating Better Performance Models Using Less Information. In Proc. of the 23rd Euro-Par Conference, Santiago de Compostela, Spain

[8] Sergei Shudler, Alexandru Calotoiu, Torsten Hoefler, Felix Wolf: Isoefficiency in Practice: Configuring and Understanding the Performance of Task-based Applications. In Proc. of the ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP), Austin, TX, USA, 2017

[9] Manuel Baumgartner & Peter Spichtinger: Local Interactions by Diffusion between Mixed-Phase Hydrometeors: Insights from Model Simulations. *Mathematics of Climate and Weather Forecasting*, 3(1), pp. 64-89., 2017