



Research Center High Performance Computing

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DK+ Winterschool, January 29, 2019

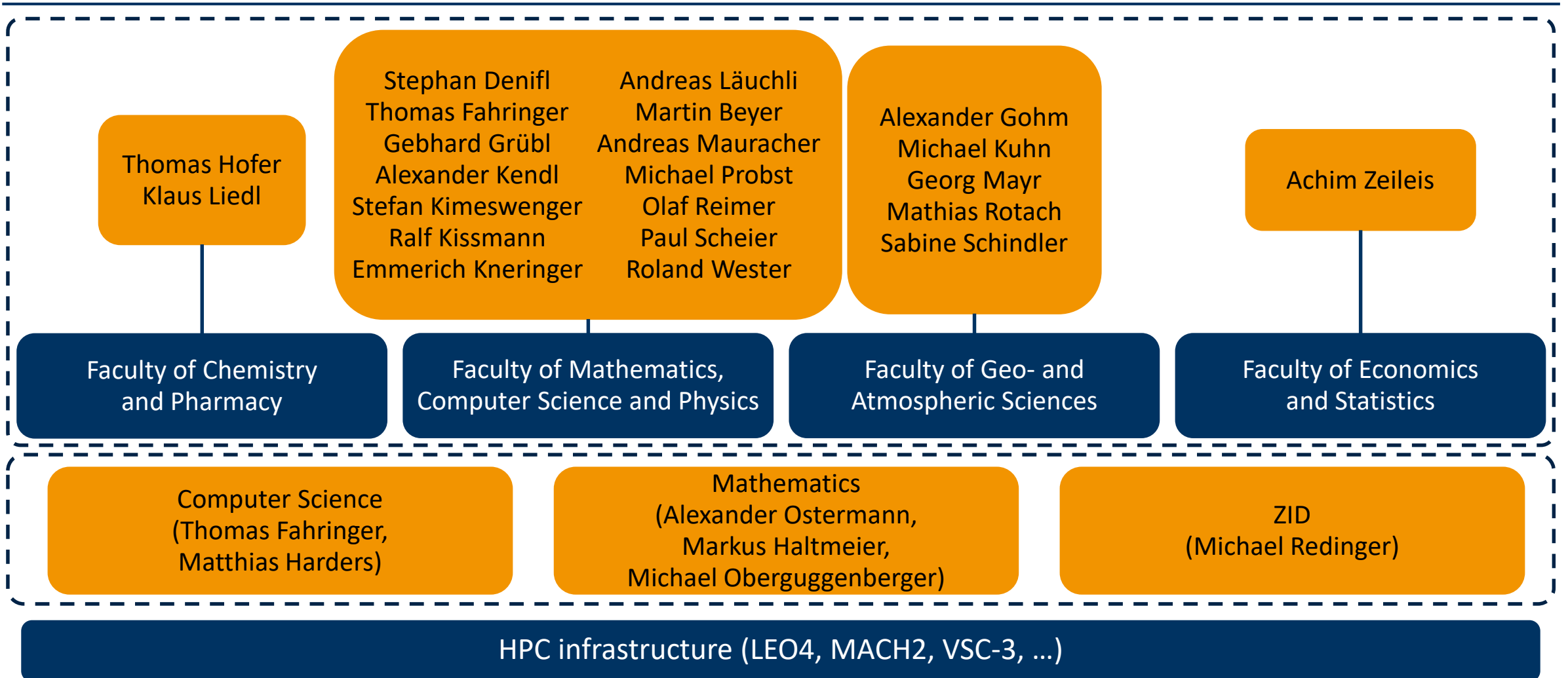
Objectives of the Research Center

Organization and support of various activities for the dissemination and efficient use of high-performance computing at the University of Innsbruck.

- HPC for application sciences
- Access to HPC expertise and resources
- National and international networking and collaboration

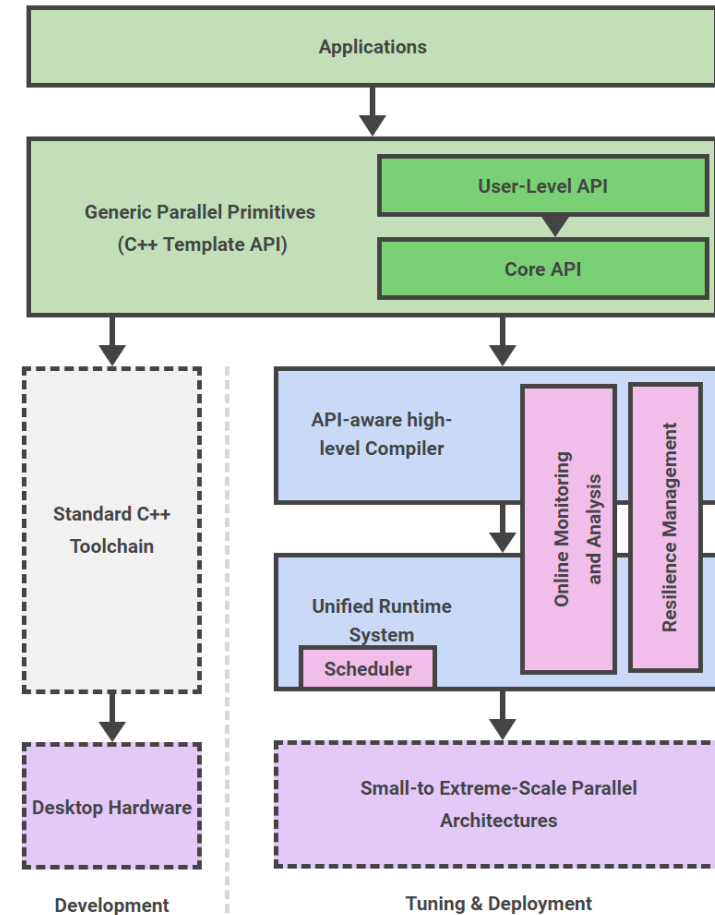


Partners of the Research Center



Project: AllScale (H2020)

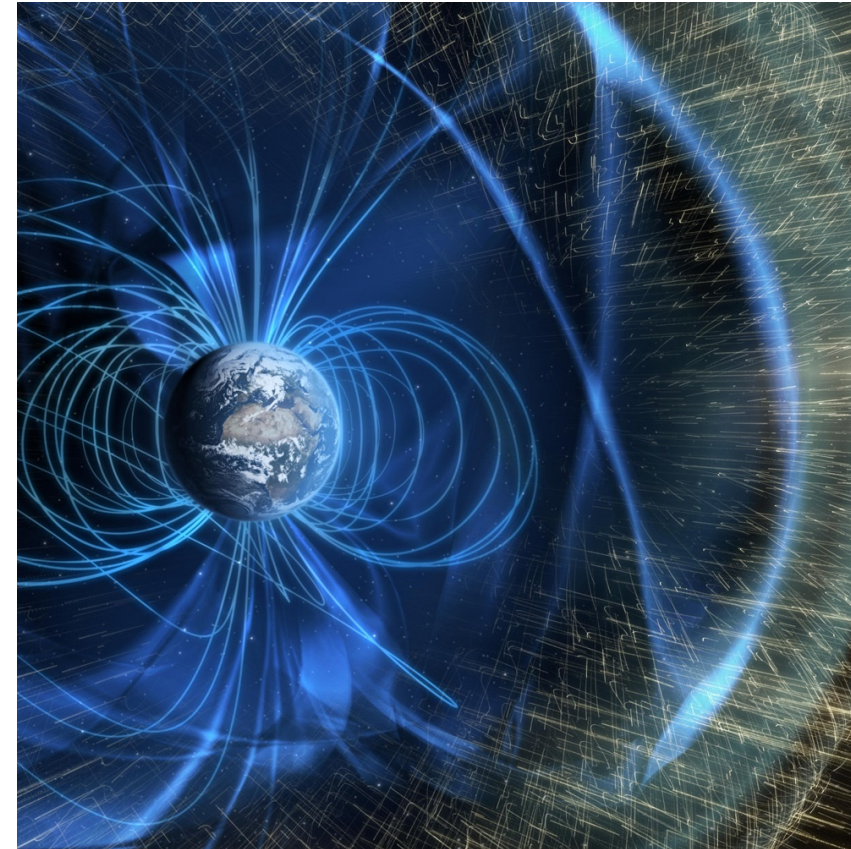
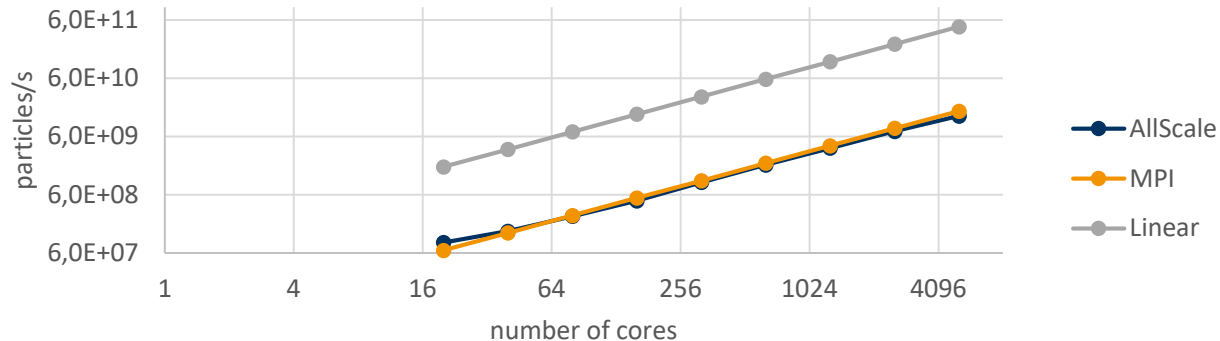
- Extreme Scale Computing
- Five international, academic and industry partners
- Improves productivity in application sciences via intuitive interface (e.g. parallel loops)
- Improves performance via recursively nested parallelism
- Hands control over data distribution to runtime system and enables e.g. automatic load balancing



AllScale Use Case – iPiC3D

- FetHPC H2020 project AllScale (coordinator: Dept. of Computer Science, UIBK)
- Space weather prediction, developed with KTH Stockholm
- Particle-in-Cell simulation
- Performance improvement compared to MPI reference implementation

iPiC3D auf Meggie (FAU)

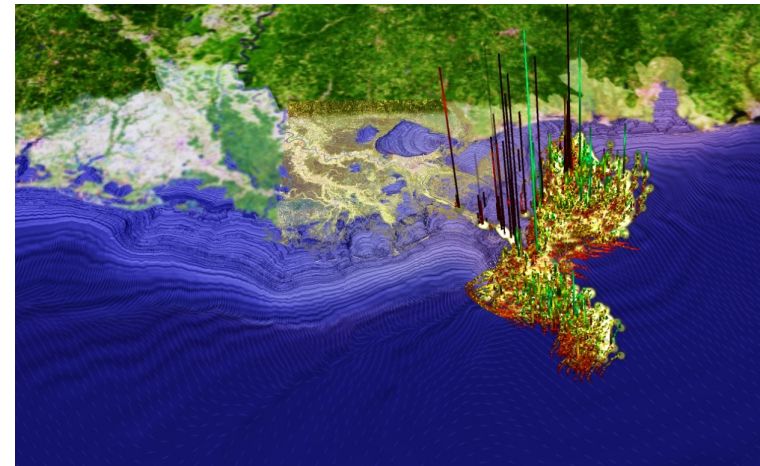
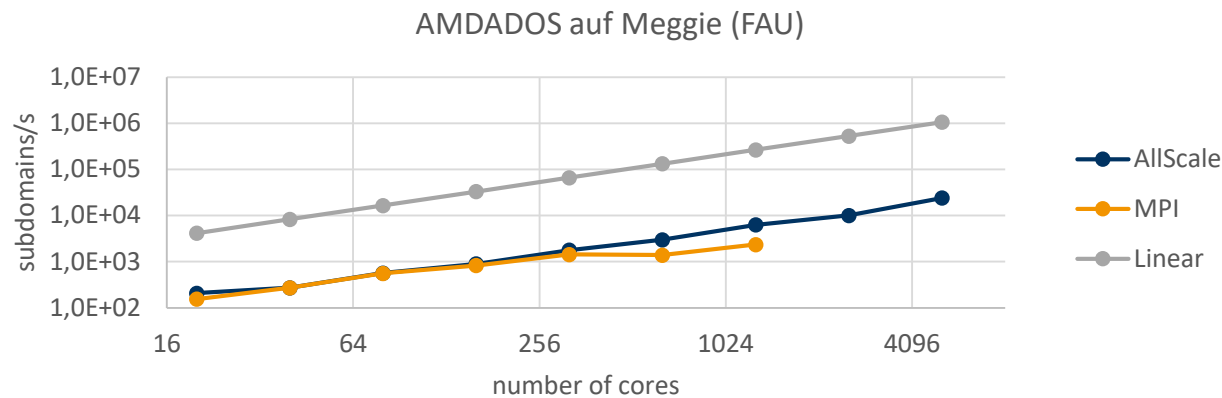


Source:

<https://twitter.com/maven2mars/status/9844440044659159040>

AllScale Use Case – AMDADOS

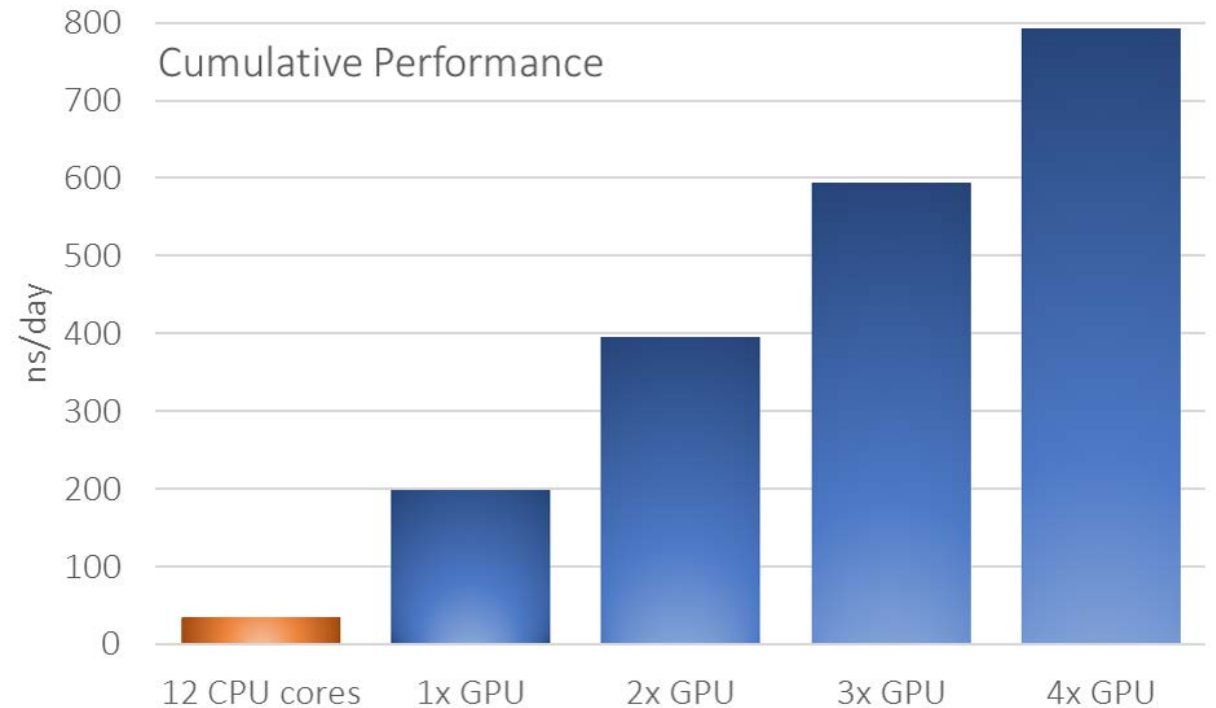
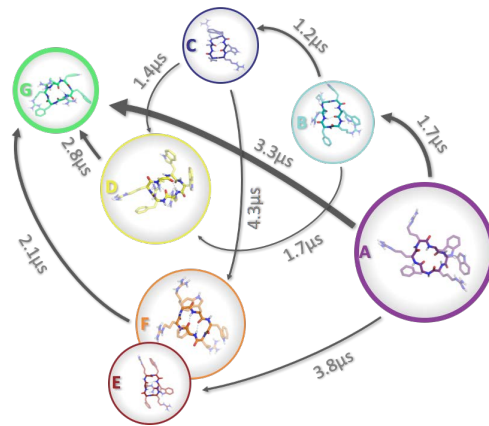
- FetHPC H2020 project AllScale (coordinator: Dept. of Computer Science, UIBK)
- Oil spill simulation, developed with IBM Ireland
- Stencil and kalman filter for assimilating sensor data
- AllScale exceeds performance of MPI reference implementation



Sources: <https://www.chemistryworld.com/features/oil-spill-cleanup/3008990.article>, Marcel Ritter (UIBK)

GPU Use Case – Amber16

- Theoretical Chemistry (UIBK) research, Anna Kamenik, Klaus Liedl
- Prediction of macrocycle conformations
- Simulation of molecular dynamics
- Performance increase on GPUs compared to CPUs: 200x



New Concept of the Research Center HPC

- Parallelization + Optimization
 - numerical methods
 - algorithms
 - data structures
- Research collaborations
 - partner in project proposals
 - networking with international computing centers and centers of excellence
- Training and consulting
 - programming concepts and languages
 - performance analysis and optimization
 - debugging



Dedicated support

- Senior Scientist

Benefit for application sciences

- Performance
- Productivity
- Sustainability



PRACE Computers and Extreme Scale Computing

universität
innsbruck



LEO 4:
1.344 Cores, 50 TFlops

- shorter simulation times
- higher problem complexity
- real-world, competitive research

VIENNA
SCIENTIFIC
CLUSTER



VSC-3:
32.320 Cores, 596 TFlops



Piz Daint:
387.872 Cores, 21 PFlops



Summit:
>2 Mio. Cores, 200 PFlops



exascale computer:
 10^{18} Flops