



Erlangen Regional
Computing Center



Friedrich-Alexander-Universität
Erlangen-Nürnberg

KONWIHR

Competence Network for Scientific High-Performance Computing in Bavaria

Gerhard Wellein, Hans-Joachim Bungartz
Katrín Nusser, Gerasimos Chourdakis



The Idea

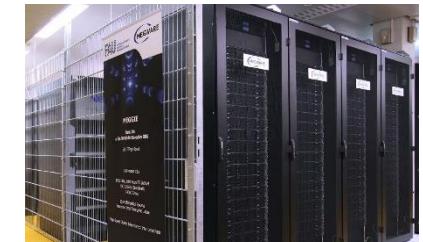
Work closely with a Bavarian computing center to improve runtime and scalability of your code:

- Analyze your code's performance
- Discover bottlenecks
- Parallelize & optimize your code
- Optimize your algorithms
- Evaluate alternative architectures



This means:

- Get funding
- Contact person assigned at either RRZE or LRZ
- Work for some time at the compute center on your project
- Get personal support from HPC experts



The Structure

Funding: Bavarian Ministry for Science and the Arts

Bayerisches Staatsministerium für
Wissenschaft und Kunst



North: FAU (Prof. Gerhard Wellein, Dr. Katrin Nusser), RRZE / NHR@FAU



Friedrich-Alexander-Universität
Erlangen-Nürnberg



South: TUM (Prof. Hans-Joachim Bungartz, Gerasimos Chourdakis), LRZ



How To

- Application deadlines: 1st of March / 1st of September
- Types of projects
 - Small (up to 3 months) - 10.000€
 - Large (up to 12 months) - 50.000€
 - Basis projects - 10.000€
 - Establish contacts at further compute centers (currently Regensburg, Würzburg, Deggendorf)
- Details on konwihr.de
- Apply via email to info@konwihr.de
- At the end:
 - A project report, including references to any publications
 - A short description and a figure for our website

COMPETENCE NETWORK FOR SCIENTIFIC HIGH PERFORMANCE COMPUTING IN BAVARIA

KONWIHR

ABOUT KONWIHR HOW TO APPLY PROJECTS CONTACT

News

KONWIHR Workshop: New Projects 2019

Being in a KONWIHR project means having open communication channels with your host computer centers, as well as being a member of a research community with common challenges and goals...>



New issue #93 of Quartl published
Issue #93 of the KONWIHR Quartl is now available. It contains articles on the following topics:

Keywords: Modellierung, Simulation, Parallel, Algorithmen

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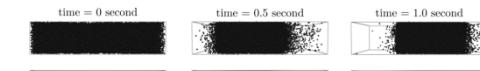
Optimizing the Parallel Granular Gas Solver to study the crater formation

Applicant
Prof. Dr. Thorsten Pöschel
Institute for Multiscale Simulation
Friedrich-Alexander Universität Erlangen-Nürnberg

Project Summary

The moving cone theory, evanescence and the dense granular rings are granular systems which consist of countless number of particles. The study of such large systems is impossible with current particle based methods such as Discrete Element Method (DEM) and Event Driven Molecular Dynamics (EDMD). However, a hydrodynamic (HD) method is a surface sensitive to study these phenomena. The hydrodynamic relaxation of the granular flow determines the system by average force exerted per particle number density, flow velocity and temperature. The time evolution of these quantities is governed by hydrodynamic equations. The solution to these equations provides valuable information about the granular systems.

We developed a granular flow solver that is based on C++ and遵循了MPI standard to solve the hydrodynamic equations of the granular flow. We did several optimizations to increase the performance and parallel efficiency of the Granular Flow Solver. The optimizations include modifying the MPI communication pattern, the timing of the functions, memory management and eliminating the expensive operations. These optimizations improved the single-core and parallel efficiency of the solver significantly.



Software projects funded through KONWIHR

- **ALF** (finite-temperature auxiliary-field quantum Monte Carlo), via Univ. Würzburg
- **ALPACA** (compressible multiphase flow), via TUM AER
- **deal.II** (FEM), via TUM LNM
- **EMPIRE** (molecular-orbital package), via FAU CCC
- **HyTeG** (FEM, matrix-free geometric multigrid), via FAU LSS
- **LIKWID** (performance tools), via RRZE / FAU
- **MARQOV** (equilibrium spin systems Monte Carlo), via Univ. Würzburg
- **MGLET** (Multi Grid Large Eddy Turbulence), via TUM BGU
- **preCICE** (coupling library for partitioned multi-physics), via TUM SCCS
- **PVSC-DTM** (stencil code generator), via RRZE / FAU
- **SCITE** (mutation histories of somatic cells), via FAU / Univ. Regensburg.
- **SWEET** (PDE solver environment, time integration), via TUM CAPS
- **waLBerla** (Lattice Boltzmann), via FAU LSS

... and more (see <https://www.konwihr.de/software/>).

Communication

Mailing Lists:

- **KONWIHR projects:** build a community (opt-out)
<https://lists.lrz.de/mailman/listinfo/konwihr-projects>
- **KONWIHR announcements:** hear the news first (opt-in)
<https://lists.lrz.de/mailman/listinfo/konwihr-announcements>

Workshop for new projects: discuss goals and find contacts, twice per year

Quartl: the official newsletter of KONWIHR and BGCE, 4x year

<https://www.cs.cit.tum.de/en/sccs/further-activities/quartl/>

Latest Projects - 2022/1

- Improving FAIRness of HPC research data – Prof. Stemmer (Technical University of Munich)
 - HPC mixed precision quantization of encoder-decoder deep neural networks – Prof. Kist (FAU)
 - Porting of Lattice QCD simulation software to GPUs – Prof. Wettig (University of Regensburg)
 - ALPACA in Florence – first steps towards the Ponte Vecchio": Porting ALPACA to Intel's upcoming GPU architecture Ponte Vecchio – Dr. Stefan Adami (Technical University of Munich)
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- Continuous Benchmarking for the GHODESS framework – Prof. Köstler (FAU)
 - Massively parallel solvers for geophysical flow problems with strong viscosity variations – Nils Kohl (FAU)
 - Optimization of the ALF implementation of the auxiliary-field quantum Monte Carlo algorithm: porting to GPUS and symmetry considerations – Prof. Assaad (University of Würzburg)
 - Largescale data processing and mass production of cosmicray background simulations for H.E.S.S. – Prof. Christopher van Eldik, Dr. Andreas Specovius (FAU)
 - HPC-Stützpunkt at the University of Regensburg – Prof. Wetting (University of Regensburg)