Performance portable and scalable particulate flow simulations using the waLBerla framework

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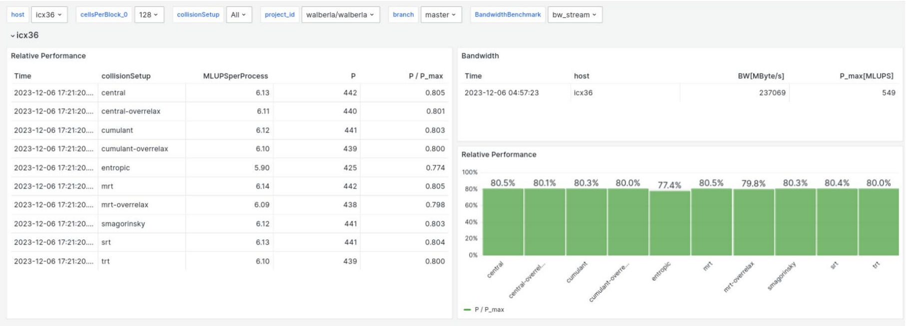
Friedrich-Alexander-Universität
Technische Fakultät

Efficient and Scalable Software Packages for multiphysics simulations

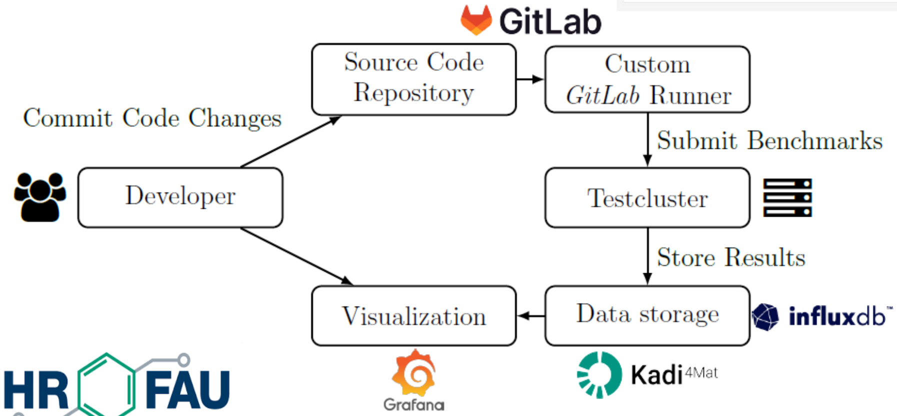
Performance Engineering and Continuous Benchmarking

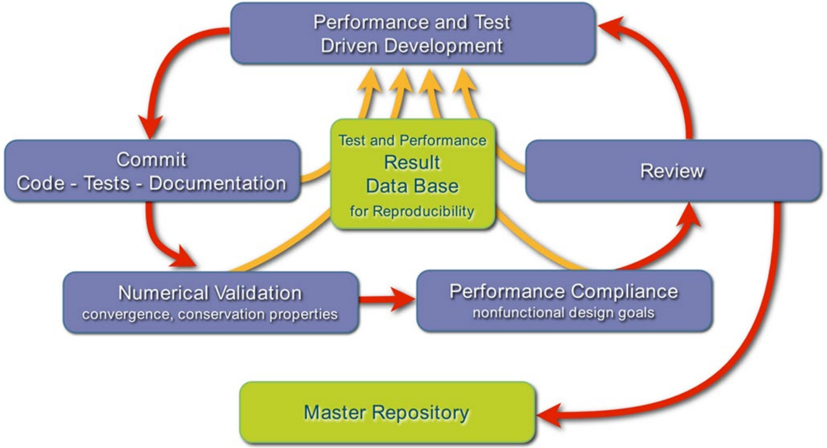
- Structured Performance Engineering
    - Performance Measurement
    - Performance Modeling
    - Performance Optimization
- Continuous Benchmarking



Time	collisionSetup	MLUPSperProcess	P	P / P_max
2023-12-06 17:21:20....	central	6.13	442	0.805
2023-12-06 17:21:20....	central-overrelax	6.11	440	0.801
2023-12-06 17:21:20....	cumulant	6.12	441	0.803
2023-12-06 17:21:20....	cumulant-overrelax	6.10	439	0.800
2023-12-06 17:21:20....	entropic	5.90	425	0.774
2023-12-06 17:21:20....	mrt	6.14	442	0.805
2023-12-06 17:21:20....	mrt-overrelax	6.09	438	0.798
2023-12-06 17:21:20....	smagorinsky	6.12	441	0.803
2023-12-06 17:21:20....	srt	6.13	441	0.804
2023-12-06 17:21:20....	trt	6.10	439	0.800

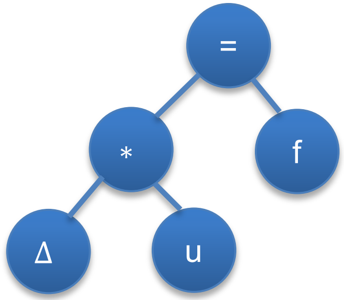
Time	host	BW[MByte/s]	P_max[MLUPS]
2023-12-06 04:57:23	icx36	237069	549

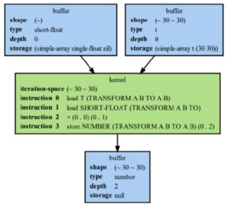




Performance Portability via Code Generation

Tree representation





Mathematical representation

$$\Delta u = f$$

Code representation 1

Field u,f
Laplace(u) = f

Code representation 2

mov EAX, [ebp+8]
add EAX, EBX

Abstract equations:
symbolic algebra

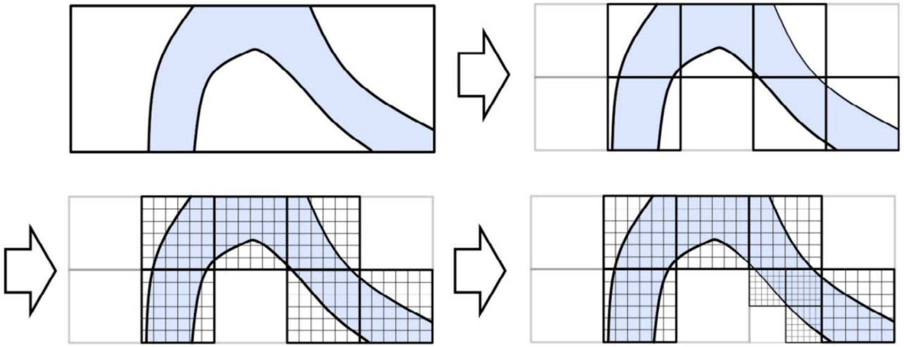
Abstract code descriptions:
includes data structures and numerical calculations

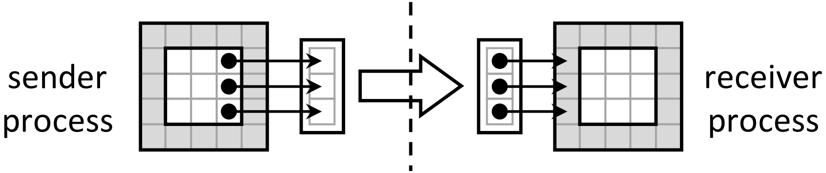
Low-level code:
architecture-specific machine code

Implement transforms to switch between different intermediate representations

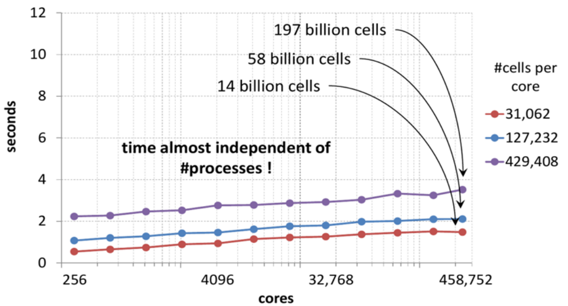
Scalability via (Block)-Structure

- The concept of block forests
  - Regularly partitioned subdomains act as root nodes for an octree
  - Leaf nodes of the refined forest of octrees make up final simulation subdomains (blocks)
  - The blocks can readily be distributed among available MPI processes
  - Support of static and dynamic mesh refinement
- Communication: distributed-memory systems
  - MPI-based halo exchange
  - support for asynchronous communication: overlapping communication and computation
  - GPU and CPU





JUQUEEN – diffusion load balancing

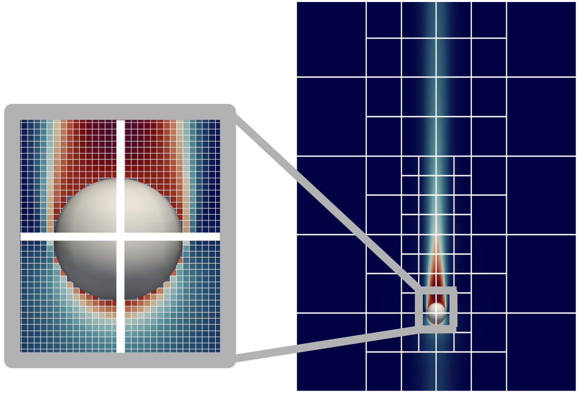


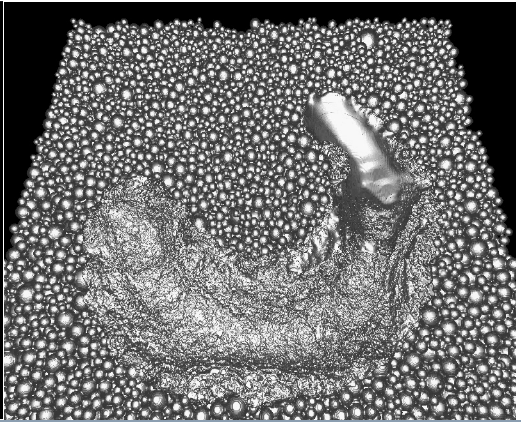
M. Bauer, et al. *waLBerla: A block-structured high-performance framework for multiphysics simulations.* Computers & Mathematics with Applications, 81, 478-501, 2021.

waLBerla framework

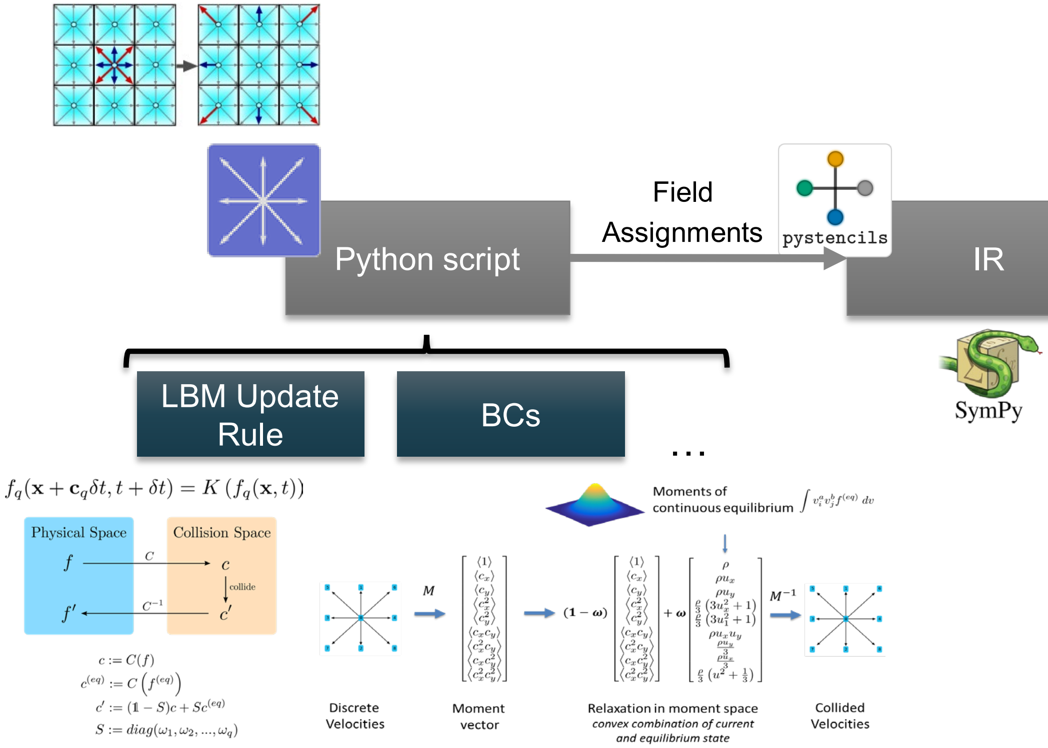
Open Source: https://walberla.net/

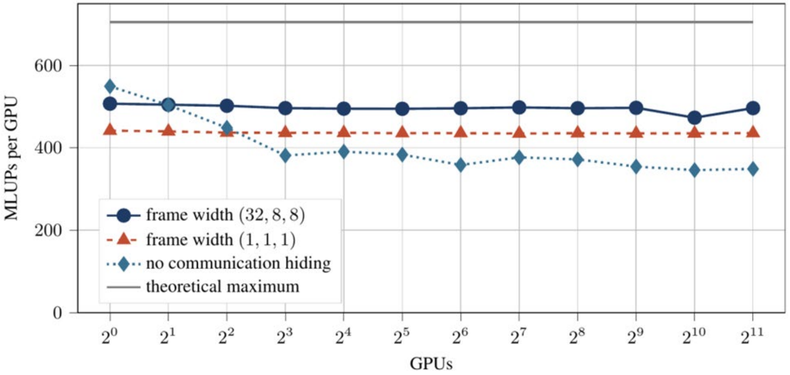
- Modular **C++17 multiphysics** framework
- CFD using the lattice Boltzmann method (**LBM**)
- Adaptive mesh refinement and load balancing
- Application scenarios e.g. rigid-particle dynamics, free-surface flows, solidification of material





Code Generation for Lattice Boltzmann Method





Bauer, M., Koestler, H., Ruede, U. (2021). lbmpy : Automatic code generation for efficient parallel lattice Boltzmann methods. Journal of Computational Science, 49.

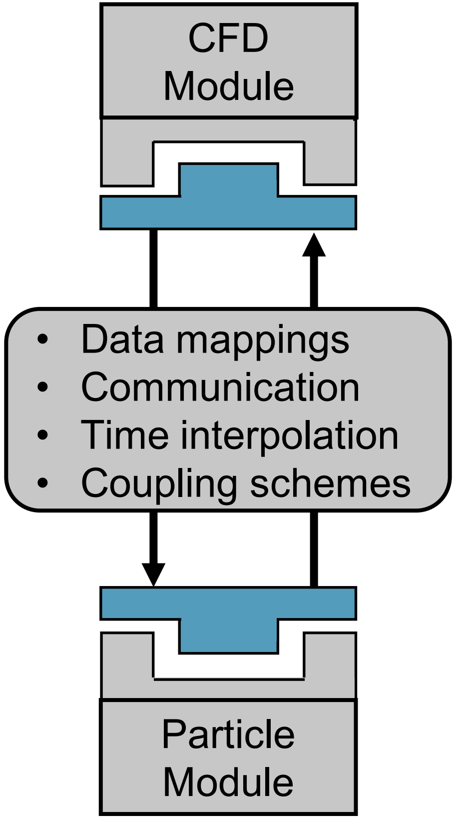
Multiphysics Simulations – Complexity

- Simulation frameworks are inherently **domain-specific**
- Put multiple simulation codes into **one program**
- Different domains
  - **Algorithms**, **discretizations** and **datastructures**
  - Discretizations space and time **scales**
  - **Target platforms** for execution
- ➢ Highly specialized and complex coupling codes

Challenge: software for multi-domain problems

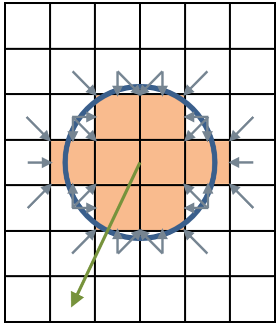
Software Couplings

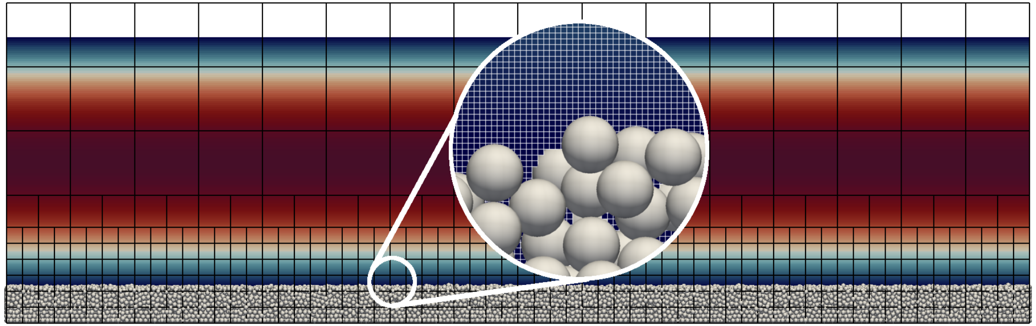
- **Hand-crafted** coupling codes
  - Often done in ad-hoc fashion
  - Tightly coupled, not very flexible
- Coupling **Libraries**, e.g. preCICE, MUSCLE
  - Minimal invasive, high-level APIs
  - Peer-to-peer, client/server designs
- **Generating** coupling codes
  - High-level description on DSL
  - On-the-fly conversions and data mappings
  - Performance-portable target code



Fluid-particle coupling

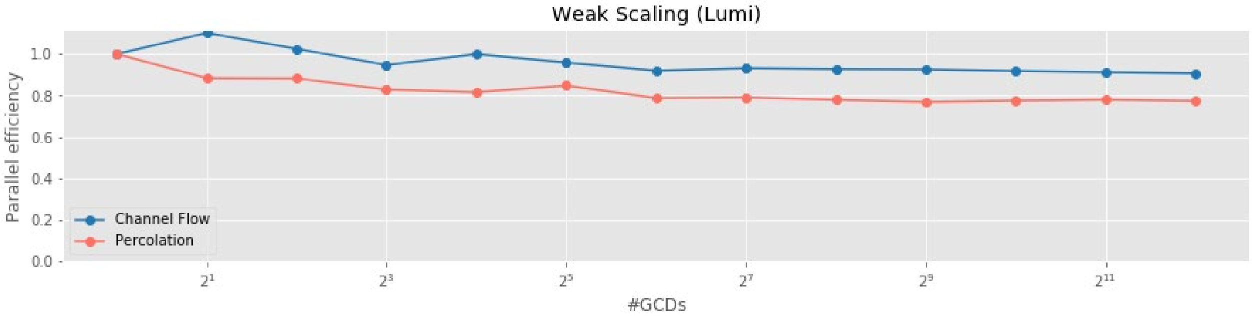
- Algorithms for rigid particle dynamics
  - Different algorithms for the broad and narrow phase collision detection of particles, soft and hard contact models
  - Euler or Velocity Verlet integration schemes
  - Different communication schemes, e.g. for regular and strongly polydisperse settings
  - Code generation for particle data structures and algorithms using the *MESA-PD* framework
- Fluid-particle coupling
  - Particles are mapped into the computational grid
  - No-slip (bounce-back) boundary conditions at the particle's surface
  - Hydrodynamic forces on particles computed from PDFs' momentum

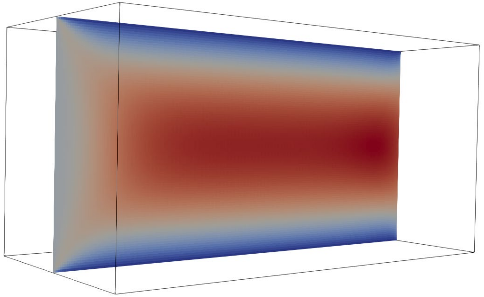




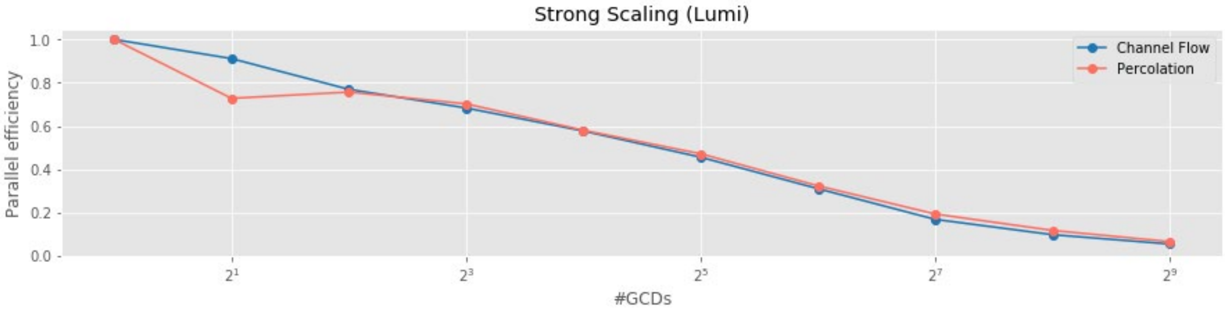
Rettinger, C., Godenschwager, C., Eibl, S., Preclik, T., Schruff, R., Frings, R., Ruede, U. (2017). Fully resolved simulations of dune formation in riverbeds. ISC 2017.

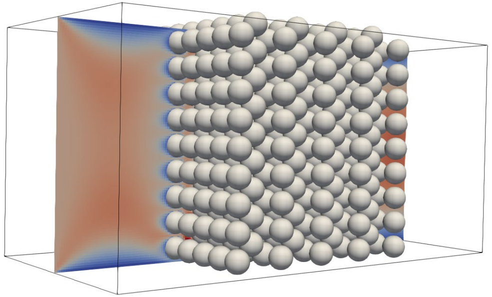
Particulate flow simulation on LUMI





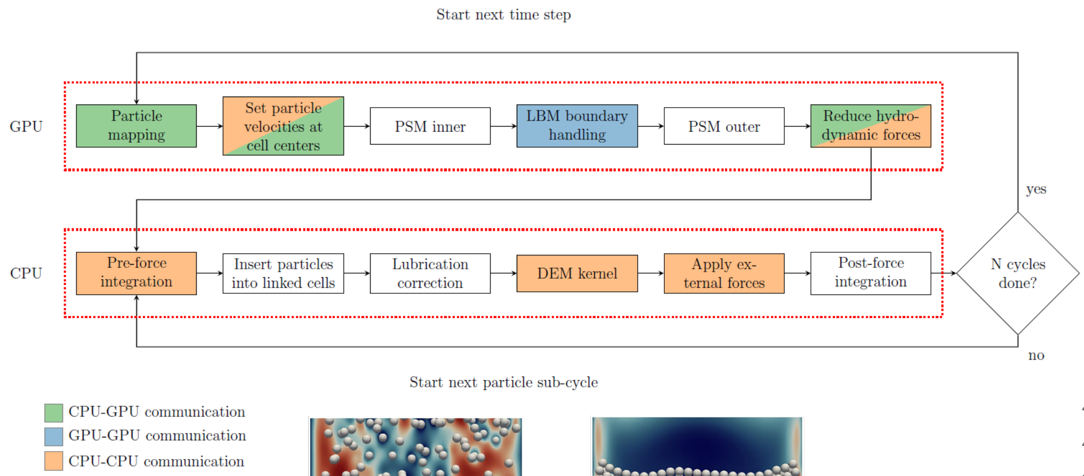
Channel flow

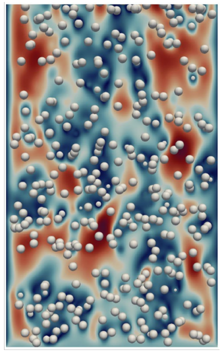




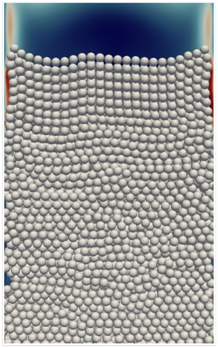
Percolation

Hybrid GPU-CPU implementation

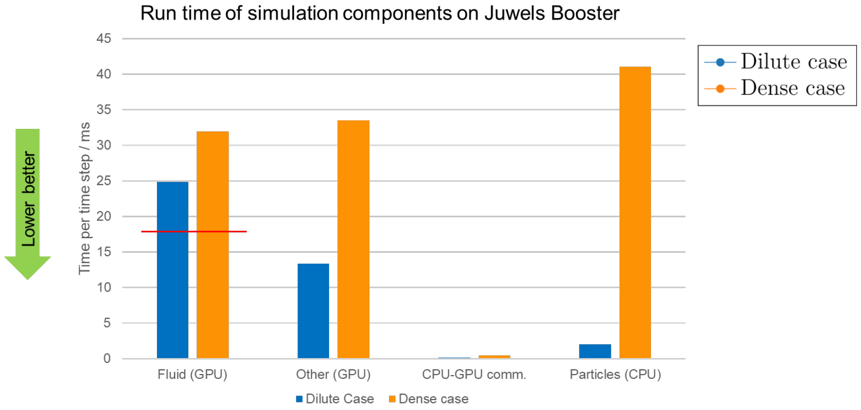




Dilute case (~600 particles)



Dense case (~8000 particles)

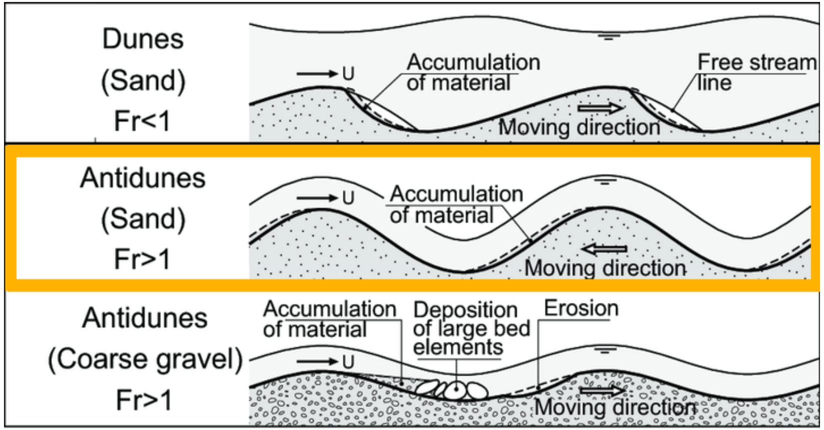


Challenges: particles + fluid + X

Example application: Antidunes

Includes Free Surface Flow

- Bedform: periodic structures developing at interface between granular bed and fluid flow in motion
- Dunes: sinusoidal shaped bedform
- Antidunes: dunes for which the liquid surface is in phase with the bed undulations



Froude number Fr = speed-length ratio $Fr = \frac{u}{\sqrt{gL}}$

https://www.researchgate.net/publication/312652397_Bed_morpholgy_and_stability_of_steep_open_channels

Extend multi-physics coupling

Challenges

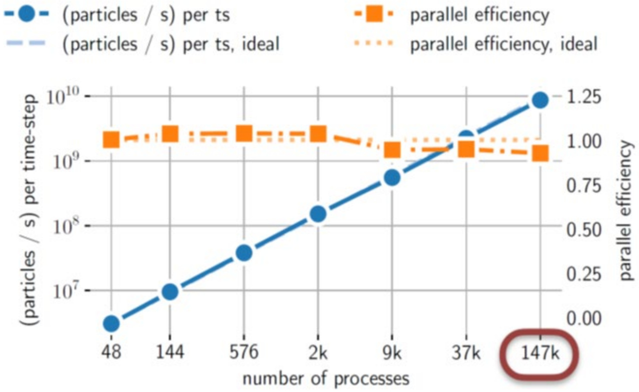
- Environmental challenges often involve **complex interactions between water, solids, and gases**

Use Case

- Progress beyond **sediment transport** to include pollutant transport and temperature effects

Approaches

- Euler-Euler coupling for macroscopic FE-models (Stokes equation, Energy equation)
- Euler-Lagrange coupling: FE and particle methods for transport of material
- Euler-Lagrange coupling: macroscopic transport models with mesoscopic Lattice Boltzmann methods (different time scales)



(b) weak scaling, $\approx 3.55 \times 10^5$ temperature DoFs (i. e. particles) per process

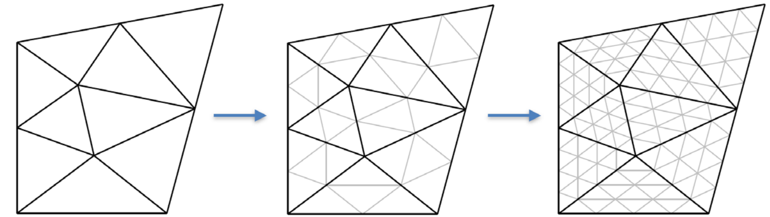
[4] Kohl, N., Mohr, M., Eibl, S., and Rüde, U., A massively parallel Eulerian-Lagrangian method for advection-dominated transport in viscous fluids. *SIAM J. Sci. Comput.*, *44*(3), C260-C285. (2022)

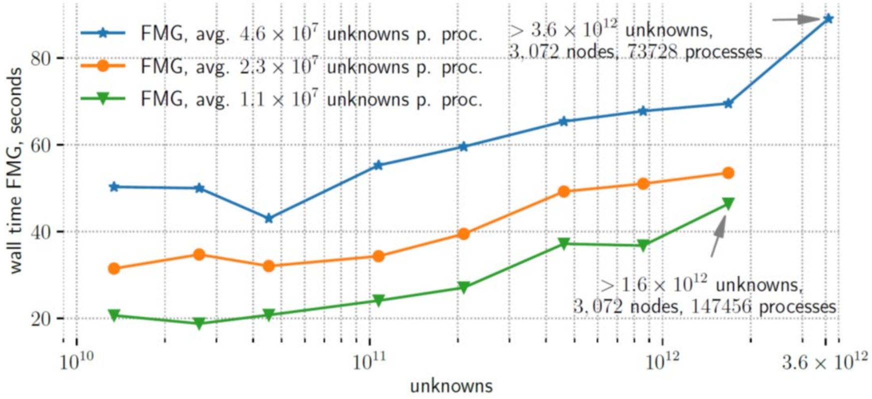
HyTeG

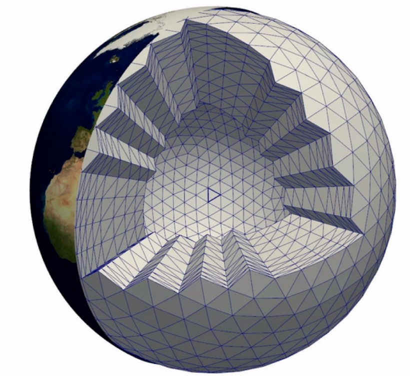
https://terraneo.fau.de/

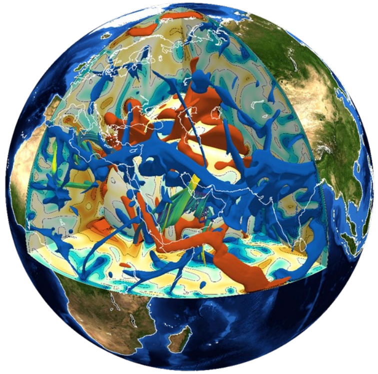
Hybrid Tetrahedral Grids (HyTeG)

- Uniform refinement of unstructured tetrahedral grids
- “Automatic” multigrid hierarchy
- matrix-free, stencil-based kernels for finite element discretizations
- Open-source C++ software, MPI parallelization for CPU clusters



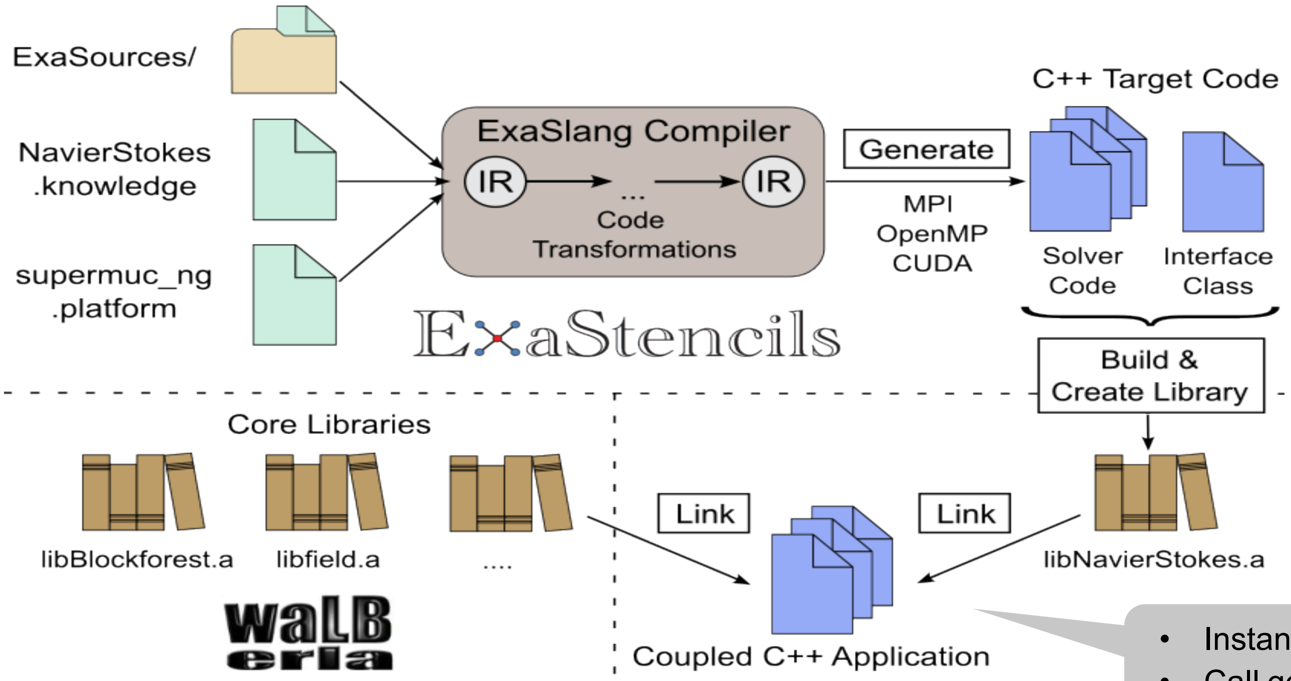






Earth mantle circulation simulation

Coupling – whole-solver code generation



- Instantiate interface class
- Call generated solver

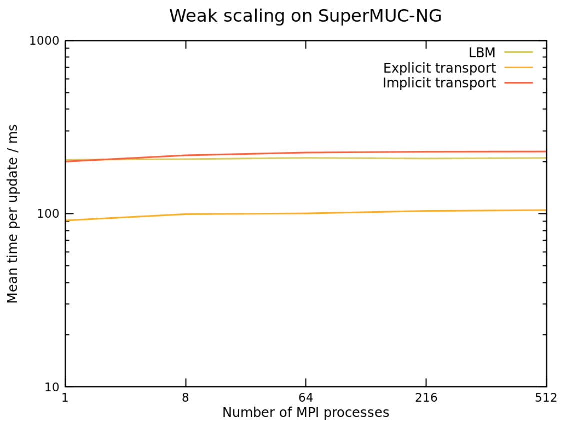
Application Scenarios – Coupled 3D Transport

- Transport of concentrations in fluid
- Advection-diffusion-reaction equation

$$\frac{\delta c}{\delta t} = Q + D\nabla^2 c - \mathbf{u} \cdot \nabla c$$

- Euler-Lagrange Coupling
- Two (FVM) variants: **explicit** and **implicit**

```
loop over c {
  c<next> = c + ( dt / vf_cellVolume ) *
              ( Q
              - D * Laplace * c
              - ( integrateOverEastFace ( c * u ) +
                  integrateOverWestFace ( c * u ) + ...
                )
              )
}
```



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