WaLBerla: Massively Parallel Lattice Boltzmann Simulations

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Motivation

Widely Applicable Lattice Boltzmann Solver from Erlangen

- Massively Parallel LB Framework
- Designed to
  - support a wide range of functionalities required by CFD applications
  - minimize the integration effort of new functionality

Outline

Requirements

- Fluidization processes
- Nanofluids

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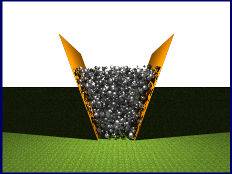
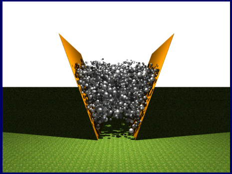
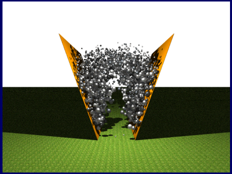
Motivation







Fluidization Processes

- Solid particles will behave like fluid
- Important in chemical engineering
- Limited understanding of fluidization behavior
- Number of particles for a representative setup $> 100K - 1M$

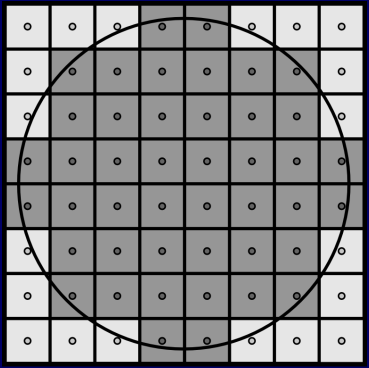
Objective

Simulate the **motion** of up to **one million fully resolved particles** to gain a deeper understanding of the **fluidization behavior**

Particulate Flows

LBM Scheme for Particulate Flows

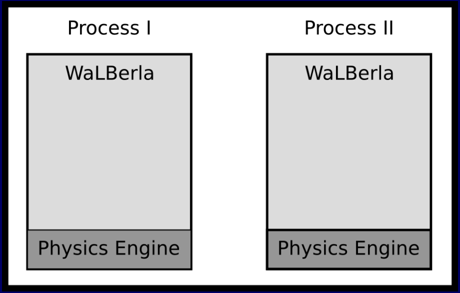
- Fully resolved particles
- Using "LB in fluid" for the particle treatment
- Second order velocity bounce back boundary conditions applied at the particle surface
- Calculation of hydrodynamic forces with the momentum exchange method
- Single relaxation time operator, D3Q19



Particulate Flows

Time Loop

- Mapping of the particles and application of the boundary conditions
- LBM stream and collide (Communicate PDFs)
- Determine hydrodynamic forces (Synchronize forces)
- Move and collide particles (Communicate contacts, positions and velocities)



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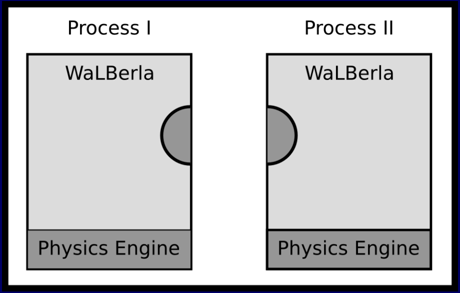

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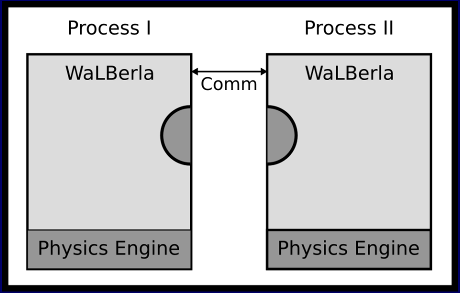

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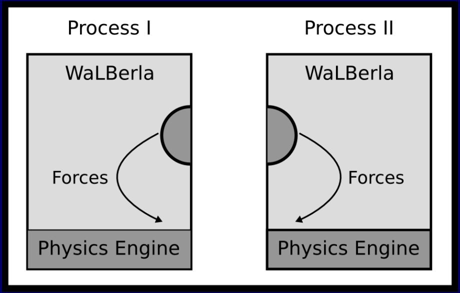

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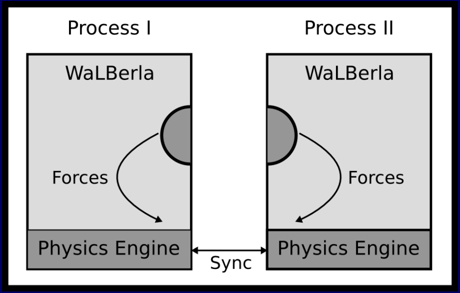

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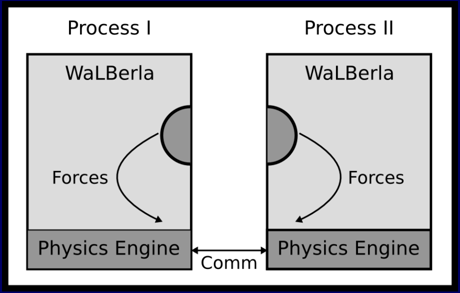

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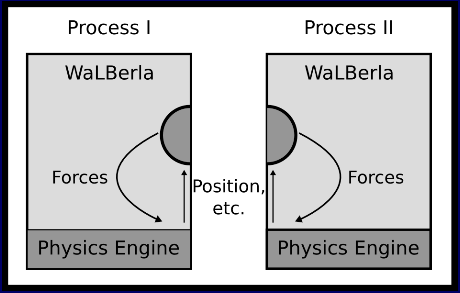


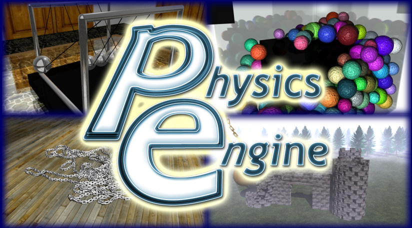
Particulate Flows

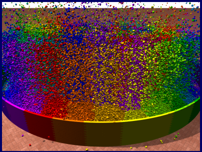
The Pe Physics Engine - Features

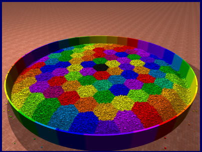
- Massively parallel framework for multi body simulations
- Several predefined primitive geometries
- Volumetric objects, not point masses
- Compound geometries
- Frictional collision response:

  Parallel fast frictional dynamics
  - Strictly local collision response calculation
  - Perfectly suited for parallelization
- Largest multi body simulation:

  1.1 billion rigid bodies



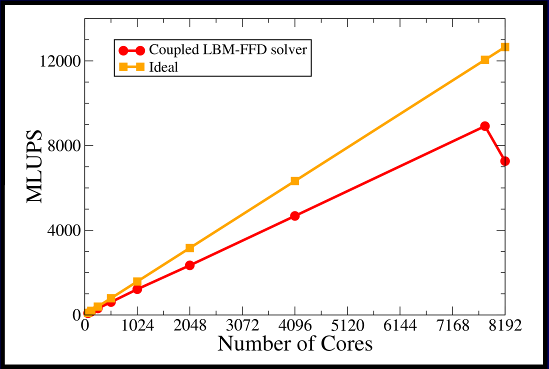




Particulate Flows

Weak Scaling Results

- Measurements conducted on HLRB-2,
  Leibniz Supercomputing Center, Garching, Germany,
  9728 cores, Itanium 2 (Montecito)
- 8 M lattice nodes and 2100 spherical particles per process
- Serial performance of 1.5 MLUPS
- We can simulate: $3.7 \cdot 10^7$ bodies, $6.6 \cdot 10^{10}$ nodes on 8192 cores



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- Nanofluids

Motivation

Nanofluids

- Colloidal suspensions of particles in the nanometer range [1 - 100 nm]
- Interesting properties: enhanced energy transfer, reduced sedimentation, reduced erosion in flow systems, etc.

Reference	System	ϕ	Size nm	Δk_{eff}
Eastman et al. (1997)	CuO-Water	5.0%	36	60%
Eastman et al. (2001)	Cu-EG	0.3%	<10	40%
Patel et al. (2003)	Au-Water	0.00026%	15	21%

- Temperature and particle size dependence

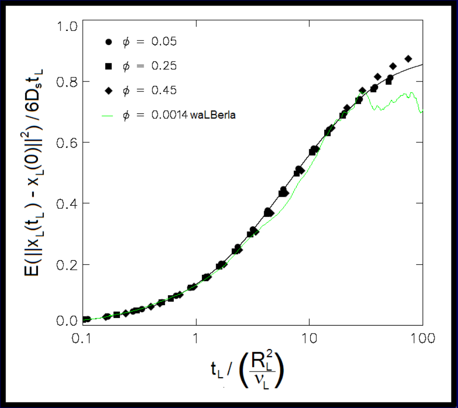
Objective

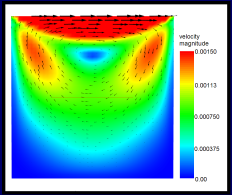
Determine the contribution of **Brownian motion** on nanofluid **transport properties**

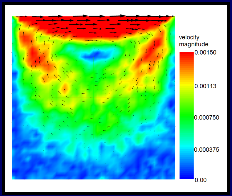
Nanofluids

Fluctuating LBM

- Introduction of thermal fluctuations to the fluid
- Method based on work reported by Dünweg et al., Phys. Rev. E., 2007
- MRT scheme with additional statistical noise
- Self-diffusion results published by Ladd, Phys. Rev. L., 1992



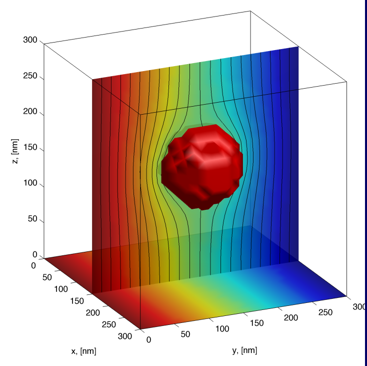




Nanofluids

Temperature

- Hybrid approach:
  - **Fluid and Particle motion**: Fluctuating Lattice Boltzmann Method
  - **Energy Transport**: Implicit Finite Volume



Acknowledgments

THANK YOU FOR YOUR ATTENTION !

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