# Walberla: A Framework for Simulating Complex Flows on 10,000 Cores and Beyond

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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

- Lattice Boltzmann Method
- Patch and Parallelization Concept
- Particulate Flows

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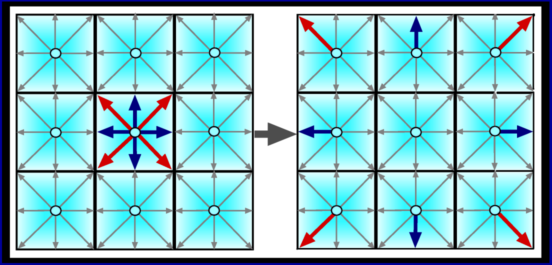
# Lattice Boltzmann Method

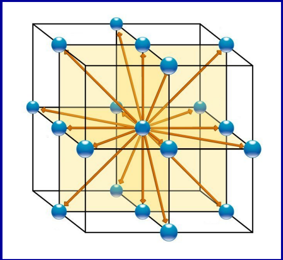
## Brief Introduction

- Mesoscopic method for CFD simulations
- Equivalent to a finite difference Navier-Stokes scheme
- Two major steps: Stream step and collision step

$$f_\alpha(x_i + e_{\alpha,i}\delta t, t + \delta t) - f_\alpha(x_i, t) = -\frac{\delta t}{\tau}\left[f_\alpha(x_i, t) - f_\alpha^{(eq)}(\rho(x_i, t), u_i(x_i, t))\right]$$

$$\rho u_i = \sum_{\alpha=0}^{18} e_{\alpha,i} \cdot f_\alpha \qquad \rho = \sum_{\alpha=0}^{18} f_\alpha$$





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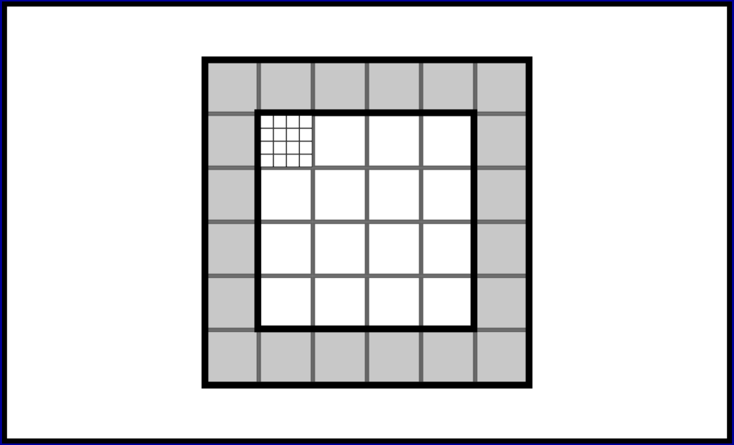
- Lattice Boltzmann Method
- **Patch and Parallelization Concept**
- Particulate Flows

# Patch Concept and Parallelization



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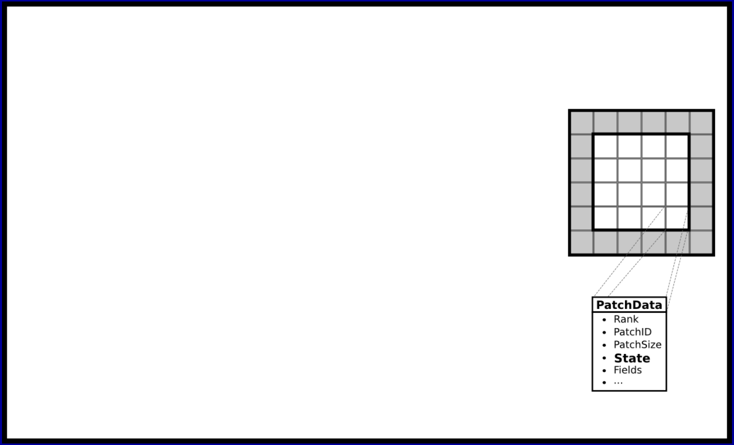

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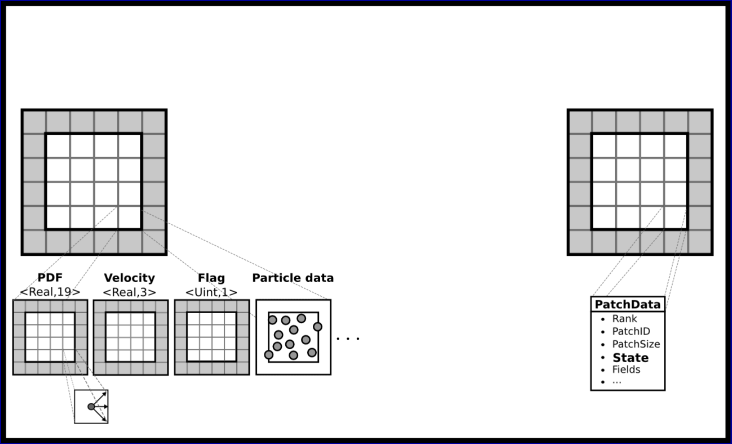

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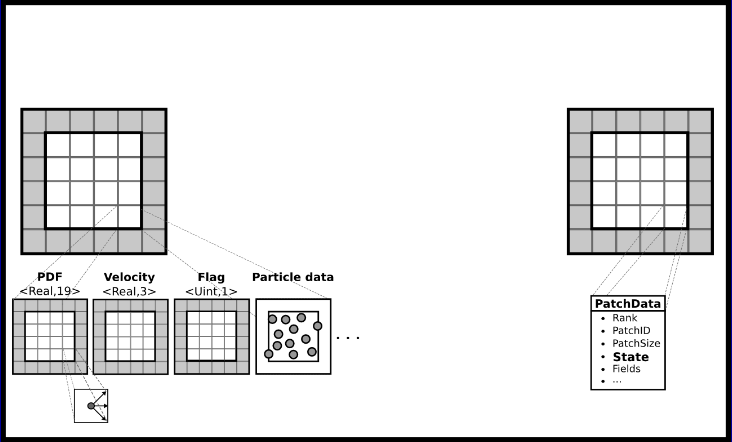


## Parallelization Features

- Send/Recv of arbitrary grid data via MPI
- Support of messages with variable size
- Bundling of MPI messages to reduce start up times

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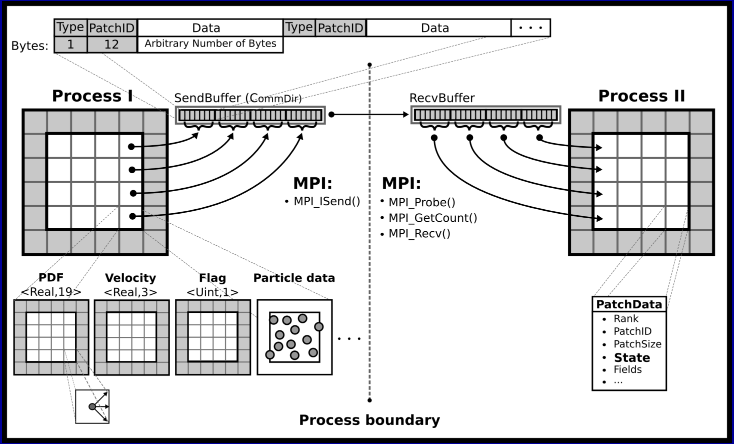


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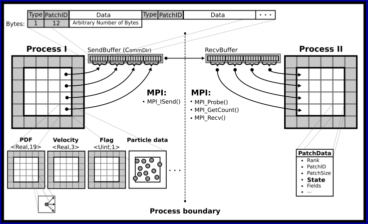



## Utilization

- Various complex LBM applications
- Poisson and convection-diffusion problems
- Jacobi and Gauss-Seidel solvers
- Multigrid solver

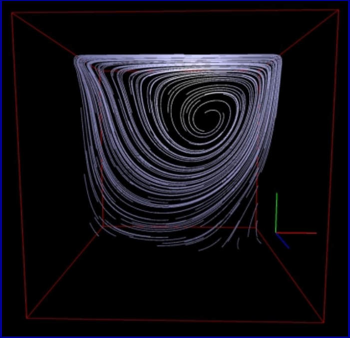
# Weak Scaling Results

## LBM

- D3Q19
- SRT
- Lid Driven Cavity

## Node Performance on Woodcrest Cluster

- 217 Intel Xeon (Woodcrest) CPUs
- Duel-socket, duel-core
- Peak performance: 10.3 TFlops



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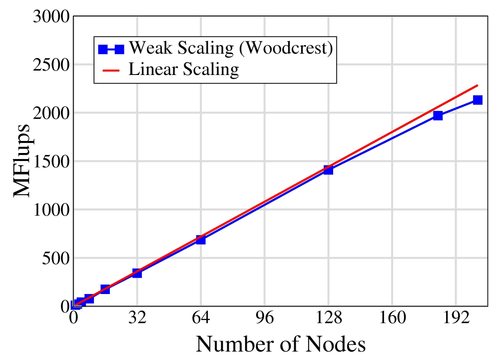


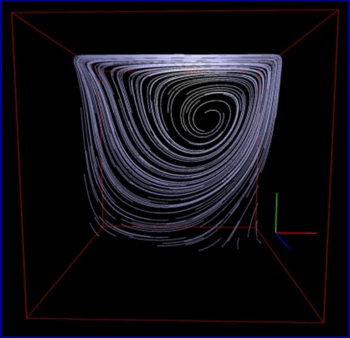

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- Lattice Boltzmann Method
- Patch and Parallelization Concept
- **Particulate Flows**

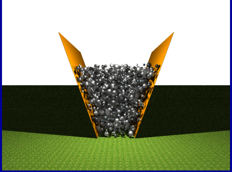
# Motivation

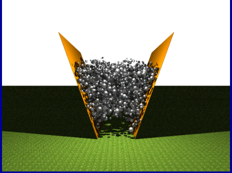
## Fluidization Processes

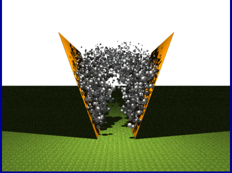
- Solid particles will behave like fluid
- Important in chemical engineering
- Limited understanding of fluidization behavior
- Number of particles for a representative setup $> 100K - 1M$

## Objective

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







# Particulate Flows

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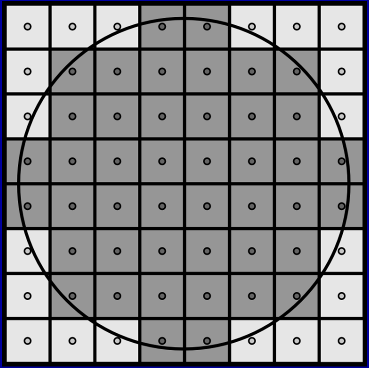
## LBM Scheme for Particulate Flows

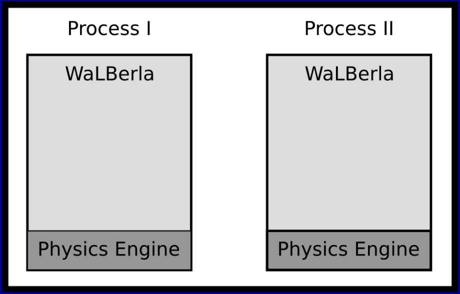
- Fully resolved particles
- Using "LB in fluid" for the particle treatment
- Second order velocity bounce back boundary conditions applied at the particle surface
- Calculation of hydrodynamic forces with the momentum exchange method
- Single relaxation time operator, D3Q19



# 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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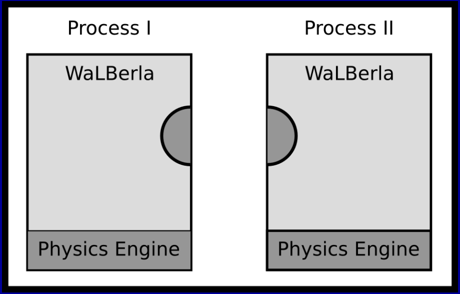

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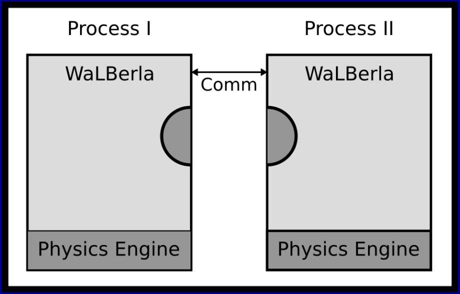

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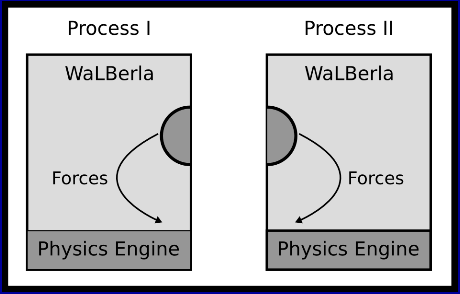

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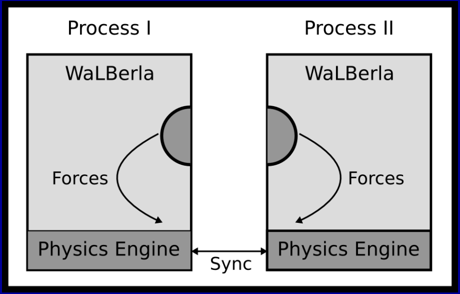

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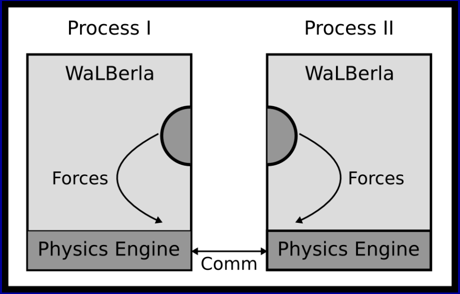

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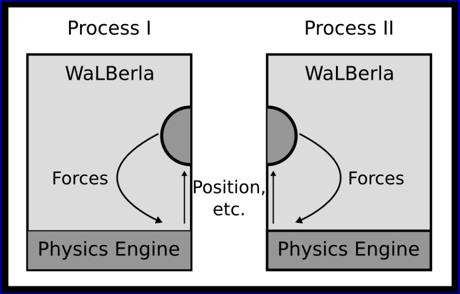

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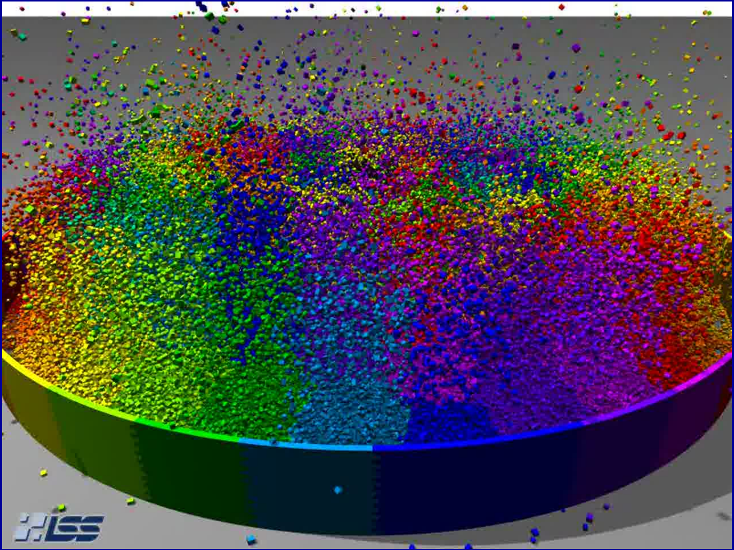


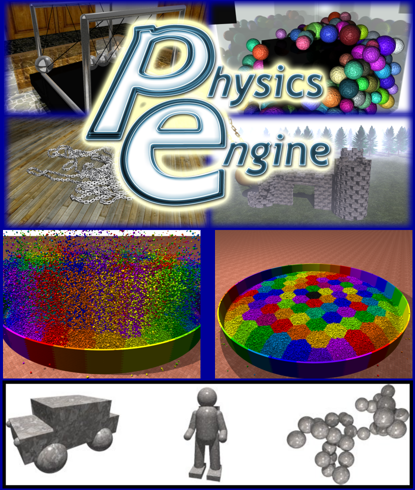
# Particulate Flows

### 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:

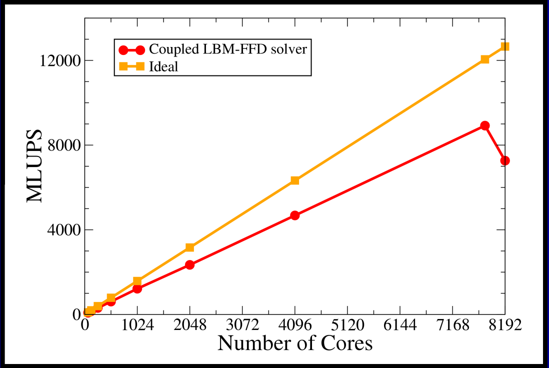
  **1.1 billion rigid bodies**



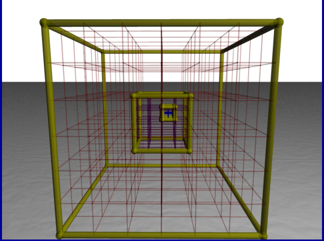
# Particulate Flows

## 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

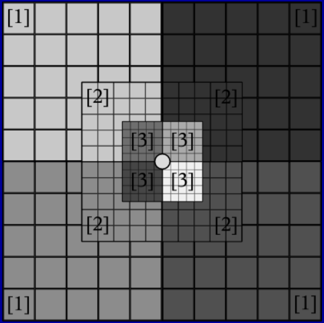


# Outlook



**Further Improvements of WaLBerla**

- Adaptive grid refinement
- Load balancing
- Hybrid parallelization
- New architectures and systems




# Acknowledgments

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