Massively Parallel Multiphysics Simulations with the waLBerla Software Framework

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Outline

- The waLBerla Simulation Framework
- The Lattice Boltzmann Method (LBM)
- Fluid-Particle Interaction for Elongated Particles
- Charged Particles in Fluid Flow
The waLBerla Simulation Framework
waLBerla

- Widely applicable lattice Boltzmann framework
- Suited for various flow applications
- Large-scale, MPI-based parallelization:
  - Domain partitioned into Cartesian grid of blocks, blocks assigned to different processes
  - MPI communication between the blocks, based on ghost layers
- New: Adaptivity and load balancing (for LBM)
Fluid-Particle Interaction with LBM
and tumbling spherocylinders in Stokes flow
Lattice Boltzmann Method

\[ f_q(\vec{x}_i + \vec{c}_q dt, t_n + dt) - f_q(\vec{x}_i, t_n) = dt \, C_q (f_q(\vec{x}_i, t_n)) \]

- Discrete lattice Boltzmann equation with collision operator \( \Omega_q = dt \, C_q \)
  Note: two relaxation time (TRT) collision model used for the simulations
- Domain discretized in cubes (cells)
- Discrete velocities \( \vec{c}_q \) and associated distribution functions \( f_q \) per cell

D3Q19 model
Stream-Collide

The equation is solved in two steps:

- **Stream step:**
  \[ f_q(\vec{x}_i + \vec{e}_q, t_n + dt) = \tilde{f}_q(\vec{x}_i, t_n) \]

- **Collide step (SRT):**
  \[ \tilde{f}_q(\vec{x}_i, t_n) = f_q(\vec{x}_i, t_n) - \frac{1}{\tau} \left( f_q(\vec{x}_i, t_n) - f_{eq}^q(\vec{x}_i, t_n) \right) \]
Hydrodynamic Interactions – 4-Way Coupling

- Particles mapped onto fixed lattice Boltzmann grid
- Each lattice node with cell center inside object is treated as moving boundary
- Hydrodynamic forces of fluid on particle computed by momentum exchange method*

Tumbling Spherocylinders in Stokes Flow

- Tumbling motion of elongated particles in Stokes flow
- Four spherocylinders in periodic domain, aspect ratio \( \frac{1}{\varepsilon} = \frac{\text{length}}{\text{radius}} = 12 \)

LBM simulation validation and comparison against slender body formulation (examining influence of aspect ratio, inertia, wall effects, and particle shape)*


Typical runs on SuperMUC:
1 thin island (8192 cores) for 15 to 48 hrs (70 000 to 605 000 time steps)
Charged Particles in Fluid Flow

for particle-laden electrokinetic flows
Motivation

Separation (or agglomeration) of charged particles in micro-fluid flow, influenced by external electric fields

Medical applications:
- Optimization of Lab-on-a-Chip systems, e.g. separation of different cells
- Deposition of charged aerosol particles in respiratory tract (e.g. drug delivery)

Multiphysics simulation of three mutually coupled phenomena
Charged Particles – 6-Way Coupling

● Long-range electrostatic interactions:
  ● Poisson equation for electrostatic potential, particle charge on right-hand side
  ● Finite volume discretization, solved with cell-centered multigrid in waLBerla
  ● Resulting electrostatic force on particle

\[-\Delta \Phi(\vec{x}) = \frac{q_{\text{particles}}(\vec{x})}{\epsilon_r \epsilon_0}\]

\[\vec{F}_q = -q_{\text{particle}}(\vec{x}) \cdot \nabla \Phi(\vec{x})\]

● Overall coupling:
Simulation Results and Scaling

- Charged particle separation in bisecting micro-channel:

- Weak scaling:
  - Thin islands, 16 cores/node @ 2.5 GHz
  - Constant size per core
    - $128^3$ cells
    - 9.4% moving obstacle cells
  - Cell-centered MG:
    - $V(3,3)$ with 7 levels
    - 10 to 45 CG coarse-grid iterations
  - Convergence rate: 0.07
Weak Scaling for 240 Time Steps

Parallel efficiency @2048 nodes:
- Overall: 83 %
- LBM: 91 %
- MG - 1 V(3.3): 64 %

MG performance restricted by coarsest-grid solving

Summary

- SuperMUC used for scaling experiments and productivity runs
- Validation and study of hydrodynamic interactions of elongated particles (4-way coupling)
- Parallel multi-physics algorithm for charged particles in fluid flow (6-way coupling)
- Scaling experiments for charged particles algorithm

- Further simulations on SuperMUC: Validation experiments for electrophoresis of charged particles, including ions (7.5-way coupling)

- We would like to thank

![Irz Logo]
Thank you for your attention!