Fast Multigrid Solvers for Long Range Potentials

Dominik Bartuschat, Boston, USA
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D. Bartuschat, H. Köstler, U. Rüde

Chair for System Simulation, FAU Erlangen-Nürnberg
Outline

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- Charged Particles in Fluid Flow
- Multigrid Solver
- Validation
- Results
Motivation

Simulating agglomeration of charged particles in (micro-)fluid flow on charged plane.

- Industrial applications:
  - Filtering particulates from exhaust gases.
  - Charged particle deposition in cooling systems of fuel cells.

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

© Kang and Li „Electrokinetic motion of particles and cells in microchannels“ Microfluidics and Nanofluidics
Multi-Physics Simulation

Electro (quasi) statics

- Electrostatic force
- Charge density
- Force on ions
- Ion convection

Rigid body dynamics

- Object movement
- Hydrodynamic force

Fluid dynamics
The waLBerla Simulation Framework
waLBerla

- Widely applicable Lattice Boltzmann framework.
- Suited for various flow applications.
- Large-scale, MPI-based parallelization.
- Dynamic application switches for different functionalities and optimization.
waLBerla Concepts

Block concept:
- Domain partitioned into cartesian grid of blocks.
- Blocks can be assigned to different processes.
- Blocks contain:
  - cell data, e.g. electric potential.
  - global information e.g. MPI rank, location.

Communication concept:
- Simple communication mechanism on uniform grids, utilizing MPI.
- Ghost layers to exchange cell data with neighboring blocks.

Sweep concept:
- Sweeps are work steps of a time-loop, performed on block-parallel level.
- Example: MG sweep, contains sub-sweeps (restriction, prolongation, smoothing).
Charged Particles in Fluid Flow
Lattice Boltzmann Method

\[ f_i(\bar{x} + \bar{c}_i \Delta t, t + \Delta t) - f_i(\bar{x}, t) = -\frac{1}{\tau}(f_i - f_i^{eq}). \]

- Discrete lattice Boltzmann equation (single relaxation time).
- Domain discretized in cubes (cells).
- Discrete velocities \( \bar{c}_i \) and associated distribution functions \( f_i \) per cell.

D3Q19 model
Stream-Collide

The equation is solved in two steps:

- **Stream step**
  \[ f_i(\bar{x} + \bar{c}_i \Delta t, t + \Delta t) = \tilde{f}_i(\bar{x}, t + \Delta t) \]

- **Collide step**
  \[ \tilde{f}_i(\bar{x}, t + \Delta t) = f_i(\bar{x}, t) - \frac{1}{\tau}(f_i - f_i^{eq}) \]
Fluid-Particle Interaction - waLBerla and pe

- Particles mapped onto 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*.

Poisson Equation and Force on Particles

- Electric potential described by Poisson equation, with particle’s charge density on RHS:

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

- Discretized by finite volumes.
- Solved with cell-centered multigrid solver.
- Subsampling for computing overlap degree to set RHS accordingly.

- Electrostatic force on particle:

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

foreach time step, do

// solve Poisson equation with particle charge density
set RHS of Poisson equation
while residual too high do
  perform multigrid v-cycle to solve Poisson equation
end

// solve lattice Boltzmann equation considering particle velocities
begin
  perform stream step
  compute macroscopic variables
  perform collide step
end

// couple potential solver and LBM with pe
begin
  apply hydrodynamic force to particles
  apply electrostatic force to particles
  pe moves particles depending on forces
end
Multigrid Solver
Multigrid

- Iterative method for efficient solution of sparse linear systems.

- Based on
  - Smoothing principle: High-frequency error elimination by iterative solvers (e.g. GS).
  - Coarse grid principle: Restriction to coarser grid transforms low-frequency error components to relative higher-frequency ones.
  - Smoothing on coarse grids.
  - Prolongation of obtained correction terms to finer grid.

- Applied recursively, $V(v_{\text{pre}}, v_{\text{post}})$-cycle.
Cell-Centered Multigrid - Implementation

- All operations implemented as compact stencil operations.

- Design goals:
  - Efficient and robust black-box solver.
  - Handling complex boundary conditions on coarse levels.
  - Naturally extensible to jumping coefficients.

  ➡ Method of choice: Galerkin coarsening.

- (FV) Stencils stored for each unknown.
- On finest level: quasi-constant stencils.

- Averaging restriction, constant prolongation.
  - Preserves D3Q7 stencil on coarse grids.
  - Convergence rate deteriorates.
  - Workaround for Poisson problem: Overrelaxing prolongation*

Validation
Validation of Electric Potential

Analytical solution for homogeneously charged particle:

\[
\Phi(\vec{x}) = \begin{cases} 
\frac{1}{4\pi\varepsilon} \cdot \frac{Q}{|\vec{x}|} & \text{for } |\vec{x}| \geq R \\
\frac{1}{4\pi\varepsilon} \cdot \frac{Q}{2R} \left(3 - \left(\frac{|\vec{x}|}{R}\right)^2\right) & \text{for } |\vec{x}| < R
\end{cases}
\]

Particle in 256\(^3\) domain
- MG: 5 V(2,2)-cycles.
- Dirichlet BCs: exact solution.
- Relative error: in order of 10\(^{-3}\)

- Radius: 60 µm.
- Charge: 8000 \cdot e.
- Subsampling: factor 4.
Validation of Electric Potential

Determination of residual threshold:

Error hardly reduced after residual norm smaller than $10^{-9}$

Residual threshold for simulations: $2 \cdot 10^{-9}$
Results
Charged Particles in Fluid Flow

Agglomeration of charged particles on charged plane in water flow.

- Channel: 2.56 x 5.76 x 2.56 mm
  - $D_x = 10 \mu m$, $D_t = 4 \cdot 10^{-5} s$, $\tau = 1.7$
- Particle radius: 60$\mu m$
- Inflow velocity: 1 mm/s
- Particle charge: 8000e
- Potential: Bottom -100V, Top 0V
- Other walls: No-slip BCs
- Other walls: homogen. Neumann BCs
- Computed on 144 cores (12 nodes) of RRZE - LiMa
- 71,600 time steps
- $64^3$ unknowns per core
- 6 MG levels
Scaling Setup and Environment

Weak scaling:
- **Costant size per core:**
  - 128³ cells.
  - 9.4% moving obstacle cells.
- **Size doubled** (y-dimension).
- **MG** (Residual $L_2$-Norm $\leq 2 \cdot 10^{-9}$):
  - V(3,3) with 7 levels.
  - 10 to 45 CG coarse-grid iterations.
  - Convergence rate: 0.07.
- 2x4x2 cores per node.

Executed on LRZ‘s SuperMUC:
- 9216 compute nodes (thin islands), each:
  - 2 Xeon "Sandy Bridge-EP" chips @2.7 GHz,
  - 32 GB DDR3 RAM,
  - Infiniband interconnect.
- Currently ranked #6 in TOP500.
Single Node Performance

Weak scaling (first time-step, size doubled here in different dimensions)

- LBM scales very well.
- MG scales reasonably well.

Highest performance with 16 cores
- used for further scaling experiments.

<table>
<thead>
<tr>
<th>Time loop</th>
<th>LBM</th>
<th>MG - 5 V(3,3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.10s</td>
<td>0.67s</td>
<td>2.08s</td>
</tr>
</tbody>
</table>

Contact: dominik.bartuschat@fau.de
Weak Scaling for First Time Step

- Parallel efficiency @512 nodes:
  - LBM: 60%
  - MG - 5 V(3,3): 57%

- Reasonably good scaling for both, MG and LBM.
Weak Scaling for 240 Time Steps

- Parallel efficiency @512 nodes:
  - LBM 94 %
  - MG - 1 V(3,3) 59 %

- LBM scales nearly ideally, MG scales reasonably well,
  - MG performance restricted by coarsest-grid solving

8192 cores
1.77M particles

Boston, 01.03.2013 - Dominik Bartuschat - System Simulation Group - Fast Multigrid Solvers for Long Range Potentials (Contact: dominik.bartuschat@fau.de)
Summary

- Parallel multi-physics algorithm for charged particles in fluid flow.
- Cell-centered multigrid with variable stencils for Poisson problem.
- Validation of Poisson problem solution.
- Performance results of main components.
  - Performance evaluation on single (many-core) node.
  - Weak scaling experiments on several nodes.
- Possible MG improvements:
  - Redistribution of coarse grid unknowns / Optimize CG.
  - Higher order prolongation scheme, conserving seven-point stencils.
Thank you for your attention!