Massively Parallel Simulations of Particulate Electrokinetic Micro-fluid Flows

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Advanced Measurements and Multiscale CFD Simulations for Intensification of Multiphase Flow Processes
Motivation

Interactions of large numbers of charged particles in fluid flows, influenced by external electric fields

• Medical applications
  • Optimization of Lab-on-a-Chip systems
    • Sorting of different cells
    • Trapping cells and viruses
  • Deposition of charged aerosol particles in respiratory tract

• Industrial applications
  • Filtering particulates from (exhaust) gases
  • Particle deposition in cooling systems
  • …

© Kang and Li “Electrokinetic motion of particles and cells in microchannels“ Microfluidics and Nanofluidics
waLBerla

- Widely applicable Lattice Boltzmann framework
- Suited for various flow applications
- Large-scale, distributed memory parallelization:
  - Domain partitioned into Cartesian grid of blocks
  - Blocks can be assigned to different processes
  - Ghost layers to exchange cell data between blocks
Hydrodynamic Interactions

Electro-quasi-statics

Rigid body dynamics

Fluid dynamics

Hydrodynamic force

force on ions

ion motion

electrostatic force

charge density

object motion

hydrodynamic force

charge density

ion motion

electrostatic force

force on ions
The Lattice Boltzmann Method

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

- Discrete lattice Boltzmann equation
  - Describes probabilities \( f_q \) that fluid molecules move with given discrete velocities
  - Molecule collisions represented by collision operator \( \Omega_q \)

- Domain discretized into cubic cells
- Discrete velocities \( \vec{c}_q \) and associated distribution functions \( f_q \) per cell

D3Q19 model
Illustration by Klaus Iglberger
The Lattice Boltzmann Method

The equation is solved in two steps:

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

- **Collide step:**
  \[
  \tilde{\tilde{f}}_q(\tilde{x}_i, t_n) = f_q(\tilde{x}_i, t_n) - \frac{1}{\tau} \left( f_q(\tilde{x}_i, t_n) - f^\text{eq}_q(\tilde{x}_i, t_n) \right)
  \]

\[\Omega_q\] with single relaxation time

Fluid viscosity \(\nu_f\) determined by \(\tau\), fluid velocity \(\tilde{u}\), and density \(\rho_f\)
Fluid-Particle Interaction

- Hydrodynamic forces computed by momentum exchange method*
- Four-way coupling

Tumbling Spherocylinders

- Tumbling motion of elongated particles in Stokes flow
- Spherocylinders in periodic domain, aspect ratio $1/\varepsilon = \frac{L}{R} = 12$

Typical runs on SuperMUC:
- on 8192 cores
- for 15 to 48 hrs
- (70 000 to 605 000 time steps)

- Comparison against slender body formulation [*]

Two Tumbling Spherocylinders

Flow field for spherocylinders of $1/\varepsilon = 12$

- Time steps: 600,000
- Runtime on LiMa: 16 h, 768 cores
- Domain size: $[576 \text{dx}]^3$
- Fluid: Water (20 °C)
- $\text{dx} = 4.98 \mu\text{m}$, $R = 4 \text{dx}$
- $\rho_P = 1492 \text{kg/m}^3$
Charged Particles in Fluid Flow

- Electro-quasi-statics
  - Electrostatic force
  - Charge density

- Rigid body dynamics
  - Object motion
  - Hydrodynamic force

- Fluid dynamics
  - Force on ions
  - Ion motion
Electrostatic Force on Particles

- Electric potential described by Poisson equation with particle’s charge density $\rho_e$ on RHS:
  \[- \Delta \Phi(\vec{x}) = \frac{\rho_e(\vec{x})}{\varepsilon_e}\]

- Discretized by finite volumes on lattice
- Solved with cell-centered multigrid (MG) solver implemented in waLBerla
- Supersampling for computing overlap degree to set RHS more accurately

- Electrostatic force on particle:
  \[\vec{F}_c = -q_{\text{particle}} \cdot \nabla \Phi(\vec{x})\]
6-Way Coupling Approach

- Charge distribution
  - Finite volumes
  - MG
    - treat BCs
    - V-cycle
  - Electrostatic force
- Object motion
  - Object distance
  - Newtonian mechanics
  - Collision response
- LBM
  - Velocity BCs
  - Stream-collide step
  - Correction force
  - Lubrication correction

Validation of Electric Potential

Analytical solution for homogeneously charged particle in infinite domain:

\[ \Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \frac{q_e}{|\vec{r}|} \quad \text{if } |\vec{r}| \geq R \]

\[ \Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \frac{q_e}{r} \quad \text{if } r \geq R \]

\[ q_e = 8000 \, e \]

\[ R = 600 \, \mu\text{m} \]

Domain: \([256 \, \text{dx}]^3\)
- Dirichlet BCs: exact solution
- MG: 5 V(2,2)-cycles
- Residual threshold \(2 \cdot 10^{-9}\)

Supersampling: factor 3
Charged Particles in Fluid Flow

- Computed on 144 cores (12 nodes) of RRZE - LiMa
- 210,000 time steps
- 15.7h runtime
- $64^3$ unknowns per core

Channel: $2.56 \text{ mm} \times 7.68 \text{ mm} \times 1.92 \text{ mm}$

dx = 10µm, $\tau = 1.7$, dt = 40µs

Particles: $R = 80\mu\text{m}$, $q_e = \pm 40,000\text{ e}$

Water (20°C), Inflow 1 mm/s, Outflow 0 Pa

Charged plates: $\Phi = \pm 76.8\text{ V}$

else: no-slip & insulating BCs
Parallel Scaling Experiments

Experiments on SuperMUC:
- 18 thin islands with 512 compute nodes, each:
  - 16 cores (2 Xeon chips) @2.5 GHz
  - 32 GB DDR3 RAM
  - Ranked #6 in TOP500 during experiments

Weak scaling:
- Constant size per core:
  - $128^3$ cells
  - 9.4% moving obstacle cells
- Size doubled (in all dimensions)
- Cell-centered multigrid
  - $V(3,3)$ with 7 levels
  - 6 to 116 CG coarse-grid iterations
  - Convergence rate: 0.07
- 2x4x2 cores per node
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


32 768 cores
7.1M particles
Electrophoresis

Electro-quasi-statics

Rigid body dynamics

Fluid dynamics

Equilibrium description of electrical double layer → 7.5-way coupling
**Electrical Double Layer Effect**

**Electrical double layer potential**

Symmetric Poisson-Boltzmann equation (PBE)

\[-\Delta \psi = -\frac{2 z e n_\infty}{\varepsilon_e} \sinh \left( \frac{z e \psi}{k_B T} \right)\]

Debye-Hückel approximation (DHA) for $|\zeta| < 25 \text{ mV}$

\[-\Delta \psi = -\kappa^2 \psi, \quad \kappa = \lambda_D^{-1}\]

**Electrostatic force on double layer charge**

\[\vec{f}_b = \rho_e(\psi) \cdot \vec{E}_{\text{ext}}\]

**Lattice Boltzmann equation with body force term**

\[f_q(\vec{x}_i + \vec{c}_q \, \text{dt}, t + \text{dt}) - f_q(\vec{x}_i, t) = \Omega_q + \text{dt} \, F_q(\vec{f}_b)\]
Validation of Electric Potential

Analytical solution for sphere with uniform surface charge in infinite domain (DHA):

\[ \psi(\vec{r}) = \zeta \frac{R}{|\vec{r}|} e^{-\kappa(|\vec{r}| - R)} \text{ if } |\vec{r}| \geq R \]

Domain: \([128 \, dx]^2 \times 256 \, dx\]

- SOR solver
- Dirichlet BCs: exact solution
- Residual reduction \(2 \times 10^{-7}\)

Radius: \(R = 120 \, \text{nm}\)
Charge: \(q_s = -124 \, e\)
Fluid: Water (20 °C)
\(\kappa R \approx 0.89\)
Electrophoretic Velocity Validation

Analytical solution for sphere with uniform surface charge in infinite domain (Stokes flow):

\[
\vec{U}_{EP} = \frac{2\varepsilon_e \zeta}{3\mu_f} \left( 1 + \frac{1}{2\left[1 + \frac{2.5}{\kappa R \left(1 + 2e^{-\kappa R}\right)}\right]^3} \right) \vec{E}_{ext}
\]

- Validation in large, finite domains (SuperMUC, up to 8192 cores):

<table>
<thead>
<tr>
<th>(R_L)</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>9</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\kappa R)</td>
<td>0.27</td>
<td>0.40</td>
<td>0.53</td>
<td>0.60</td>
<td>0.80</td>
</tr>
<tr>
<td>Retardation / %</td>
<td>-21</td>
<td>-28</td>
<td>-34</td>
<td>-36</td>
<td>-43</td>
</tr>
<tr>
<td>dev. from (U_{EP})/%</td>
<td>-2.56</td>
<td>-2.48</td>
<td>-3.59</td>
<td>-3.51</td>
<td>-3.91</td>
</tr>
<tr>
<td>dev. from (U_{Stokes})/%</td>
<td>-3.04</td>
<td>-2.65</td>
<td>-2.98</td>
<td>-2.89</td>
<td>-3.00</td>
</tr>
<tr>
<td>difference /%</td>
<td>0.5</td>
<td>0.2</td>
<td>-0.6</td>
<td>-0.6</td>
<td>-0.9</td>
</tr>
</tbody>
</table>

- Relative error in electric effects below 1%

dx = 5 nm
\(\zeta = 10\) mV
\(E_{ext} = 99 \cdot 10^6\) V/m
Fluid: Water (20°C)
\(\lambda_D = 75\) nm
\(\Re_{p,d} = 0.018 \ldots 0.057\)
Electrophoresis in Micro-Channel

Electrophoresis of charged particle along channel axis
- Result after 30,000 time steps
- Flow field, double layer potential, and ion charge distribution

Channel: 1.28 µm × 2.56 µm × 1.28 µm
Fluid: Water (20 °C), $c_\infty = 5 \mu$mol/l
Particle: $R = 120$ nm, $q_e = -124$ e
$dx = 10$ nm, $\tau = 6.5$, $dt = 0.2$ ns
$\zeta = -10$ mV, $E_y = -4.7 \cdot 10^6$ V/m
BCs: Periodic in axial direction, else insulating & no-slip BCs

$U_{EP}^* = 0.21 \frac{m}{s}$
Weak Scaling for 240 Time Steps

Parallel efficiency @ 4096 nodes:
- Overall: 87%
- LBM: 94%
- SOR: 82%

Thank you for your attention!