Moving Nano-particles with the LBM in 3D

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The basic Lattice Boltzmann Algorithm

- A Form of Cellular Automaton
- Regular Grid with a fixed Number of Velocities
- Timestep and Cellsize are normalized
- Optimized Implementation/Parallelization possible
- The common 2D/3D Models:
  - D2Q9
  - D3Q19

During one time step:
1) **Stream**: Movement of fluid particles during one time step along their respective velocities
2) **Collide**: Fluid particle collisions during movement are calculated

Rigid Body physics engine

- Simulation of arbitrarily complex particle agglomerates
- Focus on physically correct simulations:
  - Störmer-Verlet method for the equations of motion
  - Quaternions for the rotation handling
  - Exact rigid body collision handling
- Determining the contact points at a certain point in time
- Distinguishing colliding and resting contacts
- Example resting contacts: calculate contact forces to avoid particles to penetrate each other
- Rigid body collisions
- Calculation of internal force and torque in contact points
- Dynamic agglomeration and rupture
- Easy to use C++ framework

LBM Extensions for moving particles

- Dynamic flag status due to moving particles → flag calculation in each time step
- Handling of the curved particle surfaces
- Force interaction between the fluid and the particle surface
- Momentum Exchange Method:

  \[ F = \sum \sum e^i \left( f^i(x,t) + f^i(x,t) \right) \cdot [1 - \Delta v] \Delta x / \Delta t \]

- Calculation of momenta and forces in contact points
- Calculation of angular momentum: Determining the contact points at a certain point in time
- Flag change from PARTICLE to FLUID cell: Use local density interpolation and the
- Dynamic flag status due to moving particles: flag calculation in each time step
- Handling of the curved particle surfaces
- Force interaction between the fluid and the particle surface
- Momentum Exchange Method:

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Coupling of the rigid body physics engine and the LBM

- Successful coupling of a rigid body physics engine with the Lattice Boltzmann method
- For simple settings, the simulation shows the analytical results
- Despite the LBM extensions, 25% of the maximal performance can be conserved
- Extreme memory requirements for exact simulations with a negligible boundary influence
- So far only very small time steps possible → no long lasting processes (sedimentations)
- Current work: adding electrostatic forces