Computational Statistical Physics

Part II: Interacting particles and molecular dynamics

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Particles in fluids

Particles in Fluids

Simulations of particle dynamics in fluids is highly relevant for optimizing certain structures in the sense of minimizing friction and turbulence effects. We therefore consider an incompressible fluid of density ρ and dynamic viscosity μ. It is described by the incompressible *Navier-Stokes equations*

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\left(\nabla \mathbf{u}\right) = -\frac{1}{\rho}\nabla p + \mu \Delta \mathbf{u} \tag{1}$$

The velocity and pressure fields are denoted by $\mathbf{u}\left(\mathbf{x}\right)$ and $p\left(\mathbf{x}\right)$, respectively. In the case of constant density ρ, the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla\left(\rho \mathbf{u}\right) = 0 \tag{2}$$

yields $\nabla \mathbf{u} = 0$.

Particles in Fluids

We classify the fluid flow according to the *Reynold's number*

$$\mathrm{Re} = \frac{uh}{\mu} = \begin{cases} \ll 1 & \text{Stokes limit,} \\ \gg 1 & \text{turbulent flow,} \end{cases} \tag{3}$$

where u and h represent a characteristic velocity and length scale, respectively.

Particles in Fluids

There are two possibilities of modeling particle-fluid interactions. First, in a continuum approach the fluid is described by differential equations such as Eqs. 1 and 2. Second, it is possible to use particle-based models of fluids. Different methods are applicable to solve such problems. Some examples include

- Penalty method with MAC
- Finite volume method (FLUENT)
- $k - \epsilon$ model or spectral methods for the turbulent case
- Lattice-Boltzmann methods
- Discrete simulation methods

Particles in Fluids

Based on the fluid motion described by the Navier-Stokes equations, we are able to extract the forces exerted on the particles which enables us to solve their equations of motion. The total drag force is obtained by integrating **the stress tensor** Θ of the fluid over the particles' surfaces

$$\mathbf{F}_D = \int_\Gamma \Theta \mathrm{d}\mathbf{A}. \tag{4}$$

The stress tensor of the fluid is given by:

$$\Theta_{ij} = -p\delta_{i,j} + \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{5}$$

where $\eta = \rho\mu$ is the static viscosity and p the hydrostatic pressure.

Particles in Fluids

In the Stokes limit for $\mathrm{Re} \ll 1$, the drag law is given by:

$$F_D = 6\pi\eta R u, \tag{6}$$

where η is the viscosity of the fluid, R the radius of the particle, u the velocity of the fluid relative to the particle. The Stokes law is exact for $\mathrm{Re} = 0$. In the case of turbulent flow for $\mathrm{Re} \gg 1$, the drag force is (Newton's law)

$$F_D = 0.22\pi\rho R^2 u^2. \tag{7}$$

Particles in Fluids

The general drag law is

$$F_D = \frac{\pi \eta^2}{8\rho} C_D \mathrm{Re}^2. \tag{8}$$

where C_D denotes the drag coefficient. It depends on the velocity of the particle in the fluid, and on the density and the viscosity of the fluid.

Particles in Fluids

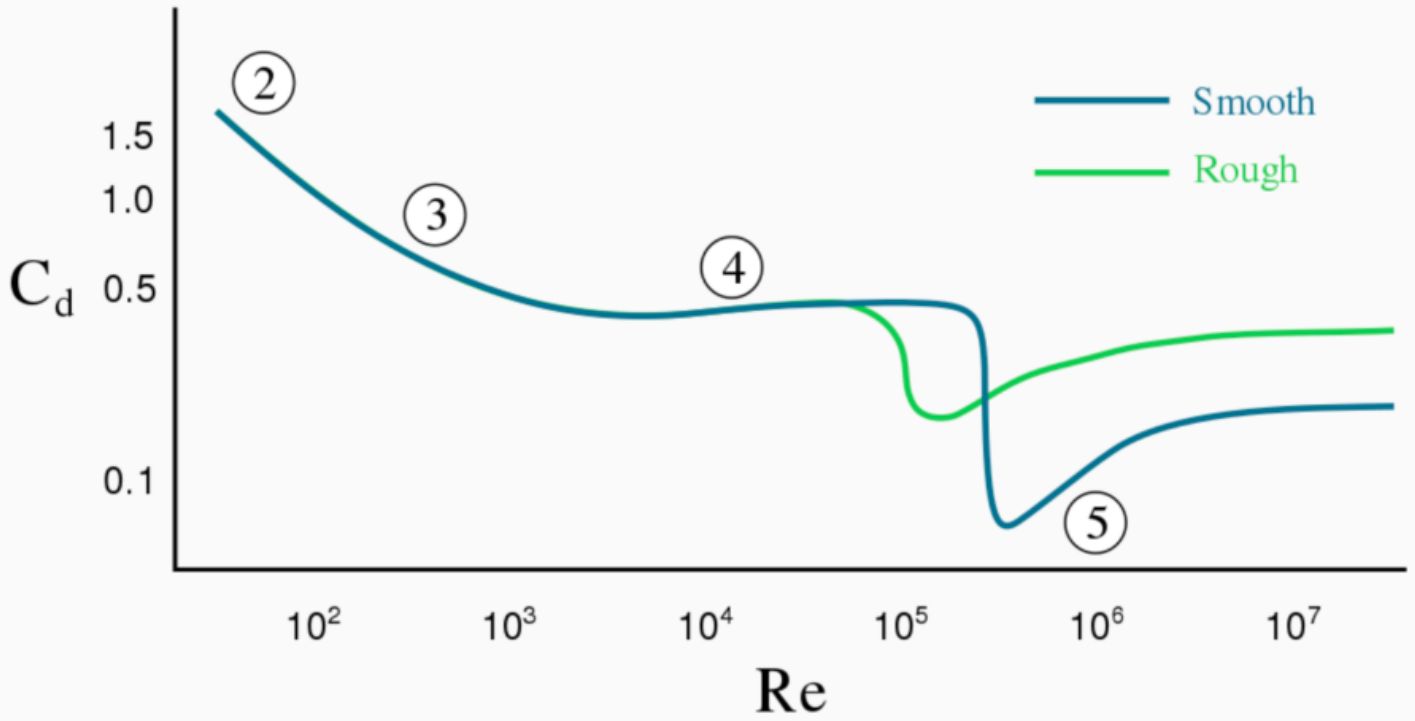


Figure 1: Dependence of the drag coefficient C_D on the Reynold's number.

These laws are based on the assumption of spherical particles and other simplifications, and we may encounter substantial deviations in experiments. In certain cases, it is important to also consider the influence of pressure or velocity gradients which lead to lift forces

$$F_L = \frac{1}{2} C_L \rho A u^2, \tag{9}$$

where C_L denotes the lift coefficient.

Particles in Fluids

In addition to drag and lift forces, rotating particles experience a torque

$$T = \int_{\Gamma} \mathbf{r}_{\mathrm{cm}} \wedge \Theta \mathrm{d}\mathbf{A} \tag{10}$$

For cylinder of radius R and angular velocity ω, the corresponding Magnus force is

$$F_M = 2\pi R^2 \rho u \omega. \tag{11}$$

Particles in Fluids

There exist empirical relation for drag coefficient in certain Reynold's numbers regimes. For example, one may addopt the following drag coefficient dependence:

$$C_D = \begin{cases} 1 & \mathrm{Re}_\rho < 1000, \\ 0.44 & \mathrm{Re}_\rho \geq 1000, \end{cases} \tag{12}$$

where $\mathrm{Re}_\rho = \frac{\rho_f |\mathbf{v}-\mathbf{u}| D_s}{\nu}$. Here D_s is the diameter of the particle, and $|\mathbf{v} - \mathbf{u}|$ is the absolute value of the particle velocities compared to the fluid.

Stokesian Dynamics [Brady, Bossis 1985]

In a method to study Stokesian dynamics ($\mathrm{Re} \ll 1$), we start from the Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\rho}\nabla p + \mu \Delta \mathbf{u} \tag{13}$$

The Green's function of the Stokes equation is the Stokeslet

$$G^S_{\alpha\beta}(\mathbf{r}) = \frac{1}{8\pi\eta}\left(\frac{\delta_{\alpha\beta}}{r} + \frac{r_\alpha r_\beta}{r^3}\right). \tag{14}$$

Stokesian Dynamics [Brady, Bossis 1985]

A general solution for the velocities fields of N particles is then

$$\mathbf{u}(\mathbf{x}) = -\sum_{i=1}^{N} \int_{\Gamma_i} G^S \Theta \, \mathbf{n} \, \mathrm{d}\Gamma_i \tag{15}$$

The drag force on a surface element ijk is determined according to

$$\mathbf{f}_{ijk} = \Theta^{ijk} \mathbf{n}. \tag{16}$$

Lattice Boltzmann Method

Based on the Chapman–Enskog theory, it is possible to derive the Navier-Stokes equations from the Boltzmann equation. This connection between fluid dynamics and Boltzmann transport theory allows us to simulate the motion of fluids by solving the corresponding Boltzmann equation on a lattice. The basic idea is that we define on each site x of a lattice on each outgoing bond i a velocity distribution function $f(x, v_i, t)$ whose updates are given by

$$f(x + v_i, v_i, t + 1) - f(x, v_i, t) + F(v_i) = \frac{1}{\tau}[f_i^{\mathsf{eq}} - f(x, v_i, t)] \quad (17)$$

the equilibrium distribution is

$$f_i^{\mathsf{eq}} = n\omega_i \Big[1 + \frac{3}{c^2}\mathbf{u}\mathbf{v}_i + \frac{9}{2c^4}(\mathbf{u}\mathbf{v}_i)^2 - \frac{3}{2c^2}\mathbf{u}\mathbf{u}\Big]. \quad (18)$$

One possible choice of the weights in two dimensions is

$$\omega_i = \begin{cases} 4/9 & i = 0, \\ 1/9 & i = 1, 2, 3, 4, \\ 1/36 & i = 5, 6, 7, 8. \end{cases} \tag{19}$$

Lattice Boltzmann Method

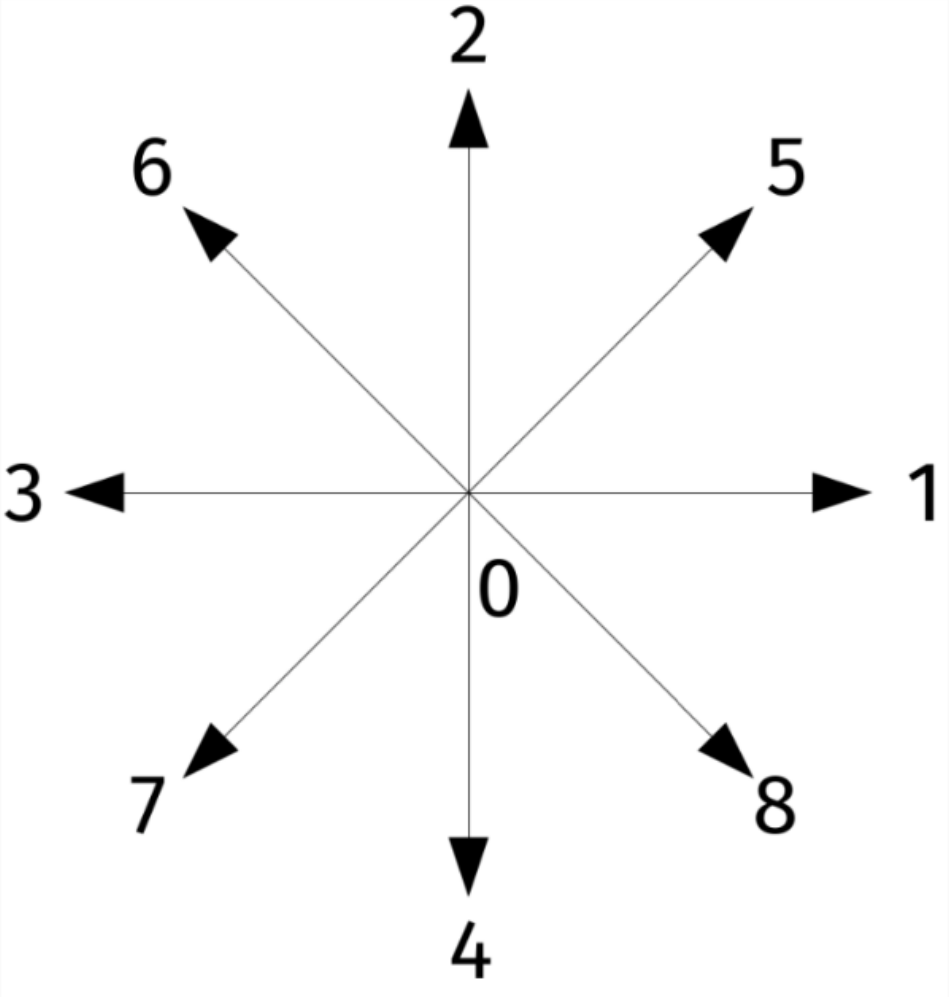


Figure 2: Lattice Boltzmann weights in 2 dimensions

Stochastic rotation dynamics

Stochastic Rotation Dynamics (SRD) is a particle-based fluid modeling approach [Malevanets, Kapral, 99]. This technique is also known as Multi-particle Collision Dynamics (MPC). In this method, we discretize the space into cells and model the fluid as a system composed of N particles with mass m and coordinates x_i and v_i. The particle positions and velocities are updated according to

$$\mathbf{x_i}' = \mathbf{x_i} + \Delta t \mathbf{v_i}, \tag{20}$$

$$\mathbf{v_i}' = \mathbf{u} + \Omega(\mathbf{v_i} - \mathbf{u}) + \mathbf{g} \tag{21}$$

where $\mathbf{u} = \langle \mathbf{v} \rangle$ is the mean velocity of particles in the respective cell and Ω is the rotation matrix.

Stochastic rotation dynamics

The rotation matrix is given by

$$\Omega = \begin{pmatrix} \cos(\alpha) & \pm\sin(\alpha) & 0 \\ \mp\sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{22}$$

The collective fluid particle interaction is modeled by rotations of local particle velocities. In this model, Brownian motion is intrinsic. These very simple dynamics recovers hydrodynamics correctly.

Direct simulation Monte Carlo

Direct Simulation Monte Carlo (DSMC) is a particle-based simulation technique which is appropriate to model particle systems at large Knudsen numbers

$$\mathrm{Kn} = \frac{\lambda}{L} \tag{23}$$

where λ is the mean free path and L a characteristic system length scale. It is very popular in aerospace modeling, because the atmosphere is very thinned out at high altitudes and the corresponding Knudsen numbers are large.

Direct simulation Monte Carlo

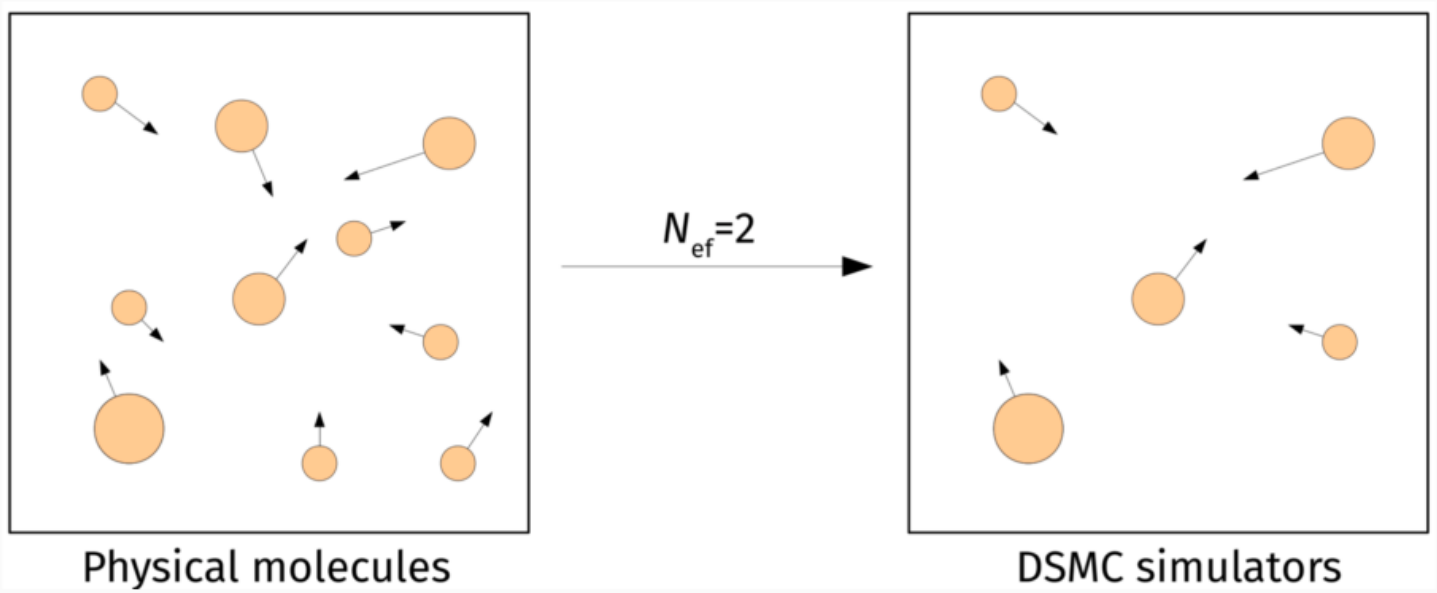


Figure 3: In DSMC N_{ef} simulators represent one physical particle.

Direct simulation Monte Carlo

Collision are modeled by sorting particles into spatial collision cells. We then iterate over all cells and

1. compute the collision frequency in each cell,
2. randomly select collision partners within cell,
3. process each collision.

We note that collision pairs with large relative velocity are more likely to collide but they do not have to be on a collision trajectory.

Direct simulation Monte Carlo

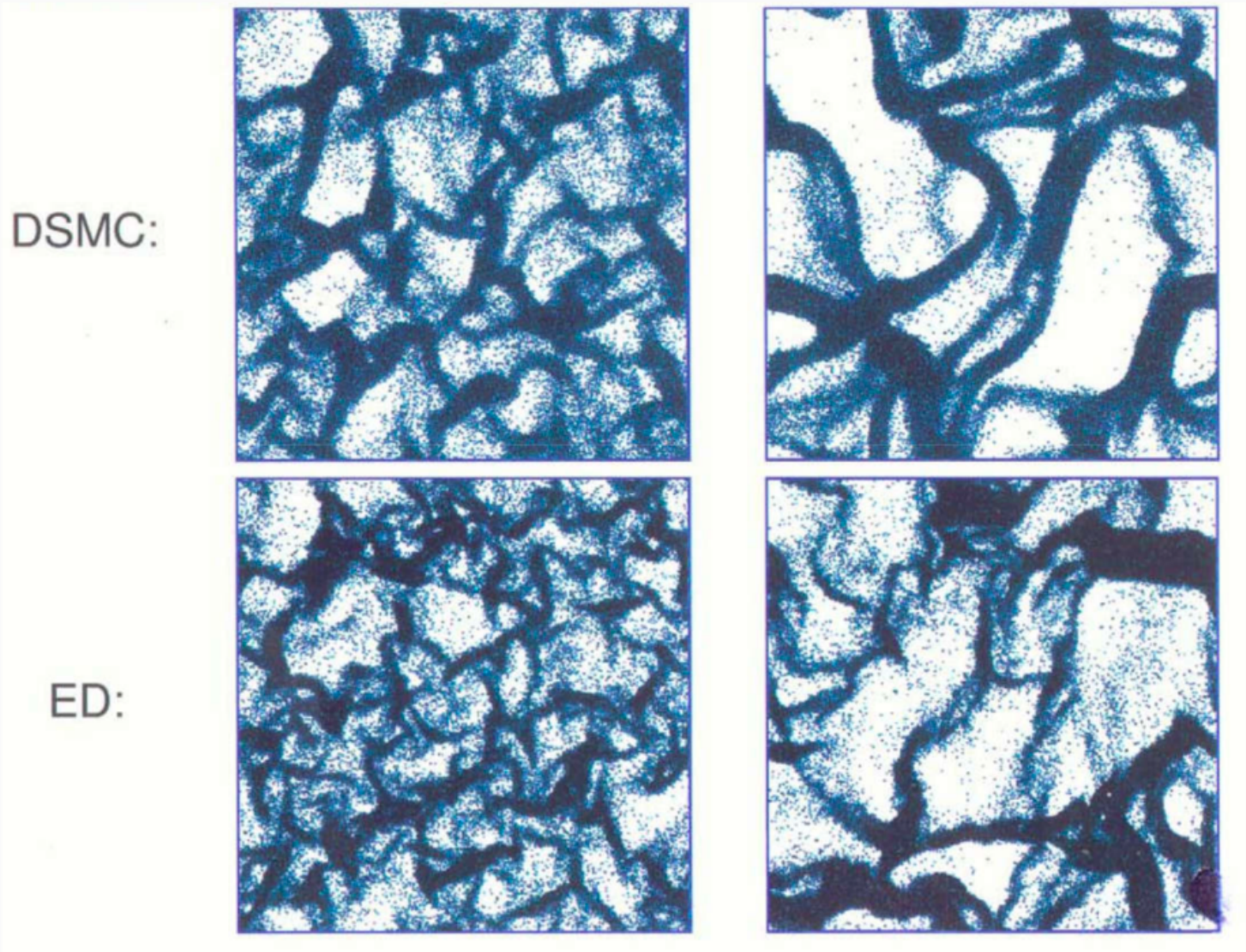
The material surface may be treated with a thermal wall, which resets the velocity of a particle as a biased-Maxwellian distribution

$$P_{v_x}(v_x) = \pm \frac{m}{k_B T_W} v_x e^{-\frac{m v_x^2}{2 k_B T_W}} \tag{24}$$

$$P_{v_y}(v_y) = \sqrt{\frac{m}{2\pi k_B T_W}} e^{-\frac{m(v_y - u_W)^2}{2 k_B T_W}} \tag{25}$$

$$P_{v_x}(v_x) = \sqrt{\frac{m}{2\pi k_B T_W}} e^{-\frac{m v_z^2}{2 k_B T_W}} \tag{26}$$

Direct simulation Monte Carlo



Dissipative Particle Dynamics [Hoogerbrugge, Koelman, '92]

Another particle-based fluid simulation approach is the so-called Dissipative Particle Dynamics (DPD). The particle interactions are described by

$$\mathbf{F}_i = \sum_{i \neq j} (\mathbf{f}_{ij}^C + \mathbf{f}_{ij}^R + \mathbf{f}_{ij}^D), \tag{27}$$

where $\mathbf{f}_{ij}^C$ represents the conservative forces (e.g., momentum transfer), $\mathbf{f}_{ij}^R$ a random force and $\mathbf{f}_{ij}^D$ the dissipative forces, proportional to the velocity of the particles. The weights of the random and dissipative forces must be chosen such that thermal equilibrium is reached

Smoothed Particle Hydrodynamics

Another important technique in the field of computational fluid dynamics is Smoothed Particle Hydrodynamics (SPH). This method uses smooth kernel functions W to represent properties of particles in a weighted sense. Instead of localized positions and velocities, the particle characteristics are smoothened over a smoothing length h. An arbitrary quantity A is then given by

$$A(r) = \int_{\Omega} W\left(\left|r - r'\right|, h\right) A\left(r'\right) \mathrm{d}r' \approx \sum_{j} \frac{m_j}{\rho_j} W\left(\left|r - r_j\right|, h\right) A_j.$$

Smoothed Particle Hydrodynamics

In this method, no spatial discretization is necessary and even complex geometries can be interpolated and simulated with SPH. This makes this method broadly applicable in many different fields where fluids interact with complex structures. Example of a kernel functions include Gaussians or quadratic functions

$$W(r,h) = \frac{3}{2\pi h^2}(\frac{1}{4}q^2 - q + 1) \tag{28}$$

with $q = \frac{h}{r}$ and $r = |r_a - r_b|$. Another advantage of this method is that kernels may be changed without much effort for a given simulation framework.