Stochastic Smoothed Particle Hydrodynamics Method for Multiphase Flow and Transport

Alexandre Tartakovsky,
Pacific Northwest National Laboratory
Challenges in SPH and SDPD

- Boundary (no-slip and Navier) Conditions
- Parameterization (with respect to surface tension and static contact angle) of multiphase SPH/SDPD models
Flow and Transport at Mesoscale

Continuity and momentum equations:

\[
\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}, \quad \rho \frac{D\mathbf{v}}{Dt} = -\nabla \cdot \mathbf{T} \quad \mathbf{r} \in \mathbb{R}^N
\]

Stochastic diffusion equation:

\[
\frac{DC}{Dt} = \frac{1}{\rho} \nabla \cdot (\rho D^F \nabla C) + \frac{1}{\rho} \nabla \cdot \mathbf{J}.
\]

\[\mathbf{T} = P\mathbf{I} - \mu [\nabla \mathbf{v} + \nabla \mathbf{v}^T] - \mathbf{s} \text{ is stress tensor}\]

\[
\frac{s^{ik}(\mathbf{r}_1, t_1)s^{lm}(\mathbf{r}_2, t_2)}{\sigma^2} = \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2) \quad \sigma^2 = 2\mu k_B T\delta^{im}\delta^{kl}
\]

\[
\frac{J^i(\mathbf{r}_1, t_1)J^j(\mathbf{r}_2, t_2)}{\tilde{\sigma}^2} = \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2) \quad \tilde{\sigma}^2 = 2m_0 DC(1 - C)\rho \delta^{ij}
\]

Landau and Lifshitz
Non-Local Continuity Equation

Continuity equation defined on infinite domain $\mathbb{R}^N$

$$\frac{D\rho^h}{Dt} = -\rho^h \int_{\mathbb{R}^N} \left( \mathbf{v}^h(r') - \mathbf{v}^h(r) \right) \cdot \nabla_r W^h(r - r') dr'$$

If $W$ satisfies the conditions:

$$W^h(r - r') = \frac{1}{h^d} W\left(\frac{r - r'}{h}\right)$$

$$W(y - x) = W(x - y), \quad W \geq 0, \quad \int_{\mathbb{R}^N} W(z) dz = 1,$$

then

$$\rho = \rho^h + \mathcal{O}(h^2)$$

Lehoucq, Du et al
Non-Local Momentum Equation

\[
\frac{Dv^h}{Dt} = -\frac{1}{\rho^h} \int_{\mathbb{R}^N} \left( \frac{P^h(r')}{\rho^h(r')} + \frac{P^h(r)}{\rho^h(r)^2} \rho^h(r') \right) \nabla_r W^h(r - r') \, dr'
\]
\[
+ \frac{2\mu}{\rho^h} \int_{\mathbb{R}^N} \left( v^h(r') - v^h(r) \right) \frac{r - r'}{|r - r'|^2} \cdot \nabla_r W^h(r - r') \, dr'
\]
\[
+ \frac{1}{\rho^h} \int_{\mathbb{R}^N} \left( \frac{s(r')}{\rho^h(r')} + \frac{s(r)}{\rho^h(r)^2} \rho^h(r') \right) \cdot \nabla_r W^h(r - r') \, dr'
\]

\[
v = v^h + O(h^2)
\]
Non-Local Diffusion Equation

\[
\frac{DC^h}{Dt} = \frac{DF}{\rho h} \int_{\mathbb{R}^N} \left( \rho^h(r) + \rho^h(r') \right) \left( C^h(r') - C^h(r) \right) \frac{r - r'}{|r - r'|^2} \cdot \nabla_r W^h (r - r') \, dr' \\
+ \frac{1}{\rho h} \int \left( \frac{J^h(r')}{\rho h(r')} + \frac{J^h(r)}{\rho h(r)^2} \rho^h(r') \right) \cdot \nabla_r W^h (r - r') \, dr'
\]

\[c = c^h + \mathcal{O}(h^2)\]

SPH discretization

Discretize domain with $N$ uniformly spaced points (or particles)
$r_i(t = 0) (i = 1, N)$ - positions of particles
$\Delta$ is the spacing between particles ($\Delta < h$)
$V_i(t = 0) = \Delta^d$ - volume occupied by particle $i$
$m_i = \rho_i(t = 0)\Delta^d$ - mass of particle $i$, does not change with time

$$\frac{D\rho^h_i}{Dt} = -\rho^h_i \sum_{i=1}^{N} \frac{1}{n_j} \left( v^h_j - v^h_i \right) \cdot \nabla r_i W^h (r_i - r_j)$$

$$\frac{Dv^h_i}{Dt} = -\sum_{i=1}^{N} \left( \frac{T^h_j}{n_j^2} + \frac{T^h_i}{n_i^2} \right) \cdot \nabla r_i W^h (r_i - r_j)$$

$$\frac{Dr_i}{Dt} = v^h_i, \quad \frac{1}{n_j} = V_j(t) = \frac{m_j}{\rho^h_j(t)}$$

EoS: $P_i = P(\rho^h_i)$
SPH discretization error

\[ e \leq e_{\text{integral}} + e_{\text{quadrature}} + e_{\text{anisotropy}} \]

Error due to integral approximation:

\[ e_{\text{integral}} \leq C_1 h^2 \]

Quadrature error:

\[ e_{\text{quadrature}} \leq C_2 \frac{\Delta}{h} \]

Anisotropy error due to particle disorder:

\[ e_{\text{anisotropy}} \leq C_3 \frac{\chi}{h^\rho} \left( \frac{\Delta}{h} \right)^\beta \]

\( \chi \) - deviation from the cartesian mesh, \( \rho \) - order of differential operator, \( \beta \) - order of polynomial form of \( W \)
A scalable consistent second-order SPH solver for unsteady low Reynolds number flows


Discretization error:

\[ e = e_{\text{integral}} \leq C_1 h^2 \]
Boundary-value problems

Consider diffusion equation subject to the Neuman and Dirichlet BCs:

\[
\begin{align*}
\frac{\partial}{\partial t} c(\boldsymbol{x}, t) &= \nabla \cdot [k(\boldsymbol{x}) \nabla c(\boldsymbol{x}, t)] & \boldsymbol{x} \in \Omega, \ t > 0 \\
c(\boldsymbol{x}, t) &= g_\tau(\boldsymbol{x}, t) & \boldsymbol{x} \in \partial\Omega_d, \ t > 0 \\
\frac{\partial}{\partial n} c(\boldsymbol{x}, t) &= f_\tau(\boldsymbol{x}, t) & \boldsymbol{x} \in \partial\Omega_n, \ t > 0 \\
c(\boldsymbol{x}, 0) &= c_0(\boldsymbol{x}) & \boldsymbol{x} \in \Omega,
\end{align*}
\]

where \( \Omega \subseteq \mathbb{R}^N \) is an open region.
Non-local operator

Let \( \Gamma := \mathbb{R}^N \setminus \Omega \) and \( \Gamma = \Gamma_n \cup \Gamma_d \)
Define the integral operator:

\[
\mathcal{L} c^h(x, t) := \int_{\Omega \cup \Gamma_d} \left( k(x) + k(y) \right) \left( c^h(y, t) - c^h(x, t) \right) \frac{x - y}{|x - y|^2} \nabla W^h(x - y) \, dy, \quad x \in \Omega, t > 0
\]
Non-local boundary-value problems

\[ \frac{\partial}{\partial t} c^h(x, t) = \mathcal{L} c^h(x, t) + f(x, t) \int_{\Gamma_n} (n(x) + n(y)) \nabla W^h dy \quad x \in \Omega \]

\[
\begin{cases}
  c^h(x, t) = g(x, t) & x \in \Gamma_d, t > 0 \\
  \mathcal{L} c^h(x, t) = 0 & x \in \Gamma_n, t > 0 \\
  c^h(x, 0) = c_0(x) & x \in \Omega,
\end{cases}
\]

\[ g(x, t) = g_\tau(x, t) \text{ for } x \in \partial\Omega_d \text{ and } f(x, t) = f_\tau(x, t) \text{ for } x \in \partial\Omega_n. \]

Then,

\[ c = c^h + O(h^2) \]

Application to NS Eq subject to partial-slip Robin (Navier) BC

Navier BC: $\tau \cdot n = \beta v$ and $v \cdot n = 0$; $\tau$ - viscous stress; $\mu/\beta$ - slip length $\approx 10 - 15 \eta m$.

Example: flow around cylinder subject to Navier BC.

Pan, Bao, Tartakovsky, JCP (2014)
Multiphase flow

Young-Laplace boundary condition at the fluid-fluid interface:

\[(P_\alpha - P_\beta)\mathbf{n} = (\tau_\alpha - \tau_\beta) \cdot \mathbf{n} + \kappa \sigma_{\alpha\beta} \mathbf{n}\]

Fluid-solid interface: no-slip, \(\mathbf{v} = 0\)

Contact line (Fluid-fluid-solid interface): Contact angle \(\theta\) is prescribed (\(\mathbf{v}\) is unknown)

Fundamental Challenges:

- Divergence of stress \(\tau\) at the contact line
- Unknown \(\mathbf{v}\)-dependent dynamic contact angle
- Empirical models for \(\theta\) are accurate for a narrow range of conditions (\(Ca < 1\))
Hybrid models to remove singularity and model dynamic contact angle

Approximate models to relieve the stress singularity near the contact line

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesoscopic precursor film</td>
<td>Hervet and de Gennes, 1984</td>
</tr>
<tr>
<td>Molecular film</td>
<td>Eres et al., 2000</td>
</tr>
<tr>
<td>Navier slip</td>
<td>Huh and Scriven, 1971</td>
</tr>
<tr>
<td>Nonlinear slip</td>
<td>Thompson and Troian, 1997</td>
</tr>
<tr>
<td>Surface roughness</td>
<td>Hocking, 1976</td>
</tr>
<tr>
<td>Shear thinning</td>
<td>Weidner and Schwartz, 1993</td>
</tr>
<tr>
<td>Evaporation and condensation</td>
<td>Wayner, 1993</td>
</tr>
<tr>
<td>Diffuse interface</td>
<td>Seppecher, 1996</td>
</tr>
<tr>
<td>Normal stresses</td>
<td>Boudaoud, 2007</td>
</tr>
</tbody>
</table>

Bonn et al., 2009

Main disadvantages:

- Approximate models: require a phenomenological model for dynamic contact angle
- Multiscale models: computationally demanding, limited to small length and time scales
SPH Multiphase Flow Models

- Continuous Surface Force Model (*Morris* 2000)
  - Replace Young-Laplace BC $\Delta P = \sigma \kappa$ with the source term $|\nabla \phi| \sigma \kappa$ (*Brackbill* 1992)
  - Contact Line Force Model for dynamic contact angles (*Huber, Hassanzadeh et al*)
  - Challenge: Curvature calculation requires fine resolution

- Phase Field Model (*Xu, Tartakovsky and Meakin* 2010)

- Pairwise Force SPH Model (*Tartakovsky and Meakin* 2005)
  - Advantages: easy to implement, robust, free surface and multiphase flow problems
Lagrangian mesoscale model for multiphase flow
Tartakovsky and Meakin, 2005; Bondara et al, 2013

Continuum Surface Force formulation of the NS equation (Brackbill, 1992):

\[ \rho \frac{D\mathbf{v}}{Dt} = -\nabla P + \nabla \cdot \mathbf{\tau} + \kappa \sigma |\nabla \gamma| + \rho \mathbf{g}, \quad \gamma(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_\alpha(t) \\ 0, & \mathbf{x} \in \Omega_\beta(t) \end{cases} \]

\[ \frac{Dx_i}{Dt} = v_i, \quad m_i \frac{Dv_i}{Dt} = \sum_j f_{ij} + \sum_j F_{ij}^{int} + m_i g \]

- Fluid and solid phases are discretized by separate sets of particles with mass \( m_i \)
- \( F_{ij}^{int} \) is a pairwise force creating surface tension
Interaction forces

\[ F^{\text{int}}(x_i, x_j) = s(x_i, x_j) \phi(|x_i - x_j|) \frac{x_i' - x_j''}{|x_i' - x_j''|} \]

\( \phi \) is the shape function

\[ s(x_i, x_j) = s_{\alpha \beta} \text{ for } x_i \in \alpha\text{-phase and } x_j \in \beta\text{-phase}. \]

Forces are scaled as to generate the same surface tension

**Surface tension:** \( \sigma_{\alpha \beta} = T_{\alpha \alpha} + T_{\beta \beta} - 2T_{\alpha \beta} \)

**Specific interfacial energy:** \( T_{\alpha \beta} = -\frac{1}{8} \pi n_\alpha n_\beta s_{\alpha \beta} \int_0^\infty z^4 \phi(z) dz \)

**Static contact angle:** \( \sigma_{\alpha \beta} \cos \theta_0 + \sigma_{s\alpha} = \sigma_{s\beta} \)
Relationship between surface tension, contact angle and pairwise forces

\[
F^{\text{int}}(x_i^\alpha, x_j^\beta) = s_{\alpha\beta}\phi(|x_i^\alpha - x_j^\beta|) \frac{x_i^\alpha - x_j^\beta}{|x_i^\alpha - x_j^\beta|}
\]

\[
s_{\alpha\alpha} = s_{\beta\beta} = 10^4 s_{\alpha\beta} = \frac{1}{2} n^{-2} \left( \frac{h}{3} \right)^{-5} \frac{\sigma}{\lambda}
\]

\[
s_{s\alpha} = \frac{1}{2} n^{-2} \left( \frac{h}{3} \right)^{-5} \frac{\sigma}{\lambda} \left( 1 + \frac{1}{2} \cos \theta_0 \right)
\]

\[
s_{s\beta} = \frac{1}{2} n^{-2} \left( \frac{h}{3} \right)^{-5} \frac{\sigma}{\lambda} \left( 1 - \frac{1}{2} \cos \theta_0 \right),
\]

\[
\lambda = \int z^4 \phi(z) dz
\]

and \( n \) is the average particle number density.
“Force - surface tension” relationship

Stress tensor Hardy, 1982

\[ \mathbf{T}(\mathbf{x}) = \mathbf{T}(c)(\mathbf{x}) + \mathbf{T}(int)(\mathbf{x}) \]

Convection stress

\[ \mathbf{T}(c)(\mathbf{x}) = \sum_{j=1}^{N} m_j (\mathbf{v}(\mathbf{x}) - \mathbf{v}_j) \otimes (\mathbf{v}(\mathbf{x}) - \mathbf{v}_j) \psi_\eta(\mathbf{x} - \mathbf{r}_j) \]

Virial stress:

\[ \mathbf{T}(v)(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} f_{ij} \otimes (\mathbf{r}_j - \mathbf{r}_i) \int_0^1 W_\eta(\mathbf{x} - s\mathbf{r}_i - (1 - s)\mathbf{r}_j) ds \quad \eta > h \]

Continuum approximation:

\[ \mathbf{T}^{int}(\mathbf{x}) \approx \frac{n_{eq}^2}{2} \int \int g(\mathbf{x}', \mathbf{x}'') \mathbf{F}^{int} \otimes (\mathbf{x}'' - \mathbf{x}') \int_0^1 \psi_\eta(\mathbf{x} - s\mathbf{x}' - (1 - s)\mathbf{x}'') ds dx' dx'' \]
Analytical evaluation of surface tension

\[
\sigma_{\alpha\beta}(x) = \int_{-\infty}^{+\infty} \left[ T_\tau(r) - T_n(r) \right] dr
\]

Then,

\[
\sigma_{\alpha\beta} = \tau_{\alpha\alpha} + \tau_{\beta\beta} - 2\tau_{\alpha\beta},
\]

Specific interfacial energy \(\tau_{\alpha\beta}\) is

\[
3D : \quad \tau_{\alpha\beta} = -\frac{1}{8} \pi n_\alpha n_\beta s_{\alpha\beta} \int_0^\infty z^4 \phi(z) dz
\]

\[
2D : \quad \tau_{\alpha\beta} = -\frac{1}{3} n_\alpha n_\beta s_{\alpha\beta} \int_0^\infty z^3 \phi(z) dz
\]

\[\text{The 3D result agrees with Rayleigh, 1890.}\]
Pressure due to $\mathbf{F}_{ij}^{\text{int}}$ forces

\[
p^{\text{int}} = -\frac{1}{3} \text{tr}(\mathbf{T}^{\text{int}})
\]

3D: \[
p_{\alpha}^{\text{int}} = \frac{2}{3} \pi n_{\alpha}^{2} s_{\alpha \alpha} \int_{0}^{\infty} z^{3} \phi(z) dz
\]

2D: \[
p_{\alpha}^{\text{int}} = -\frac{1}{2} \pi n_{\alpha}^{2} s_{\alpha \alpha} \int_{0}^{\infty} z^{2} \phi(z) dz
\]
Effect of thermal fluctuations on surface tension

\[ \sigma^F(k_BT) = \sigma_0 \left(1 - b \left(\frac{k_BT}{n_{eq}\epsilon}\right)^2\right)^2 \]

\( \epsilon \) - potential energy

Huan Lei
Effect of $F_{\alpha\beta}$ on particle distribution

Figure: Particle distribution obtained from simulations of a bubble of one fluid surrounded by another fluid with: (a) cosine pairwise force; (b) gaussian pairwise force with $\varepsilon_0 = 0.5\varepsilon/2$; and (c) gaussian pairwise force with $\varepsilon_0 = 0.8\varepsilon/2$. 
Fluctuations of “immiscible” interfaces due to thermal fluctuations

$$\rho_{\text{top}}/\rho_{\text{bottom}} = 1$$

$$\rho_{\text{top}}/\rho_{\text{bottom}} = 0.5$$

$$\rho_{\text{top}}/\rho_{\text{bottom}} = 2$$

Structure factor (hight-hight correlation function). Good agreement with theory for stable and unstable fluids configurations.

Huan Lei
PF-SPH accurately models dynamic contact angles

Withdrawal of a plate from the bath of liquid (green fluid)

Dynamic contact angle satisfies the Cox-Voinov law $\theta_0^3 - \theta_r^3 = a_r Ca$.

$\theta_0$ - prescribed static contact angle
$\theta_r$ - resulting receding dynamic angle

Tartakovsky and Panchenko, 2015 JCP
Effect of wettability on distribution of fluid phases and possible implications for the long-term CO$_2$ storage

![Figure: Distribution of non-wetting CO$_2$ at 4 different dimensionless times: (a) $t^*=204$ (during injection); (b) $t^*=983$ (after injection); (c) $t^*=1022$ (after injection); and (d) $t^*=251524$ (after equilibrium stage is achieved).](image)

![Figure: Distribution of neutrally-wetting CO$_2$ in Case 1b at 4 different dimensionless times: (a) $t^*=776$; (b) $t^*=73891$; (c) $t^*=308796$; and (d) $t^*=536426$.](image)
Effect Of Thermal Fluctuations on Miscible Fronts

“Giant fluctuations” of interface between miscible fluids

Figure 1 | Development of nonequilibrium fluctuations during diffusion processes occurring on Earth and in space. False-colour shadowgraph images of nonequilibrium fluctuations in microgravity (a-d) and on Earth (e-h) in a 1.00-mm-thick sample of polystyrene in toluene. Images were taken 0, 400, 800 and 1,600 s (left to right) after the imposition of a 17.40 K temperature difference. The side of each image corresponds to 5 mm. Colours map the deviation of the intensity of shadowgraph images with respect to the time-averaged intensity.
Power spectra of the miscible front

\[ \frac{S(q)}{S^\infty} = \left( q^4 + B(\Lambda)q^2 + \Lambda^4 \right)^{-1} \] (Ortiz de Za` rate, 2004)

- SPH results agree with theory for \( g = 0 \)
- Gravity reduces low wave number fluctuations

Kordilla, Pan, Tartakovsky, JCP 2014
Rayleigh-Taylor Instability. Comparison with analytical solutions.

\[ D^F = 3.6 \times 10^{-4}, \ D^\xi = 0 \]
\[ D^F = 2.4 \times 10^{-4}, \ D^\xi = 1.2 \times 10^{-4} \]
\[ D^F = 2.4 \times 10^{-4}, \ D^\xi = 1.2 \times 10^{-4} \ (SDPD) \]
Conclusions

“The particle method is not only an approximation of the continuum fluid equations, but also gives the rigorous equations for a particle system which approximates the molecular system underlying, and more fundamental than the continuum equations.”

Von Neumann (1944) in connection with the use of particle methods to model shocks.