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

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Flow and Transport at Mesoscale

Continuity and momentum equations:

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

Stochastic diffusion equation:

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

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

$$\overline{s^{ik}(\mathbf{r_1},t_1)s^{lm}(\mathbf{r_2},t_2)} = \sigma^2\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(t_1-t_2) \quad \sigma^2 = 2\mu k_B T\delta^{im}\delta^{kl}$$

$$\overline{J^i(\mathbf{r_1},t_1)J^j(\mathbf{r_2},t_2)} = \tilde{\sigma}^2\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(t_1-t_2) \quad \tilde{\sigma}^2 = 2m_0DC(1-C)\rho\delta^{ij}$$

Landau and Lifshitz

Non-Local Continuity Equation

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

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

If W satisfies the conditions:

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

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

then

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

Lehoucq, Du et al

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Non-Local Momentum Equation

$$\begin{aligned}\frac{D\mathbf{v}^h}{Dt} &= -\frac{1}{\rho^h}\int_{\mathbb{R}^N}\left(\frac{P^h(\boldsymbol{r}')}{\rho^h(\boldsymbol{r}')}+\frac{P^h(\boldsymbol{r})}{\rho^h(\boldsymbol{r})^2}\rho^h(\boldsymbol{r}')\right)\nabla_{\boldsymbol{r}}W^h\left(\boldsymbol{r}-\boldsymbol{r}'\right)d\boldsymbol{r}' \\ &+ \frac{2\mu}{\rho^h}\int_{\mathbb{R}^N}\left(\mathbf{v}^h(\boldsymbol{r}')-\mathbf{v}^h(\boldsymbol{r})\right)\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\cdot\nabla_{\boldsymbol{r}}W^h\left(\boldsymbol{r}-\boldsymbol{r}'\right)d\boldsymbol{r}' \\ &+ \frac{1}{\rho^h}\int_{\mathbb{R}^N}\left(\frac{\mathbf{s}(\boldsymbol{r}')}{\rho^h(\boldsymbol{r}')}+\frac{\mathbf{s}(\boldsymbol{r})}{\rho^h(\boldsymbol{r})^2}\rho^h(\boldsymbol{r}')\right)\cdot\nabla_{\boldsymbol{r}}W^h\left(\boldsymbol{r}-\boldsymbol{r}'\right)d\boldsymbol{r}'\end{aligned}$$

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

Non-Local Diffusion Equation

$$
\begin{aligned}
\frac{DC^h}{Dt} &= \frac{D^F}{\rho^h}\int_{\mathbb{R}^N}\left(\rho^h(\boldsymbol{r})+\rho^h(\boldsymbol{r}')\right)\left(C^h(\boldsymbol{r}')-C^h(\boldsymbol{r})\right)\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^2} \\
&\cdot \quad \nabla_{\boldsymbol{r}} W^h\left(\boldsymbol{r}-\boldsymbol{r}'\right)d\boldsymbol{r}' \\
&+ \quad \frac{1}{\rho^h}\int\left(\frac{\mathbf{J}^h(\boldsymbol{r}')}{\rho^h(\boldsymbol{r}')}+\frac{\mathbf{J}^h(\boldsymbol{r})}{\rho^h(\boldsymbol{r})^2}\rho^h(\boldsymbol{r}')\right)\cdot\nabla_{\boldsymbol{r}} W^h\left(\boldsymbol{r}-\boldsymbol{r}'\right)d\boldsymbol{r}'
\end{aligned}
$$

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

Du, Lehoucq, Tartakovsky, Comp Meth in Appl Mech and Eng (2015); Kordilla et al, JCP (2014)

SPH discretization

Discretize domain with N uniformly spaced points (or particles)
$\boldsymbol{r}_i(t=0)$ $(i=1,N)$ - positions of particles
Δ 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

$$\frac{D\rho_i^h}{Dt} = -\rho_i^h \sum_{i=1}^{N} \frac{1}{n_j} \left(\mathbf{v}_j^h - \mathbf{v}_i^h\right) \cdot \nabla_{\boldsymbol{r}_i} W^h \left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)$$

$$\frac{D\mathbf{v}_i^h}{Dt} = -\sum_{i=1}^{N} \left(\frac{\mathbf{T}_j^h}{n_j^2} + \frac{\mathbf{T}_i^h}{n_i^2}\right) \cdot \nabla_{\boldsymbol{r}_i} W^h \left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)$$

$$\frac{D\boldsymbol{r}_i}{Dt} = \mathbf{v}_i^h, \qquad \frac{1}{n_j} = V_j(t) = \frac{m_j}{\rho_j^h(t)}$$

EoS: $P_i = P(\rho_i^h)$

SPH discretization error

$$e \leq e_{integral} + e_{quadrature} + e_{anisotropy}$$

Error due to integral approximation:

$$e_{integral} \leq C_1 h^2$$

Quadrature error:

$$e_{quadrature} \leq C_2 \frac{\Delta}{h}$$

Anisotropy error due to particle disorder:

$$e_{anisotropy} \leq C_3 \frac{\chi}{h^p} \left(\frac{\Delta}{h} \right)^{\beta}$$

χ - deviation from the cartesian mesh, p - order of differential operator, β - order of polynomial form of W

A scalable consistent second-order SPH solver for unsteady low Reynolds number flows

Trask, N.,Maxey,M., Kim, K., Perego, M., Parks,M.L., Yang, K., Xu, J., *Computer Methods in Applied Mechanics and Engineering*, 2014

Discretization error:

$$e = e_{integral} \leq C_1 h^2$$

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Boundary-value problems

Consider diffusion equation subject to the Neuman and Dirichlet BCs:

$$
\begin{cases}
\frac{\partial}{\partial t} c(\boldsymbol{x}, t) = \nabla \cdot [k(\boldsymbol{x}) \nabla c(\boldsymbol{x}, t)] & \boldsymbol{x} \in \Omega, t > 0 \\
c(\boldsymbol{x}, t) = g_\tau(\boldsymbol{x}, t) & \boldsymbol{x} \in \partial\Omega_d, t > 0 \\
\frac{\partial}{\partial \mathbf{n}} c(\boldsymbol{x}, t) = f_\tau(\boldsymbol{x}, t) & \boldsymbol{x} \in \partial\Omega_n, t > 0 \\
c(\boldsymbol{x}, 0) = c_0(\boldsymbol{x}) & \boldsymbol{x} \in \Omega,
\end{cases}
\tag{1}
$$

where $\Omega \subseteq \mathbb{R}^N$ is an open region.

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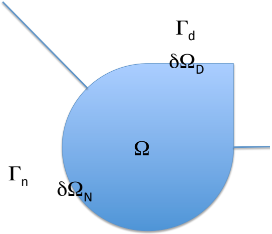
Non-local operator



Let $\Gamma := \mathbb{R}^N \setminus \Omega$ and $\Gamma = \Gamma_n \cup \Gamma_d$

Define the integral operator:

$$\mathcal{L}c^h(\boldsymbol{x},t) := \int_{\Omega\cup\Gamma_d} (k(\boldsymbol{x})+k(\boldsymbol{y}))\left(c^h(\boldsymbol{y},t)-c^h(\boldsymbol{x},t)\right) \frac{\boldsymbol{x}-\boldsymbol{y}}{|\boldsymbol{x}-\boldsymbol{y}|^2}\nabla W^h(\boldsymbol{x}-\boldsymbol{y})d\boldsymbol{y}, \quad \boldsymbol{x}\in\Omega, t>0$$

Non-local boundary-value problems

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

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

$g(\boldsymbol{x}, t) = g_\tau(\boldsymbol{x}, t)$ for $\boldsymbol{x} \in \partial\Omega_d$ and $f(\boldsymbol{x}, t) = f_\tau(\boldsymbol{x}, t)$ for $\boldsymbol{x} \in \partial\Omega_n$.
Then,

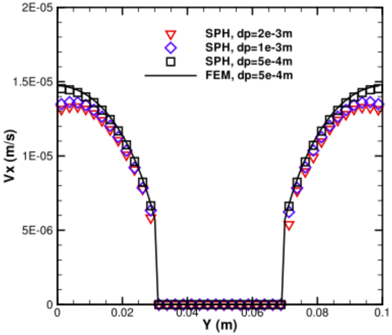
$$c = c^h + \mathcal{O}(h^2)$$

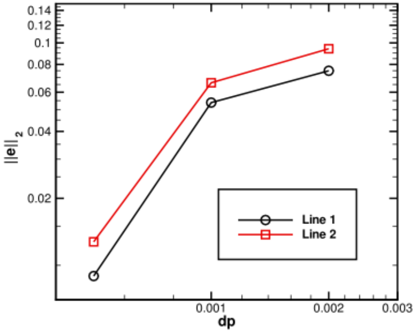
Du, Lehoucq, Tartakovsky, Comp Meth in Appl Mech and Eng (2015)

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

Navier BC: $\boldsymbol{\tau} \cdot \mathbf{n} = \beta \mathbf{v}$ and $\mathbf{v} \cdot \mathbf{n} = 0$; $\boldsymbol{\tau}$ - viscous stress; μ/β - slip length $\approx 10 - 15\ \eta$m.

Example: flow around cylinder subject to Navier BC.





Pan, Bao, Tartakovsky, JCP (2014)

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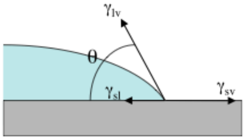
Multiphase flow



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

$$(P_\alpha - P_\beta)\mathbf{n} = (\boldsymbol{\tau}_\alpha - \boldsymbol{\tau}_\beta) \cdot \mathbf{n} + \kappa \sigma_{\alpha\beta} \mathbf{n}$$

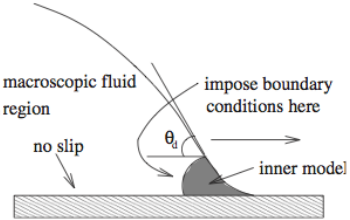
Fluid-solid interface: no-slip, $\mathbf{v} = 0$

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

Fundamental Chalenges:

- Divergence of stress τ at the contact line
- Unknown $\mathbf{v}$-dependent dynamic contact angle
- Empirical models for θ 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

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

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, Hassanizadeh* 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):

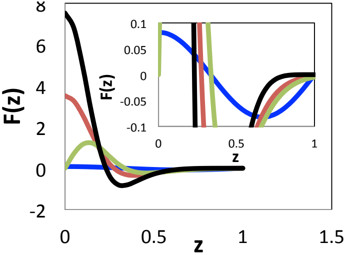
$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \kappa\sigma|\nabla\gamma| + \rho\mathbf{g}, \qquad \gamma(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_\alpha(t) \\ 0, & \mathbf{x} \in \Omega_\beta(t) \end{cases}$$

$$\frac{D\mathbf{x}_i}{Dt} = \mathbf{v}_i, \qquad m_i \frac{D\mathbf{v}_i}{Dt} = \sum_j \mathbf{f}_{ij} + \sum_j \mathbf{F}_{ij}^{int} + m_i\mathbf{g}$$

- Fluid and solid phases are discretized by separate sets of particles with mass m_i
- $\mathbf{F}_{ij}^{int}$ is a pairwise force creating surface tension

Interaction forces

$$\mathbf{F}^{int}(\mathbf{x}_i, \mathbf{x}_j) = s(\mathbf{x}_i, \mathbf{x}_j)\phi(|\mathbf{x}_i - \mathbf{x}_j|)\frac{\mathbf{x}' - \mathbf{x}''}{|\mathbf{x}' - \mathbf{x}''|}$$



ϕ is the shape function

$s(\mathbf{x}_i, \mathbf{x}_j) = s_{\alpha\beta}$ for $\mathbf{x}_i \in \alpha$-phase and $\mathbf{x}_j \in \beta$-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: $T_{\alpha\beta} = -\frac{1}{8}\pi n_\alpha n_\beta s_{\alpha\beta} \int\limits_0^\infty z^4 \phi(z) dz$

Static contact angle: $\sigma_{\alpha\beta} \cos\theta_0 + \sigma_{s\alpha} = \sigma_{s\beta}$

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Relationship between surface tension, contact angle and pairwise forces

$$\mathbf{F}^{int}(\mathbf{x}_i^\alpha, \mathbf{x}_j^\beta) = s_{\alpha\beta}\phi(|\mathbf{x}_i^\alpha - \mathbf{x}_j^\beta|)\frac{\mathbf{x}_i^\alpha - \mathbf{x}_j^\beta}{|\mathbf{x}_i^\alpha - \mathbf{x}_j^\beta|}$$

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

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

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

$$\lambda = \int z^4\phi(z)dz$$

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

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

Virial stress:

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

Continuum approximation:

$$\mathbf{T}^{int}(\mathbf{x}) \approx \frac{n_{eq}^2}{2}\int\int g(\mathbf{x}', \mathbf{x}'')\mathbf{F}^{int} \otimes (\mathbf{x}'' - \mathbf{x}')\int_0^1 \psi_\eta(\mathbf{x} - s\mathbf{x}' - (1-s)\mathbf{x}'')dsd\mathbf{x}'\mathbf{x}''$$

Analytical evaluation of surface tension

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

Then,

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

Specific interfacial energy $\tau_{\alpha\beta}$ is

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

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

The 3D result agrees with Rayleigh, 1890.

Pressure due to $\mathbf{F}_{ij}^{int}$ forces

$$p^{int} = -\frac{1}{3}\mathrm{tr}(\mathbf{T}^{int})$$

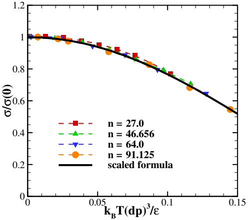
$$3D: \quad p_\alpha^{int} = \frac{2}{3}\pi n_\alpha^2 s_{\alpha\alpha}\int_0^\infty z^3\phi(z)dz$$

$$2D: \quad p_\alpha^{int} = -\frac{1}{2}\pi n_\alpha^2 s_{\alpha\alpha}\int_0^\infty z^2\phi(z)dz$$

Effect of thermal fluctuations on surface tension

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

ϵ - potential energy



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

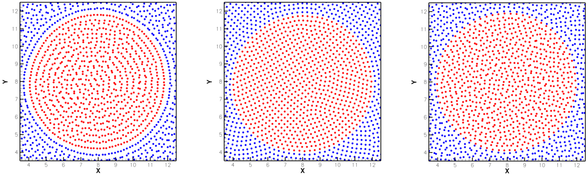

Figure: Particle distribution obtained from simulations of a bubble of one fluid surrounded by another fluid with: (a) cosine pairwise force; (b) gaussian pairwise force with $\varepsilon_0 = 0.5\varepsilon/2$; and (c) gaussian pairwise force with $\varepsilon_0 = 0.8\varepsilon/2$.

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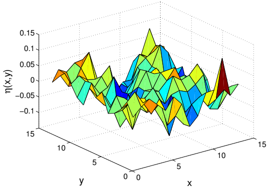
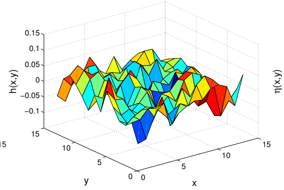
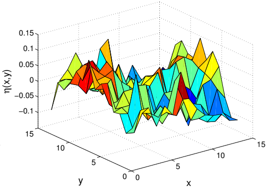
Fluctuations of “immiscible” interfaces due to thermal fluctuations



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

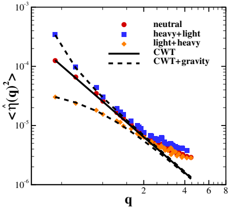


$\rho_{top}/\rho_{bottom} = 0.5$



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

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



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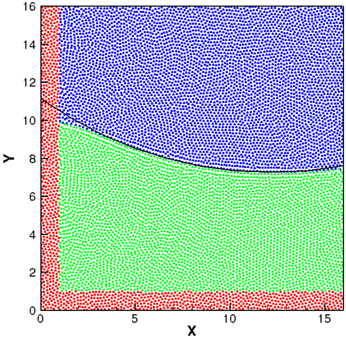
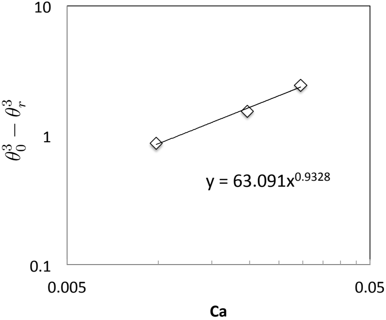
PF-SPH accurately models dynamic contact angles

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





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

θ_0 - prescribed static contact angle

θ_r - resulting receding dynamic angle

Tartakovsky and Panchenko, 2015 JCP

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Effect of wettability on distribution of fluid phases and possible implications for the long-term CO_2 storage

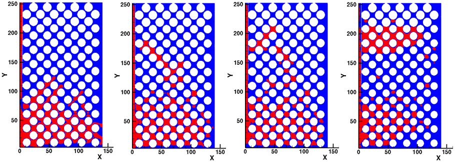

Figure: Distribution of non-wetting CO_2 at 4 different dimensionless times: (a) t^*=204 (during injection); (b) t^*=983 (after injection); (c) t^*= 1022 (after injection); and (d) t^*=251524 (after equilibrium stage is achieved).

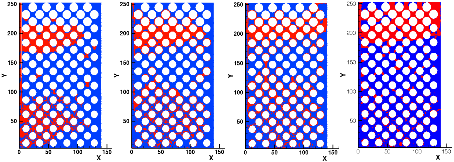

Figure: Distribution of neutrally-wetting CO_2 in Case 1b at 4 different dimensionless times: (a) t^*=776; (b) t^*=73891; (c) t^*= 308796; and (d) t^*=536426.

Effect Of Thermal Fluctuations on Miscible Fronts

"Giant fluctuations" of interface between miscible fluids

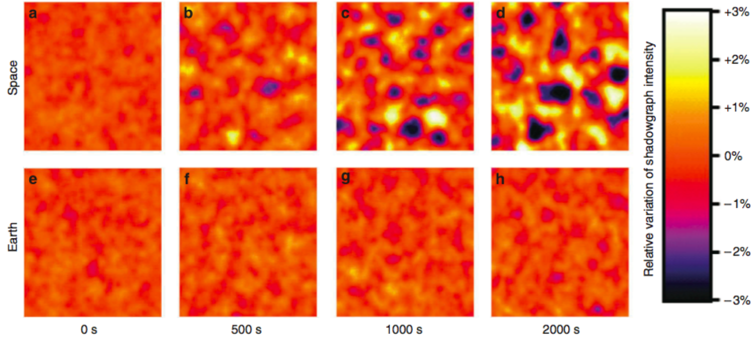

Figure 1 | Development of nonequilibrium fluctuations during diffusion processes occurring on Earth and in space. False-colour shadowgraph images of nonequilibrium fluctuations in microgravity (**a–d**) and on Earth (**e–h**) in a 1.00-mm-thick sample of polystyrene in toluene. Images were taken 0, 400, 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.

Vailaty et al, 2011

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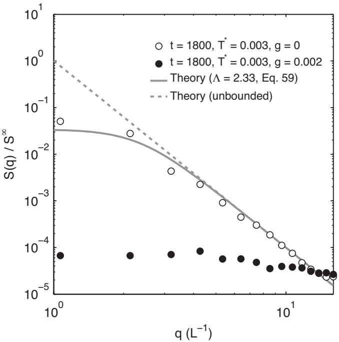
Power spectra of the miscible front

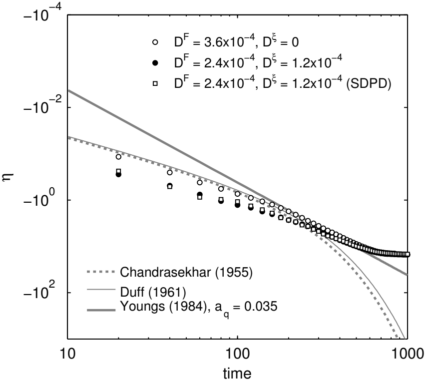
$S(q)/S^{\infty} = (q^4 + B(\Lambda)q^2 + \Lambda^4)^{-1}$ (Ortiz de Zaràte, 2004)



- 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.



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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.