IParticle methods for simulation of subsurface multiphase fluid flow and biogeochemical processes.

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SciDAC Project: Hybrid numerical methods for multiscale simulations of biogeochemical processes

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Particle methods for simulation of subsurface multiphase fluid flow and biogeological processes.

- **Motivation:**
  
  **Environmental protection:**
  water quality and the impact of fuel production and power generation

  **Oil recovery:**
  Original recoverable conventional and unconventional oil \( \approx 5 \) trillion barrels (about 1 trillion extracted so far) with current technology

  Less than half of oil in place is recovered (increase from 40% to 40.01% worth $75 billion @ $60/barrel)

  **Carbon sequestration:**
  Recoverable coal resources 1 trillion tonnes (>7 trillion BOE) + *in situ* gasification (3 trillion tonnes of coal under Haltenbanken)

  **Methane hydrate:** > 100 trillion BOE ??

US has little conventional oil – but very large amounts of unconventional oil and coal
Multiscale modeling of biogeological processes

- Scientific challenge:
  - develop adequate understanding of (very) complex systems that cannot be completely characterized
  - Identify minimal set of processes (model components) needed to model system with sufficient accuracy and reliability
- Computational challenge:
  - Large range of length scales ($\geq O(10^{14})$) for many applications
  - Much larger range of time scales ($\geq O(10^{24})$) for many applications
Particle methods for simulation of subsurface multiphase fluid flow and biogeological processes.

Particle methods are computationally inefficient relative to continuum methods and they need calibrating, so why use them?

- No need for interface trapping/capturing
- Rigorous mass conservation
- Code development effort is relatively low – and it is relatively easy to add new physics
- Can simulate complex processes such as fluid-fluid-solid contact line dynamics
- Can simulate mesoscale processes in which thermal fluctuations play an important role (polymers, colloids, biofilm)
Principles of particle and particle-based CFD

Particle microdynamics $\rightarrow$ continuum fluid dynamics (Navier–Stokes)

• Conservation of mass ($\Rightarrow$ conservation of volume in low compressibility limit)
• Conservation of momentum:
• Conservation of energy (non isothermal models)
• Galilean invariance
• $K_n (\lambda / L) \ll 1$

Essentially any microdynamics satisfying these conditions will be consistent with Navier-Stokes equation on large scales

Particle models: molecular dynamics, dissipative particle dynamics, smoothed particle hydrodynamics, Monte Carlo, lattice gas, vortex particle, fluid particle …

Particle based models: lattice Boltzmann
Molecular fluid dynamics


Liquid propane in nitrogen

E. Meiburg, Physics of fluids, 29: 3107-3113 (1986)

Hard sphere molecular dynamics


Can molecular dynamics serve as scale model for fluid dynamics?
Can molecular dynamics be used to simulate continuum fluid dynamics?


Nonequilibrium MD, sheared fluid - $r^{-12}$ repulsive potential

High strain rates can modify fluid structure and rheology


CO$_2$ at amorphous SiO$_2$ surface

Fluid has different structure near to solid boundaries

- Fluid can flow $10^4 - 10^5$ times faster in nanotube than continuum fluid dynamics with no-slip boundary conditions would predict

- Fluctuations play important role at nanoscale
Molecular dynamics simulation of multiphase fluid flow

\[ \{ \Pi^{(\text{model})} \} = \{ \Pi^{(\text{system})} \} \]

<table>
<thead>
<tr>
<th></th>
<th>Strain = 10</th>
<th>Strain = 100</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10^6 mols., 10^9 steps</td>
<td>10^9 mols., 10^6 steps</td>
</tr>
<tr>
<td>Velocity</td>
<td>O(0.1 – 1.0 m sec(^{-1}))</td>
<td>O(10(^3) – 10(^4) m sec(^{-1}))</td>
</tr>
<tr>
<td>Strain rate</td>
<td>O(10(^7) sec(^{-1}))</td>
<td>O(10(^{10}) sec(^{-1}))</td>
</tr>
<tr>
<td>Temperature rise</td>
<td>O(1 K)</td>
<td>O(10(^3) K)</td>
</tr>
<tr>
<td>g</td>
<td>O(10(^7) (g_0))</td>
<td>(10(^9) (g_0))</td>
</tr>
<tr>
<td>Re</td>
<td>O(10(^{-2}))</td>
<td>(10(^2))</td>
</tr>
<tr>
<td>Ca</td>
<td>O(10(^{-3}) – 10(^{-4}))</td>
<td>O(1 – 10)</td>
</tr>
<tr>
<td>Bo ( (\delta\rho=1.0))</td>
<td>O(10(^{-1}))</td>
<td>O(1000)</td>
</tr>
<tr>
<td>Ma*</td>
<td>O(10(^{-4}))</td>
<td>O(1)</td>
</tr>
</tbody>
</table>

\[ \text{Re} = \frac{VL\rho}{\eta} \quad \text{Ca} = \frac{\eta V}{\Gamma} \]

\[ B_o = \frac{\delta\rho g L^2}{\Gamma} \quad Ma = \frac{V}{C} \]
Dissipative particle dynamics

- Particles interact through conservative, dissipative and random forcers

\[ m \frac{dV_i}{dt} = f_i = \sum_{j \neq i} f_{ij} = \sum_{j \neq i} f_{ij}^C + f_{ij}^D + f_{ij}^R \]

- Conservative particle-particles are soft – large time steps
- Individual particles represent (very) small fluid volumes
- Interactions rigorously conserve momentum
- Fluctuation-dissipation relationship between random and dissipative interactions

\[ f_{ij}^D = \gamma w^D(r)(\hat{r}_{ij} \cdot \mathbf{v}_{ij})\hat{r}_{ij}, \quad f_{ij}^R = -\sigma w^R(r)\xi \hat{r}_{ij} \]
\[ \gamma = \sigma^2 / 2k_B T, \quad w^D(r) = (w^R(r))^2 \]

- Algorithm is like thermostatted molecular dynamics with soft potential

Short range repulsive + (relatively) long range repulsive interaction \( \Rightarrow \) phase separation
Kirkwood-Alder transition – limits physical size of DPD particles


Hard sphere molecular dynamics

Advantage vs. Molecular dynamics:

• Much larger time step

• Fluctuations play smaller role (nearer to hydrodynamic limit)
DPD simulations


Smoothed particle hydrodynamics: basic idea

\[ A_s(r) \]

A scalar field, \( A_s(r) \), can be represented by the sum of smooth “bell-shaped” functions centered on a set of points:

\[
A_s(r) = \sum_i a(r_i)W(r - r_i, h), \quad \int W(r)dr = 1
\]

\[
a \text{ is extensive variable corresponding to intensive field } A
\]

\[
A_s(r) = \sum_i A(r_i) \frac{m(r_i)}{\rho(r_i)} W(r - r_i, h)
\]

\[
A_s(r) = \sum_i \left( \frac{A(r_i)}{n_i} \right) W(r - r_i, h)
\]

The field, \( A \), is defined at a set of unstructured points – similar to defining the field at the nodes of a grid in a grid-based calculation.

\[
\nabla A_s(r) = \sum_i a(r_i)\nabla W(r - r_i, h)
\]
Smoothed particle hydrodynamics: Simulation of single phase (unconfined) fluid flow

1. Calculate fluid density from particle positions
2. Calculate pressure from density via equation of state
3. Calculate particle accelerations from pressure gradient

\[
\frac{dV}{dt} = -\nabla P / \rho \quad \frac{\nabla P}{\rho} = \nabla\left( \frac{P}{\rho} \right) + \frac{P}{\rho^2} \nabla \rho
\]

\[
F_i = -\sum_j \left( \frac{P_j}{n_j^2} + \frac{P_i}{n_i^2} \right) \nabla_i W(r_i - r_j, h)
\]

4. Update particle positions and go to step 1

Add terms to represent effects of viscosity and body forces:

\[
\frac{dV}{dt} = -\sum_j \left[ \left( \frac{P_i}{n_i^2} \right) + \left( \frac{P_j}{n_j^2} \right) \right] \nabla W(r_i - r_j, h)/m_i + \sum_j \left( \mu_i + \mu_j \right) \frac{(v_i - v_j)}{n_i n_j |r_i - r_j|^2} (r_i - r_j) \cdot \nabla_i W(|r_i - r_j|, h) + m_i g
\]

There are many ways to formulate SPH equations – just as there are many ways to solve differential equations using standard grid-based methods

Add short-range attractive and (relatively) long-range repulsive interactions for surface tension and wetting.
SPH simulations

Biofilm growth and distribution in microfractured porous medium

With Alexandre Tartakovsky, Tim Scheibe & Andy Ward - PNNL

Dispersion in fractured porous medium

Dissolution of trapped non-aqueous phase

Miscible flow, Rayleigh-Taylor instability

Precipitation in fractured porous medium
Multiscale modeling of biofilm

- Microorganism: \( O(10^{-5} - 10^{-6} \text{ m}) \)
- Small molecule: \( O(10^{-9} \text{ m}) \)
- Biopolymer chain segment: \( O(10^{-8} \text{ m}) \)
- Soil grain: \( (10^{-4} \text{ m}) \)

Adhesion of cells and biopolymer – Chemical bonding \( (O(10^{-10} \text{ m})) \), Colloidal interactions (DLVO, hydration forces, depletion forces …) \( (O(10^{-10} - 10^{-7} \text{ m})) \), Physical interactions \( (O(10^{-9} - > 10^{-6}) \text{ m})) \)
Multiscale modeling of biofilm

Soft condensed matter: gel like material

Bingham: \[ \sigma = \sigma_C + K\dot{\varepsilon} \]

Herschel Buckley: \[ \sigma = \sigma_C + K\dot{\varepsilon}^n \]

Burgers: \[ \varepsilon = \sigma\left[\frac{1}{G_1} + \frac{1}{G_2}\left(1 - e^{-t/\tau}\right) + t/\eta\right] \]

Biofilm growth

Monod kinetics: \[ \frac{dM}{dt} = MYk_s \frac{C}{k + C} \]

Double Monod kinetics: \[ \frac{dM}{dt} = MYk_s \frac{C^{(a)}}{k^{(a)} + C^{(a)}} \frac{C^{(b)}}{k^{(b)} + C^{(b)}} \]

attachment/detachment, colloidal trapping, decay….
Hybrid and multiscale models

Particle – continuum hybrid model
Adaptive particle refinement based on: conservation of mass, momentum and energy

Challenge: model fluid properties must be particle size independent (intrinsic particle contributions to fluid properties)

Decreased role of fluctuations →
Particle – particle hybrid model
Particle-particle hybrid model

Challenge:
Properties of SPH modefluid(s), MD/DPD model fluid(s) and physical fluid(s) must be the same
Conclusions

• Particle methods are versatile, and flexible

• Particle methods can be used to simulate systems over a very wide range of scales: atomistic (MD) → mesoscale (DPD) → continuum (SPH).

• From a computational point of view they are equivalent to molecular dynamics (can benefit from extensive experience in chemistry community)

• Relatively little has been done on adaptive multiscale & hybrid methods for CFD