Multiscale Flow Simulations using Particles

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with:
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SIMULATIONS WITH PARTICLES

Transport in aquaporins
Schulten Lab, UIUC

Anguiliform Swimmers
Koumoutsakos Lab, ETHZ

Growth of Black Holes
Springel, MPI - Hernquist, Harvard

-9
0
+9
Particles: “Smooth” - Discrete

Smooth = APPROXIMATE

- Smoothed Particle Hydrodynamics
- Vortex Methods
- Lagrangian level sets

Discrete = MODEL

- Molecular Dynamics (MD)
- Dissipative Particle Dynamics
- Stochastic Simulation
Particle Methods: an N-BODY problem

Particle (position, value)
\[ i, j = 1, \ldots, N \]

\[
\frac{dx_i}{dt} = U_i(q_j, q_i, x_i, x_j, \cdots)
\]

\[
\frac{dq_i}{dt} = G_i(q_j, q_i, x_i, x_j, \cdots)
\]

SMOOTH
Particles are quadrature points for continuum properties
Force Field: quadratures of integral equations

DISCRETE:
Particles are carriers of physical properties - Models
Force Field: Physical models (MD,...) - Other

• Multipole Algorithms, Fast Poisson solvers, Adaptivity, multiresolution, multiphysics
Particle Approximations

- Volumes
- Surfaces and Interfaces
- Equations
Functions on Particles

\[ \zeta_\varepsilon = \frac{1}{\varepsilon^d} \zeta \left( \frac{x}{\varepsilon} \right) \]

Particles: \( p = 1, \cdots, N \)

locations: \( x_p \) volumes: \( v_p = h_p^d \)

properties:
\[ Q_p(t) = q(x_p, t) \]

Function approximation:
\[ q_\varepsilon^h(x, t) = \sum_{p=1}^{N_p} h_p^d Q_p(t) \zeta_\varepsilon(x - x_p(t)) \]
Smoothing kernels approximate the Dirac-function

\[ \Phi(x) = \int \Phi(y) \delta(x - y) dy \]

\[ \Phi_{\epsilon}(x) = \int \Phi(y) \zeta_{\epsilon}(x - y) dy \]

For \( \Phi \) (with \( r \) continuous derivatives):

\[ \| \Phi - \Phi_{\epsilon} \| \leq C \epsilon^r \| \Phi \|_\infty \]

Cutoff Function: \( \zeta \) must satisfy the following properties:

\[ \int x^\alpha \zeta(x) dx = 0 \quad 1 \leq |\alpha| \leq r - 1 \]

\[ \int |x|^r \zeta(x) dx < \infty \]

\[ \int \zeta(x) dx = 1 \]
Particles are quadrature points - Flexible locations

\[ \Phi_\epsilon(x) = \int \Phi(y) \zeta_\epsilon(x - y) \, dy \]

\[ \Phi^h_\epsilon(x, t) = \sum_{p=1}^{N_p} h_d^p \Phi_p(t) \zeta_\epsilon(x - x_p(t)) \]

Note:

\[ \| \Phi^h_\epsilon - \Phi_\epsilon \| \leq C \left( \frac{h}{\epsilon} \right)^m \| \Phi \|_\infty \]
Linear Evolution Equation

\[ \frac{\partial \omega_i}{\partial t} + V_{ij} \frac{\partial \omega_i}{\partial x_j} = \Omega_j \frac{\partial \omega_i}{\partial x_j} + \omega_j V_{ij} + 2 \nabla^2 \omega_i \]

Initial Condition - "spherical" vortex ring

\[ \omega(x,0) = \nabla \times \left( \sigma(0) e^{-1 \frac{x^2 - x_0^2}{\sigma^2}} \right) \]
\[ = \nabla \left( e^{-1 \frac{x^2 - x_0^2}{\sigma^2}} \right) \times \sigma \omega \]

**Impulse**

\[ I = \frac{1}{2} \int \nabla \times \omega \cdot dv \sim \sigma^3 \sigma(0) \]

**Energy (Self)**

\[ E(\Phi) \sim \sigma^3 |\Phi|^2 \]
Lagrangian Adaptivity

\[ \left( \frac{\partial q}{\partial t} + \nabla \cdot (u \, q) = \mathcal{L}(q, x, t) \right) \]

Lagrangian form:

\[ \frac{Dq}{Dt} = \mathcal{L}(q, x, t) \]

PARTICLES

- no linear stability constraints
- = no CFL \((dt < dx/u)\) condition

\[ \frac{dx_p}{dt} = u(x_p, t), \quad \text{positions on lattice} \]
\[ \frac{dv_p}{dt} = v_p \, (\nabla \cdot u) (x_p, t), \quad \text{volumes} \]
\[ \frac{dQ_p}{dt} = v_p \, \mathcal{L}^{\varepsilon, h}(q, x_p, t), \quad \text{weights} \]

initial values

\[ v_p = h^d \]
\[ Q_p = q(x_p, 0) \, v_p \]
## CONTINUUM: Lagrangian Form of Governing Equations

<table>
<thead>
<tr>
<th>Position</th>
<th>( \frac{Dx_p}{Dt} = u_p )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>( \frac{Dv_p}{Dt} = v_p(\nabla \cdot u)_p )</td>
</tr>
<tr>
<td>Velocity</td>
<td>( \rho_p \frac{Du_p}{Dt} = (\nabla \cdot \sigma)_p )</td>
</tr>
<tr>
<td>Stress tensor</td>
<td>( \sigma_p = -p_p I + \bar{\sigma}_p ) evaluation depends on the constitutive model</td>
</tr>
<tr>
<td>Level set</td>
<td>( \frac{D\Phi_p}{Dt} = 0 )</td>
</tr>
</tbody>
</table>
SURFACES and INTERFACES
Level Sets for Surface Representation

Level Set: implicit surface

\[ M = \{ x : \Phi(x) = 0 \} \]

Sethian, PNAS 93:1591. 1996.

Why? Surface can be treated in space: one method
PARTICLE METHODS: Geometry

Volume particles

• Particles are quadrature points
• Easy to discretize

Surface particles

• Particle - Level Sets - COMPLEX SURFACES
• Surface Operators - Anisotropic Volume Operators

\[ \Phi = 0 \]

\[ \Phi = -1 \]

\[ \Phi = 1 \]
Extension: Level sets

\[ \frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = 0 \]

\[ \frac{\partial \phi}{\partial t} + \kappa n \cdot \nabla \phi = 0. \]

\( \kappa = \nabla \cdot n \)

Solve with particles:

\[ \frac{dx_p}{dt} = u(x_p, t) \]

\[ \frac{d\phi_p}{dt} = 0 \]

\[ \Gamma(t) = \{ x \in \Omega \mid \phi(x, t) = 0 \} \]

\[ |\nabla \phi| = 1 \]

true adaptivity for level sets (Lagrangian & Eulerian)

Hieber and Koumoutsakos, J. Comp. Phys. 2005
How Good *(robust, efficient, stable, accurate,...)* are particle methods?
Particles go to Hollywood

Rigid Fluid: Animating the Interplay Between Rigid Bodies and Fluid

Mark Carlson
Peter J. Mucha
Greg Turk

Georgia Institute of Technology

Sound FX by Andrew Lackey, M.P.S.E.
Are grid-free Particle Methods Accurate?

Solution of the Euler equation with particle methods.
**Mollification**

\[ \Phi_\epsilon(x) = \int \Phi(y) \zeta_\epsilon(x - y) \, dy \]

**Quadrature**

\[ \Phi^h_\epsilon(x, t) = \sum_{p=1}^{N_p} h^d_p \Phi_p(t) \zeta_\epsilon(x - x_p(t)) \]

\[ \| \Phi - \Phi^h_\epsilon \| \leq \| \Phi - \Phi_\epsilon \| + \| \Phi_\epsilon - \Phi^h_\epsilon \| \]
\[ \leq C_1 \epsilon^r + C_2 \left( \frac{h}{\epsilon} \right)^m \| \Phi \|_\infty \]

**NOTES:**

- **Must have** \( h/\epsilon < 1 \) for the quadrature to be accurate i.e. **PARTICLES MUST OVERLAP.**
Lagrangian distortion and REMESHING

Particles follow flow trajectories
• distortion of particle locations
• loss of overlap
• loss of convergence

Preventive action: remeshing
Reinitialize particles on a regular grid.

$$Q_i^{new} = \sum_p Q_p \zeta^h (i h - x_p)$$

Limiting: Introduction of a grid

Enabling:
• Fast Poisson solvers
• Access versatility of finite differences
• Enabling efficient multiresolution adaptivity
Remeshing = Regularization

A new regularized particle set from the old one

\[ Q_{p}^{\text{new}} = \sum_{p'} Q_{p'} M (j h - x_{p'}) \]

Interpolation Kernel \( M(x) \)
- Moment conserving
- Tensorial Product of 1D kernels

REFERENCES:
SPH: Chaniotis, Poulakakos and PK, JCP, 2002
Hybrid Particle Mesh Techniques

step 1: ADVECT Particles

step 2: REMESH Particles onto Grid nodes

step 3: SOLVE field equations / DERIVATIVES on GRID

step 4: Grid Nodes BECOME Particles
Easy to use and efficient infrastructure for Particle-mesh simulations on parallel computers
PPM + 16K processors = 10 Billion Vortex Particles

60% efficiency on 16,384 cpus
Particle Library + 16K processors = 10 Billion Vortex Particles

The Secret Life of Vortices
Particle Methods are **Adaptive yet Inefficient**

Multiresolution via Remeshing

\[ Q_p^{\text{new}} = \sum_{p'} Q_{p'} M (j h - x_{p'}) \]

Grid can have variable/adaptive size

- Moment conserving
- Tensorial Product of 1D kernels
- Programming is challenging

Key Issue: Introduction of a grid - The old “magic” is gone

Enabling: • **MULTIRESOLUTION** - New Magic
  • Fast Poisson solvers - Efficient Differential operators
  • Avoiding accumulation of energy in the small scales
Multiresolution Techniques for Particles

Adaptive Global Mappings

**Keypoints:** Adaptive mapping represented by particles

AMR-based

**Keypoints:** High-resolution particles are created on patches of refinement

Particle-Wavelet Method

**Keypoints:** Wavelets guide particle refinement. Lagrangian accounting for convection of small scales

3D curvature driven collapse of a level set dumbbell

Axisymmetrization of an elliptical vortex (2D Euler)
Wavelet-particle method

While particles are on grid locations

mollification kernel \rightarrow basis/scaling function

Multiresolution analysis \((\text{MRA})\) \(\{\mathcal{V}^l\}_{l=0}^L\) of particle quantities

Refineable kernels as basis functions of \(\mathcal{V}^l\)

Wavelets as basis functions of the complements \(\mathcal{W}^l\)

\[
\zeta^l_k = \sum_j h_{j,k}^l \zeta_{j}^{l+1}
\]

\[
\zeta^{l+1}_k = \sum_j \tilde{h}_{j,k}^l \zeta_{j}^{l} + \sum_j \tilde{g}_{j,k}^l \psi_{j}^{l}
\]

Multiresolution function representation:

Analysis (collocation): \( d_k^l \sim | \text{fine} - \text{Prediction(coarse)} | \)

\[
q^L = \sum_k c_k^0 \zeta_k^0 + \sum_{l<L} \sum_k d_k^l \psi_k^l
\]

GROUND LEVEL

WAVELETS

Each wavelet is associated with a specific grid point/particle (2D)

Compression/Adaptation:

**Discard** insignificant detail coefficients: \( |d_{k,m}^l| < \varepsilon \)

Compressed function representation:

\[
\|q^L - q_{\geq}^L\| < \varepsilon
\]

→ Adapted grid
Results: 2D Euler equations

\[ \frac{\partial \omega}{\partial t} + \nabla \cdot (u \omega) = 0 \]

\[ u = \nabla \times \Psi \]

\[ \Delta \Psi = \omega \]

CFL \( \max \approx 10 \)
Results: Crystal Growth

Simulation of Dendritic growth

The interface is driven by the jump of the temperature flux across it.

\[ \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \]

\[ T|_{\Gamma} = T_{\Gamma} \frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0 \]

\[ u|_{\Gamma} = -n[k \nabla T \cdot n]_{\Gamma} \]

\[ \Gamma = \{ x | \phi(x) = 0 \} \]
Extension: Level sets

\[ \Gamma(t) = \{ x \in \Omega \mid \phi(x, t) = 0 \} \]

\[ \frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0. \]

\[ |\nabla \phi| = 1 \]

Solve with particles:
\[ \frac{dx_p}{dt} = u(x_p, t) \quad \frac{d\phi_p}{dt} = 0 \]

→ “Narrow Band” formulation (Adalsteinsson & Sethian, 1995)

Unnecessary by virtue of adaptivity

Smooth truncation of detail coefficients:
\[ d^l,m_k \leftarrow d^l,m_k \eta (\phi(h^{l+1})^{-1}) \]

true adaptivity for level sets (Lagrangian & Eulerian)

Hieber and Koumoutsakos, J. Comp. Phys. 2005
Level set volume conservation for deformation benchmark

Enright, Fedkiw et al, 2002

dof = # grid points
+ aux. particles at t=0.0

Present Method

dof = # active gp/particles at t=0.0

dof = # active gp/particles at final time

CFL\textsubscript{max} \approx 40
Particle Methods are **Adaptive yet Inefficient**

KOumoutsakos and Leonard, JFM, 1994
Lattice Boltzmann and Impulsively Started Cylinders

Remeshing: Bad/Good News

A new regularized particle set from the old one

\[ Q_{p}^{\text{new}} = \sum_{p'} Q_{p'} M (j h - x_{p'}) \]

SIMPLE (cylinders, boxes, etc.) geometries:

Body Fitted Grids

NEW: One sided moment conserving Formulas (PK, 1992)
Boundary Conditions = Coupling

- Coupling via a Boundary Force
Immersed Boundary Method for SPH

- Enforce boundary velocity by a bodyforce \( f \) in Momentum Equation

\[
\rho \frac{Du}{Dt} = -\nabla p + \nabla \tau + \left(f\right)
\]

- Approximate Material Derivative at time step \( i \) and solve for \( f \)

\[
\rho_i \frac{u_{i+1} - u_i}{\Delta t} = -\nabla p_i + \nabla \tau_i + \left(f_i\right) \Rightarrow f_i = \rho_i \frac{u_{i+1} - u_i}{\Delta t} - \left(-\nabla p_i + \nabla \tau_i \right)
\]

- Desired Velocity field on the boundary \( u_{i+1} = u_{\text{desired}} \)

\[
u_{i+1} = u_{\text{desired}} \Rightarrow f_i = \rho_i \frac{u_{\text{desired}} - u_i}{\Delta t} - \left(-\nabla p_i + \nabla \tau_i \right)
\]
Particle-Mesh Implementation

- Compute part of forcing term on the particles

\[ f_{i,\text{part}} = \rho_i \frac{-u_i}{\Delta t} - (\nabla p_i + \nabla \tau_i) \]

- From Particles to Boundary

\[ f_{i,\text{boundary}} = \rho_i \frac{u_{\text{desired}}}{\Delta t} + f_{i,\text{part,interpolated}} \]

- Interpolate from boundary points to particles


Particules for **Fluid Mechanics @ CSE Lab**

- Vortex Rings and Vortex Wakes
- Bluff Body and Turbulent Flows
- Swimming and Flying

Cottet et al. 2002
Multi and All-scale “Hydrodynamics” - Embedding nanodevices in Macrosystems

MULTIPHYSICS: Coupling Atomistic-Continuum
Schwarz Domain Decomposition

- Iterate, until the solution in the overlap region converges.
- Conservative scheme if the transport coefficients in A and C match
Schwarz iteration

- Iterate, until the solution in the overlap region converges.
- Conservative scheme if the transport coefficients in A and C match
Description of the liquid

Atomistic: Molecular Dynamics

\[ m \frac{d^2 r}{dt^2} = F \]

\[ m: \text{ mass} \quad r: \text{ position} \quad F: \text{ force} \]

Continuum: Navier-Stokes Eqs.

\[ \frac{Du}{Dt} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 u \]

\[ \frac{D\rho}{Dt} = \rho \nabla \cdot u = 0 \]

\[ u: \text{ velocity} \quad P: \text{ pressure} \quad \rho: \text{ density} \quad \nu: \text{ viscosity} \]
BC for the atomistic system

Tests on the MD system (continuum forcing fixed)
Missing Interactions

Test I: Equilibrium

Boundary force
Specular wall
How can we replace the particles in the red domain?

Total force should be \( F = P \times A \)

Take fluid structure into account: \( g(r) \)

\[
\rho(r) = \int_0^r 4\pi r'^2 \rho g(r') dr'
\]

\[
F_m(z) = -2\pi \rho \int g(r) \frac{\partial U(r)}{\partial r} z x dx dz \quad \text{red}
\]

215 K
1.0 g cm\(^{-3}\)


Hybrid scheme vs pure MD


Streamlines

Contour lines of speed

Relative Error ~ 4%

Hybrid scheme is ~\((L/l)^3\) faster than the pure MD
MD vs Hybrid scheme

Hybrid solution

Reference MD solution

The hybrid scheme is $\sim (L/R)^3$ times faster for a computational domain of size $L$ and a MD subdomain of size $R$.

Relative Error $\sim 1.3\%$

The problem with density variations

- Density variations depend on liquid state
- **Amplitude** proportional to **structural correlations** in the liquid

\[ g(r) \]

\[ \text{distance to wall [nm]} \]

\[ \text{Red. Density} \]

\[ \text{distance to wall [nm]} \]

- \[ T = 84K, \rho = 1.5 g cm^{-3} \]
- \[ T = 131K, \rho = 1.35 g cm^{-3} \]
- \[ T = 215K, \rho = 1.0 g cm^{-3} \]
Control approach to coupling

- Controlling of the external boundary force
- measured density $\rho^m \Rightarrow$ target density $\rho^t$

Results with Control Approach

Algorithm converged after 1.7 ns (170,000 MD steps)

\[ T = 84K, \rho = 1.5 \text{g/cm}^3 \]
Goal: Extend the technique for monoatomic liquids to water.

KEY ISSUES

• Strong electrostatic forces.
• Molecule Orientation
• Bouncing
• External Boundary Force

spherical non-periodic MD in 3D
CONTROL force updated every 3 ps. The algorithm has converged after 400 ps (200,000 MD steps).
Orientation

No orientational preference in the bulk.

At the interface

At distance 0.5 nm from the interface

\[ \cos(\phi) \]

Prob. distr.

Prob. distr.

THIS EFFECT IS CAUSED BY REDUCED ELECTROSTATICS
Correct Electrostatics = Correct Orientation

Reaction Field: All molecules outside a spherical cavity of a molecular based cutoff $R_c$ are treated as dielectric continuum with a dielectric constant $\epsilon_{rf}$

$$F(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0} \left( \frac{1}{r_{ij}^3} - \frac{1}{R_c^3} \frac{2(\epsilon_{RF} - 1)}{1 + 2\epsilon_{RF}} \right) r_{ij}$$

$q_i q_j$: free charges of the interacting sites
Water Couette Flow

![Diagram of Couette Flow Model](image)

- CFD
- MD

**Graph:**
- Velocity [nm/ps] vs x [nm]
- CFD
- MD

- Values range from -0.10 to 0.10 for velocity and -6 to 6 for x.

**Legend:**
- V
- -V
I Exploring Possibilities (and bridging disciplines)

VASCULOGENESIS
blood vessel formation in embryonic development


CROWN DROPLET BREAKUP
marangoni instability

Angiogenesis
Milde F., Bergdorf M. and PK, A hybrid model of sprouting angiogenesis, Biophysical J., 2008
Hardware & Software: Need a Bridge over Troubled Waters

II. Exploring Possibilities (and bridging disciplines)
Simulations using Particles at the CSE Lab

QM/MM of water and CNTs

Cancer Modeling

Virtual Surgery

Diffusion in/on Cell Organelles

Swimming Organisms
Acknowledgements

Basil BAYATI,
Michael BERGDORF,
Mattia GAZZOLA,
Manfred QUACK,
Stefan KERN,
Florian MILDE,
Angelos KOTSALIS,
Diego ROSSINELLI

Evangelos BOUTSIANIS,
Philippe CHATELAIN,
Alexandre DUPUIS
Tobias GEBAECK,
Jens WALTHER

Simone HIEBER
Ivo SBALZARINI
Thomas WERDER
Urs ZIMMERLI