Particle-Simulation Methods for Fluid Dynamics

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WS 2012/2013: Lectures for Mechanical Engineering
Lecture 1: Introduction to Particle Methods

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Preliminary remarks

- 20 hours course on Particle Methods: Oct 2012 – Feb 2013 (approx.)
- Room 1639: 1 / week, 2 academic hours (90 min.)
- Prerequisites: basic notions of classical mechanics, thermodynamics, fluid mechanics.
- OpenSource codes for particle method.
  - Based on LAMMPS code or Parallel Particle Mesh (PPM) library
- Scope of the course: to introduce the student to Particle Methods or ....

  to show them that there are alternatives to the Finite ... Methods which are currently the workhorse of the computer modelling community worldwide.

- lecture material on UNIVIS + references + further readings
  http://www.aer.mw.tum.de  (lehre-ws-particle methods)

- Exam ?
Macroscopic range: PDEs describing collective motion in dissipative fluids (i.e. Navier Stokes equations)

Mesoscopic range: kinetic picture, continuum-molecular regime, thermal fluctuations

Microscopic (atomistic) range: ODEs (Newton) for a collection of atoms or molecules.

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The continuum picture

- **Continuum assumption**: $dV$ element of fluid: *large* enough to neglect underlying microscopic structure BUT *small* enough to be treated mathematically as infinitesimal
  - Stokes theorem:
    \[ \oint_{\partial \Sigma} \mathbf{A} \cdot d\mathbf{l} = \oint_{\Sigma} \nabla \times \mathbf{A} \cdot dS \]
  - Gauss theorem:
    \[ \oint_{\partial \Sigma} \mathbf{A} \cdot dS = \int_{\Sigma} \nabla \cdot \mathbf{A} \, dV \]

- **Conservation of mass**

  \[ \oint_{\partial \Sigma} \rho \mathbf{v} \cdot dS = -\int_{\Sigma} \partial_t \rho \, dV = \int_{\Sigma} \nabla \cdot (\rho \mathbf{v}) \, dV \]

  Continuity equation

  \[ \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \]
The continuum picture

- Conservation of momentum (inviscid fluids)
  - Def. "pressure" \( p \): force exerted by the fluid on a unit surface area
  
  1. \( -\oint_{\Sigma} p \, dS = -\int_{\Sigma} \nabla p \, dV \)
  
  2. \( \mathbf{F} = m \mathbf{a} = \int_{\Sigma} \rho \frac{d\mathbf{v}}{dt} dV \)

Euler equation

- Purely geometrical considerations (continuum assumption + conservation laws)!

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The continuum picture

- Conservation of momentum (generalization of inviscid to *dissipative* fluids)

\[
\partial_t (\rho \mathbf{v}) = (\partial_t \rho) \mathbf{v} + \rho (\partial_t \mathbf{v}) = -\nabla \cdot \Pi
\]
\[
\Pi = p I + \rho \mathbf{v} \mathbf{v}
\]

momentum flux tensor (Euler)

- Dissipative effects are introduced by modifying \( \Pi \)

\[
\Pi = p I + \rho \mathbf{v} \mathbf{v} - \rho \sigma
\]

viscous stress tensor

- Assuming that: (1) gradients of velocity change slowly in such a way \( \sigma_{ij} = f(\partial_i \mathbf{v}) \) with \( f \) being a *linear* function; (2) \( \sigma_{ij} = 0 \) under rigid body rotation

\[
\sigma = \mathbf{v} [\nabla \mathbf{v} - (\nabla \mathbf{v})^T - 2/3 (\nabla \cdot \mathbf{v}) I] + \zeta (\nabla \cdot \mathbf{v}) I
\]

\[
\nabla \cdot \mathbf{v} = 0 \quad \Rightarrow \quad \partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nabla \cdot \mathbf{v} \nabla^2 \mathbf{v}
\]

Navier-Stokes equation

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The continuum picture: discretization

The continuum NS equations must be approximated using a suitable discretization technique and solved on computers.

\[ \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \]

Continuity equation

\[ \partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nabla^2 \mathbf{v} \]

Navier-Stokes equation

Numerical approximation (i.e. FDM)

\[ (\partial_t f)_{i,j}^n \approx \frac{f_{i,j}^{n+1} - f_{i,j}^n}{\Delta t} \]

\[ (\nabla_x f)_{i,j}^n \approx \frac{f_{i+1,j}^n - f_{i-1,j}^n}{\Delta x} \]

\[ (\nabla_x^2 f)_{i,j}^n \approx \frac{f_{i+1,j}^n - 2 f_{i,j}^n + f_{i-1,j}^n}{2 \Delta x^2} \]

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The microscopic description

At the lowest level, the microscopic picture describes the fluid as a collection of atoms (or molecules) interacting via classical (or quantum-mechanics) potentials $U(r)$ and following the Newton equations of motion.

\[ \dot{r}_i = v_i, \]
\[ \dot{v}_i = -\nabla_i U(r_1, \ldots, r_N). \]

The attempt of fluid realism has an immediate difficulties: in order to describe systems at larger scales, a very large number of particles (basic constituents) should be simulated. This makes atomistic simulation useful only for very small range of spatio-temporal scales (order of nano-meters, nano-seconds).

If physical scale-separation can be assumed, an obvious strategy is to “smooth” the model and to reduce the number of freedom degrees. This strategy is called coarse-graining and it is based on the assumption that only averaged (in space and time) quantities on a large ensemble of representative systems are relevant for the dynamics while microscopic details can be neglected.
The mesoscopic description

- A possible upper level statistical description of a fluid or gas is given by the one-particle phase-space distribution function \( f(t,r,v) \)

\[
\langle n(r,t) \rangle = \int f(t,r,v) \, dv \\
\langle V(r,t) \rangle = (1/\langle n \rangle) \int f(t,r,v) \, v \, dv
\]

- One of the basic results of kinetic theory is that, under specific physical assumptions, the governing equation for \( f \) is

\[
\frac{df}{dt} = \partial_t f + \mathbf{v} \cdot \nabla f = C(f)
\]

The free-streaming term represents the local change in \( f \) due to the independent motion of particle only and it is equal to zero in absence of collisions (conservation of probability in the phase space).

- The r.h.s. term models the rate of change of the distribution caused by collisions and it must be modelled (i.e. Boltzmann operator).
Classical Computational Fluid Dynamics

- Computational Fluid Dynamics (CFD) usually based on grid-based methods (FDM, FVM, FEM)
- Need of accurate macroscopic models (i.e. Navier-Stokes) describing the flow problem.
- When do standard grid-based methods encounter difficulties and do we need particle methods?

1. Microscopic flows are intrinsically discrete (Nano-Microfluidics)
2. Mesoscopic flows are characterised by Brownian motion (thermal fluctuations)
3. Even at the macroscopic level, continuity assumption is not always satisfied: rarefied gas dynamics flows, granular flows, traffic flows.
4. Continuum flow problems characterized by very complex external/boundary conditions.
5. Multiscale flow problems (no separation of spatio-temporal scales)
Computational challenges (I)

- Nanoscale/microscale flow problems:
  - Fracture processes in materials
- Microscopic friction, wear, indentation (Deutsche Bahn train-brakes)
- Carbon nanotubes (nano-, microdevices)

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Mesoscopic flow problems:

- Clot formation in a bifurcating capillary vessel (medical applications)

- Collision-coalescence of micro-drops (vaporization, spray technology)

- Dispersion of colloidal slabs, aggregation, crystallization processes (food industry)

- Self-assembled structure: COLLOIDOSOME
Computational challenges (III)

- Macroscopic, non-continuous flow problems
  - Rarefied Gas Dynamics: atmospheric re-entry (low-density, high-velocity flow)
  - Transport, storage of granular material (corns, chemicals, iron debries etc.)
  - Traffic, pedestrian flow (evacuation modelling in architectural design)

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Computational challenges (IV)

- Macropscopic continuous flow problems:
  - Complex free-surface flows, particle-laden flows
  - Large-deformation solid flow problems, high-velocity impacts
What are Particle Methods?

Generally:

\[ \dot{r}_i = v_i \]
\[ \dot{v}_i = \sum_{i=1}^{N} \Omega_{ij} \]

- **Particles**: “objects” carrying the physical properties of the system through the solution of Ordinary Differential Equations (ODEs).

common primitives - **particles** - are defined by a set of attributes whose physical meaning depends on the specific spatio-temporal scale.

**collision operator** usually defined as a sum of short-ranged additive forces \( \Omega_{ij} \) between particles \( i \) and \( j \).

**Newton equations of motion** is a common feature of particle-based schemes.

concept of “particle” varies with the scales of the problem: atoms, molecules, \((direct\ simulation\ of\ the\ discrete\ components)\ volumes\ of\ fluid,\ moving\ mesh\ nodes\ \(\text{(Lagrangian simulation of continuum equations)}\)
Particle Methods for multiscale problems

- Microscopic methods:
  - Molecular Dynamics (MD)
  - Non-Equilibrium Molecular Dynamics (NEMD)
  - Monte-Carlo (MC), Direct Simulation Monte Carlo (DSMC)

- Mesoscopic methods:
  - Lattice Gas Automata (LGA), Lattice Boltzmann (LB)
  - Brownian Dynamics (BD), Dissipative Particle Dynamics (DPD)

- Macroscopic methods:
  - Particle-in-cells (PIC)
  - Vortex methods (VM)
  - Smoothed Particle Hydrodynamics (SPH)
Contents and scheduled plan

- Lecture 2: (07 Nov) Molecular Dynamics (I)
- Lecture 3: (14 Nov) Molecular Dynamics (II)
- Lecture 4: (21 Nov) Monte-Carlo methods
- Lecture 5: (28 Nov) Coarse-grainings, BBGKY hierarchy, Boltzmann eq., kinetic theory
- Lecture 6: (05 Dec) Lattice Gas Automata, recovering hydrodynamics, multiscale expansions
- Lecture 7: (12 Dec) Lattice Boltzmann method (I)
- Lecture 8: (19 Dec) Lattice Boltzmann method (II)
- Lecture 9: (09 Jan) Dissipative Particle Dynamics
- Lecture 10: (16 Jan) Validity macro-continuum approx. (I), rarefied gases, Direct Simulation Monte-Carlo
- Lecture 11: (23 Jan) Validity macro-continuum approx.(II), granular/pedestrian flows, Discrete Particle method
- Lecture 12: (30 Jan) Macroscopic Particle flow solvers (I): Particle-in-cell, particle-mesh methods
- Lecture 13: (06 Feb) Macroscopic Particle flow solvers (II): Smoothed Particle Hydrodynamics
- Lecture 14: (13 Feb) Smoothed Particle Hydrodynamics (II)

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