Eulerian methods for modeling gas flow in dense particle systems

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Modeling gas flow in granular systems



Three questions:

-) How model the particles? Molecular dynamics using soft-sphere model
- How model the gas phase?
 First part of this lecture
- 3) How model the gas-particle interaction?
 - Second part of this lecture

Outline

1. Models for single phase gas flow

- A. Lagrangian Models
- B. Eulerian models

2. Modeling gas-particle interaction

- A. Fully resolved (DNS)
- B. Unresolved (DEM)

3. Applications to Granular Matter research

A. Vibrated beds of bronze and glass spheresB. Vibrated shallow beds

1. Models for single phase gas flow

A. Lagrangian models



B. Eulerian models



- Molecular Dynamics
- Stochastic Rotation Dynamics
- Dissipative Particle Dynamics
- Lattice-Gas Cellular Automata

- Lattice Boltzmann Model
- Computational Fluid Dynamics

A. Lagrangian Models: Molecular Dynamics



A. Lagrangian Models: Molecular Dynamics

Hard-sphere model:

• Collision time between spheres can be calculated analytically:

b

 $\overline{v}_b t_{ab}$

 $R_a + R_b$

 \overline{r}_{ab}

 $\overline{v}_a t_{ab}$

a

R

$$t_{ab} = \frac{-\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} - \sqrt{(\mathbf{r}_{ab} \cdot \mathbf{v}_{ab})^2 - v_{ab}^2 \left[r_{ab}^2 - 4R^2\right]}}{v_{ab}^2}$$

- Evolution in time: free-flight to nearest collision event followed by instantaneous binary collision (event driven scheme)
- Collision: change of momentum does not follow from forces, but is calculated via:

$$\Delta \mathbf{v}_a = rac{\mathbf{r}_{ab} \cdot \mathbf{v}_{ab}}{4R^2} \, \mathbf{r}_{ab}$$

A. Lagrangian Models: Simplified MD models

- Dissipative Particle Dynamics (DPD)
- Stochastic Rotation Dynamics (SRD)



- Lattice-Gas Cellular Automata (LGCA)

"be wise, discretise!"

- Positions are restricted to lattice sites \rightarrow discrete velocities
- No two particles with the same velocity allowed at one site
- Update: propagation and collision



Breakthrough: from square (1973) to hexagonal (1986)



Frisch, Hasslacher & Pomeau, PRL 1986



Flow past a plate

(Frisch, Hasslacher, Pomeau, PRL 1986)

Flow past a disc

(Van der Hoef, Frenkel, & Ladd, PRL 1991)





Key aspect of LGCA:

All bit manipulation <u>no</u> floating point operations



Advantages:

- Extremely simple to program
- Fast
- Exact, no round-off errors
- Inherently stable

Disadvantages: - Noisy

- Viscosity set by collision table (cannot be tuned)

From lattice-gas to Navier-Stokes

Define velocity set $\{\vec{c}_1, \vec{c}_2, ..., \vec{c}_b\}$

Microstate of the system given by

the occupation number $n_i(\vec{r},t) = \begin{cases} 1 & \text{if i-th link occupied} \\ 0 & \text{if i-th link empty} \end{cases}$

Local densities: $\hat{\rho}(\vec{r},t) = \sum_{i}^{b} n_{i}(\vec{r},t), \quad \hat{\rho}(\vec{r},t) = \sum_{i}^{b} \vec{c}_{i} n_{i}(\vec{r},t)$

Collision rules defined by $\xi(n, n') = \begin{cases} 1 & \text{if } n \to n' \\ 0 & \text{otherwise} \end{cases}$

Equation of motion: $n_i(\vec{r} + \vec{c}_i, t+1) = n_i(\vec{r}, t) + \Delta_i(n(\vec{r}, t))$ $\sum_i \Delta_i(n) = 0, \quad \sum_i \vec{c}_i \Delta_i(n) = 0 \qquad \sum_{s,s'} (s'_i - s_i)\xi(s, s') \prod_j n_j^{s_j} (1 - n_j)^{1-s_j}$

Microscopic _____ ⟨···⟩ **____** Macroscopic $n_i(\vec{r},t)$ $f_i(\vec{r},t)$ $\rho(\vec{r},t) = \sum_{i} f_{i}(\vec{r},t)$ $\rho(\vec{r},t) \vec{u}(\vec{r},t) = \sum_{i} \vec{c}_{i} f_{i}(\vec{r},t)$ $\hat{\rho}(\vec{r},t) = \sum_{i} n_{i}(\vec{r},t)$ $\hat{\rho}(\vec{r},t) \,\hat{\vec{u}}(\vec{r},t) = \sum_{i} \vec{c}_{i} \, n_{i}(\vec{r},t)$ $\Delta_i(n)$ $\Delta_{i}(f)$ $f_{i}(\vec{r} + \vec{c}_{i}, t + 1) = f_{i}(\vec{r}, t) + \Delta_{i}(f)$ $n_{i}(\vec{r} + \vec{c}_{i}, t + 1) = n_{i}(\vec{r}, t) + \Delta_{i}(n)$ $\sum_{i} \Delta_{i}(n) = 0 , \quad \sum_{i} \vec{c}_{i} \Delta_{i}(n) = 0$ $\sum_{i} \Delta_{i}(f) = 0 , \quad \sum_{i} \vec{c}_{i} \Delta_{i}(f) = 0$

Equation of motion for f: $f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) = \Delta_i(f)$

Taylor expansion (1st order)

$$= c_{s}^{2}\rho\bar{\bar{1}} + \rho\vec{u}\vec{u} + \sum_{i}\vec{c}_{i}\vec{c}_{i}f_{i}^{neq}$$

$$\bar{\bar{\tau}} = -\mu\left[(\vec{\nabla}\vec{u}) + (\vec{\nabla}\vec{u})^{T} - \frac{2}{3}(\vec{\nabla}\cdot\vec{u})\bar{\bar{1}}\right]$$

Basic idea: solve the set of differential equations:

$$\partial_t \rho + \vec{\nabla} \rho \mathbf{u} = 0$$
$$\partial_t \rho \mathbf{u} + \vec{\nabla} \rho \mathbf{u} = -\vec{\nabla} P - \vec{\nabla} \cdot \bar{\tau}$$

by finite difference methods (CFD).

Closures for P and $\overline{\overline{\tau}}$

$$P = \frac{RT}{M}\rho$$

$$\overline{\overline{\tau}} = -(\lambda - \frac{2}{3}\mu)(\vec{\nabla} \cdot \mathbf{u})\overline{\overline{I}} + \mu((\nabla \mathbf{u}) + (\vec{\nabla}\mathbf{u})^T)$$

Discretisation of space: define cells of volume $\delta l \cdot \delta l \cdot \delta l$

Define scalar variables at the cell centers, vector variables at the cell faces



- scalar variables P, ρ
- x-velocity component u_x
- y-velocity component u_y
- z-velocity component u_z

Notation: define variables at time n and cell $\mathbf{i}=\{i,j,k\}$ by

$$p_{\mathbf{i}}^{n} P_{\mathbf{i}}^{n} u_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n}$$

with :

$$e_x = (1, 0, 0)$$

 $e_y = (0, 1, 0)$ $h = \frac{1}{2}$
 $e_z = (0, 0, 1)$

Finite difference of the mass continuity equation:

$$\partial_t \rho = - \vec{\nabla} \rho \mathbf{u}$$

$$\frac{\rho_{\mathbf{i}}^{n+1} - \rho_{\mathbf{i}}^{n}}{\delta t} = -\left[\vec{\nabla} \cdot \rho \mathbf{u}\right]_{\mathbf{i}}^{n+1}$$

$$\frac{\rho_{\mathbf{i}}^{n+1} - \rho_{\mathbf{i}}^{n}}{\delta t} = -\sum_{\beta} \frac{[\rho \mathbf{u}]_{\beta, \mathbf{i}+h\mathbf{e}_{\beta}}^{n+1} - [\rho \mathbf{u}]_{\beta, \mathbf{i}-h\mathbf{e}_{\beta}}^{n+1}}{\delta l}$$

$$\rho_{\mathbf{i}}^{n+1} - \rho_{\mathbf{i}}^{n} + \sum_{\beta} \frac{\delta t}{\delta l} \left(\left[\rho \mathbf{u} \right]_{\beta, \mathbf{i} + h \mathbf{e}_{\beta}}^{n+1} - \left[\rho \mathbf{u} \right]_{\beta, \mathbf{i} - h \mathbf{e}_{\beta}}^{n+1} \right) = 0$$

Finite difference of momentum continuity equation:

$$\partial_t \rho \mathbf{u} = -\vec{\nabla}P - \vec{\nabla} \cdot \rho \mathbf{u} \mathbf{u} - \vec{\nabla} \cdot \overline{\tau}$$

$$\frac{[\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1}-[\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n}}{\delta t} = -\left[\vec{\nabla}P\right]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1} - \left[\vec{\nabla}\cdot\rho\mathbf{u}\mathbf{u}+\vec{\nabla}\cdot\overline{\tau}\right]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n}$$

$$[\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1} = -\delta t \Big[\vec{\nabla} P \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1} - \delta t \Big[\vec{\nabla} \cdot \rho \mathbf{u} \mathbf{u} + \vec{\nabla} \cdot \overline{\overline{\tau}} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + [\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + [\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} - \rho_{\mathbf{i}}^{n+1} \Big] + A_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + A_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + [\rho \mathbf{u}]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + A_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n+1} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}^{n} + \rho_{\mathbf{i}}^{n} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n} + \rho_{\mathbf{i}}^{n} \Big] + \delta t \Big[\rho \mathbf{u} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}^{n} + \rho_{\mathbf{i}}^{n} + \rho_{\mathbf{i}}^{n} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}^{n} + \rho_{\mathbf{i}}^{n} + \rho_{\mathbf{i}}^{n} \Big]_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}^{n} + \rho_{\mathbf{i}}^{n} + \rho_{\mathbf{$$

$$\mathbf{u}_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1} = \frac{-\frac{\delta t}{\delta l}(P_{\mathbf{i}+\mathbf{e}_{\alpha}}^{n+1} - P_{\mathbf{i}}^{n+1}) + A_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n}}{\rho_{\alpha,\mathbf{i}+h\mathbf{e}_{\alpha}}^{n+1}}$$

Solution procedure to calculate variables at time n+1



B. Eulerian Models: Lattice Boltzmann Method (LBM)

Originate from the lattice-gas cellular automata

$$f_{i}(\vec{r} + \vec{c}_{i}, t + 1) = f_{i}(\vec{r}, t) + \Delta_{i}(f)$$

$$\Delta_{i}(f) = \sum_{s,s'} (s'_{i} - s_{i})\xi(s, s') \prod_{j} f_{j}^{s_{j}} (1 - f_{j})^{1 - s_{j}}$$

3D: every update requires a double sum over 16 10⁶ states! Solution: linearize the collision operator about f^{eq}

$$\Delta_{i}(f) = \Delta_{i}(f^{eq} + (f - f^{eq})) = \Delta_{i}(f^{eq}) + \sum_{i=1}^{b} \left(\frac{\partial \Delta_{i}}{\partial f_{j}}\right)_{f_{j} = f_{j}^{eq}}(f_{j} - f_{j}^{eq})$$
only needs to be calculated once

B. Eulerian Models: Lattice Boltzmann Method (LBM)

1

Lattice Boltzmann equation (1988)

$$f_i(\vec{r} + \vec{c}_i, t + 1) = f_i(\vec{r}, t) + \sum_{i=j}^{b} L_{ij} (f_j - f_j^{eq})$$

Lattice Boltzmann BGK equation (1992)

$$f_i(\vec{r} + \vec{c}_i, t + 1) = f_i(\vec{r}, t) + \frac{1}{\tau} (f_i - f_i^{eq})$$

Note: continuous BGK equation (1954 !!)

$$\partial_{t} f + \vec{v} \cdot \vec{\nabla} f = \frac{1}{\tau} (f - f^{eq}) \qquad \int_{\vec{v} d\vec{v}} \partial_{t} \rho u + \vec{\nabla} \rho u = -\vec{\nabla} P - \vec{\nabla} \cdot \vec{\tau}$$



B. Eulerian Models: Lattice Boltzmann Method (LBM)

Example of single phase flow with LBM: Poiseuille flow



2. Modeling Gas-Particle Interaction

A. Resolved Discrete Particle Models



A. Resolved Discrete Particle Models (CFD)

Resolved flow with <u>CFD</u>: Immersed Boundary Method

Define Lagrangian force points on the surface of the particle:



Each force point **m** applies a force \vec{F}_m on the fluid, such that the local velocity of the fluid is equal to the local surface velocity

The sum of all force points results in a local force density \vec{f} via a <u>Lagrangian-Eulerian</u> mapping

The momentum equation then becomes:

$$\partial_t \rho \vec{u} + \vec{\nabla} \rho \vec{u} \vec{u} = -\vec{\nabla} P - \vec{\nabla} \cdot \bar{\bar{\tau}} + \vec{f}$$

A. Resolved Discrete Particle Models (CFD)



A. Resolved Discrete Particle Models (LBM)

Resolved flow with LBM: Bounce Back at boundary nodes



Define boundary node as point halfway an exterior and interior lattice site

In the propagation step: distribution "bounces back" at boundary nodes, and returns to its original site \rightarrow average flow velocity is zero at boundary site

A. Resolved Discrete Particle Models (LBM)



Results from resolved flow simulations

- 1. Fluidized bed simulation with 3600 particles using the CFD-IB method (J.A.M. Kuipers, 2008)
- 2. Sedimentation of 6144 particles using the LBM-BB method (A.J.C. Ladd, see http://ladd.che.ufl.edu)
- 3. Measuring the gas-solid drag force using the LBM-BB method (Van der Hoef, Beetstra, Kuipers)

Conclusion

Fully resolved methods provide the most detailed level of modeling gas-particle flow, yet number of particles are limited to O(1000)









Unresolved flow with CFD: implementation similar to resolved flow



 $\partial_t \rho \mathbf{u} + \vec{\nabla} \rho \mathbf{u} \mathbf{u} = -\vec{\nabla} P - \vec{\nabla} \cdot \mathbf{\bar{\tau}} + \mathbf{f}$

$$\vec{\mathsf{F}}_{\mathsf{i}} = \frac{\beta V_i}{1 - \varepsilon} (\vec{\mathsf{v}}_{\mathsf{i}} - \vec{\mathsf{u}}) \qquad \qquad \vec{\mathsf{f}} \equiv \beta (\vec{\mathsf{u}} - \vec{\mathsf{v}})$$

Gas phase:

$$\partial_{t} \varepsilon \rho \vec{u} + \vec{\nabla} \cdot \varepsilon \rho \vec{u} \vec{u} = -\vec{\nabla} P - \vec{\nabla} \cdot \varepsilon \vec{\tau} + \vec{f} + (1 - \varepsilon) \vec{\nabla} P$$
Solid phase:
$$\frac{d}{dt} m \vec{v}_{i} = \sum_{j} \vec{F}_{ij} - \vec{F}_{i} + V_{i} \vec{\nabla} P$$

Required: correlations for β

Monodisperse systems



Bidisperse systems

Theory: $\tilde{\beta}_i/\tilde{\beta} = \varepsilon y_i + (1-\varepsilon) y_i^2$ $\tilde{\beta}_{i} = \tilde{\beta}$ Currently assumed: 6 $\left(y_{i} = \frac{d_{i}}{\langle d \rangle} \right)$ theory o simulation 0 5 8 4 0 $\tilde{\beta}_{i}$ 3 2 Re = 1001 VDH, Beetstra & Kuipers, J. Fluid Mech. 528 (2005) 0 2 3 4 5 0 $\varepsilon y_i + (1-\varepsilon) y_i^2$

Applications of unresolved discrete particle models

I. Study of gas-fluidized beds



II. Study the effect of air in granular systems

3. Application to Granular Matter research

A. Vibrated beds of bronze and glass spheres Christiaan Zeilstra, Hans Kuipers

B. Vibrated shallow beds

Henk-Jan van Gerner, Devaraj v.d. Meer, Ko v.d Weele

Vibrated bed of <u>equal-sized</u> bronze and glass spheres (100 μ m) Experiments by Burtally, King and Swift (Science 2002)

Simulations:

- Particles: "molecular dynamics" with soft-sphere model
- Gas phase: computational fluid dynamics model
- Gas-Particle interactions: unresolved, empirical drag force
- System size: $N_p = 25\ 000$, $W \times H \times D = 8 \times 6 \times 0.6\ mm^3$
- Parameters: f = 55 Hz, A = 1 mm $\Rightarrow \Gamma = \frac{A(2\pi f)^2}{g} = 12$





Burtally, King, Swift & Leaper, Gran.Mat. 2003

f = 550Hzlz A = 0.07mmm



Why do the light particles sink to the bottom?



Sandwich formation:



- Convection plays an important role
- Sensitive of the particle-particle and partice wall friction:

$\mu_{ extsf{pp}}\downarrow\ \mu_{ extsf{pw}} ightarrow $	0.0	0.1	0.4
0.0	Bottom	Bottom	Bottom
0.1	Middle (40 s)	Middle (10 s)	Тор
0.4	Middle (20 s)	Middle (10 s)	Тор

B. Faraday Heaping

with: H-J van Gerner K. van der Weele D. van der Meer

Simulations:

- Particles: soft-sphere model, 0.5 mm diameter
- Gas phase: computational fluid dynamics model
- Gas-Particle interactions: unresolved, empirical drag drag
- System size: $N_p = 14\ 000$, W x H x D = 100 x 50 x 2.1 mm³
- Parameters: f = 6.25 Hz, A = 10 mm $\Rightarrow \Gamma = \frac{A(2\pi f)^2}{g} = 1.6$
 - No air 🕨 Air 🕨 Exp 🕨

First documented by Da Vinci (1500) and Faraday (1831)

B. Faraday Heaping

Three rivaling mechanisms for steady state heap

- 1. Internal avalanche flow (Laroche et al., J. Phys., 1989)
- 2. Inward pressure gradient (Thomas and Squires, PRL, 1998)
- 3. Stability of inclined surfaces (Duran, PRL, 2000])



B. Faraday Heaping

Conclusion for the steady state heap:

Our simulations confirm the pressure gradient mechanism proposed by Thomas & Squires.

How does the heap come into existence?

Two stages:

- 1. Fast initial stage where heaps are formed from a flat surface
- 2. Slow second stage where heaps merge:



Summary: overview of gas-solid models

