Modeling the effect of interstitial air in granular matter

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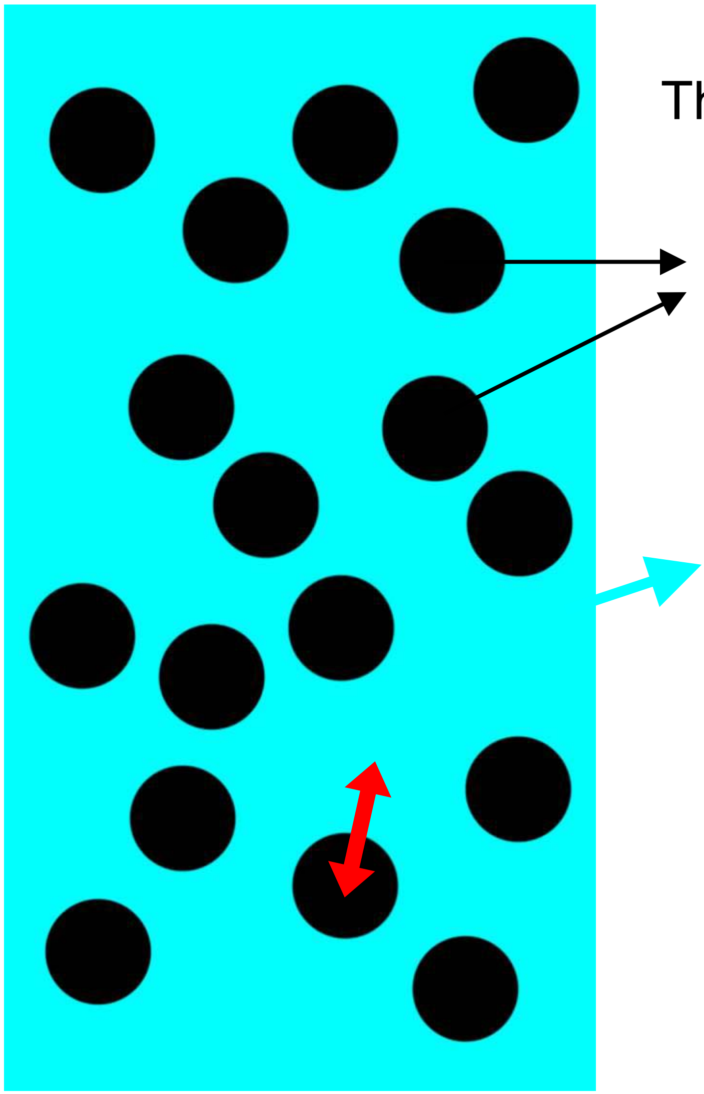
Modeling gas flow in granular systems



Three questions:

1) How model the particles?

First part of the lecture

2) How model the gas phase?

Second part of this lecture

3) How model the gas-particle interaction?

Third part of this lecture

Outline

1. Models for the solid phase

    A. Soft-sphere Models
    B. Hard-sphere Model

2. Models for the gas phase

    A. Computational Fluid Dynamics (CFD) Models
    B. Lattice Boltzmann Model (LBM)

3. Modeling gas-particle interaction

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

4. Examples of the effect of air on granular systems

    A. Density segregation in vibrated (deep) beds
    B. Heaping in vibrated (shallow) beds

1. Models for the solid phase

- Phase consists of individual particles → Lagrangian

- Methods borrowed from classical "molecular dynamics"

- Two different methods

A. Soft-sphere model

B. Hard-sphere model

1A. Solid Phase Models: Soft-Sphere

Position of particle a: $\vec{R}_a$

Newton's equation of motion: $m_a \dfrac{d^2\vec{R}_a}{dt^2} = \vec{F}_{a,tot}$

is integrated numerically: $\vec{R}_a(t+dt) = 2\vec{R}_a(t) - \vec{R}_a(t-dt) + \dfrac{\vec{F}_{a,tot}(t)}{m} dt^2$

total force: $\vec{F}_{a,tot} = \sum_b^{\text{inter}} \vec{F}_{ab} + m_a\vec{g}$

→ Time driven scheme

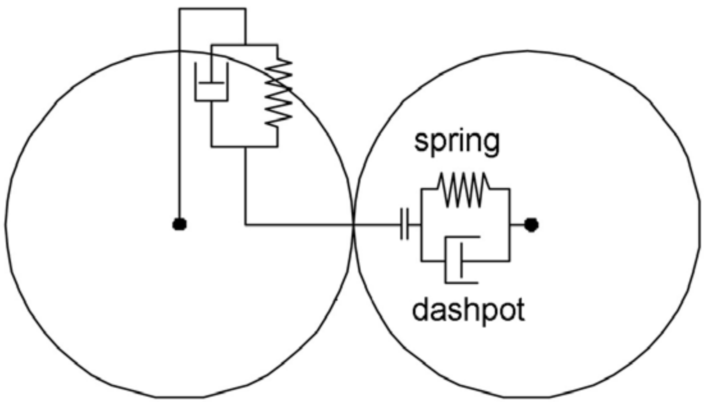
→ Interaction force $\vec{F}_{ij}$ follows from a continuous potential

→ "soft-sphere model"

1A. Solid Phase Models: Soft Sphere

Interaction force: $$\vec{F}_{ab} = \vec{F}^{coll}_{ab} + \vec{F}^{el}_{ab} + \vec{F}^{coh}_{ab}$$

- Collision force: Spring-dashpot model

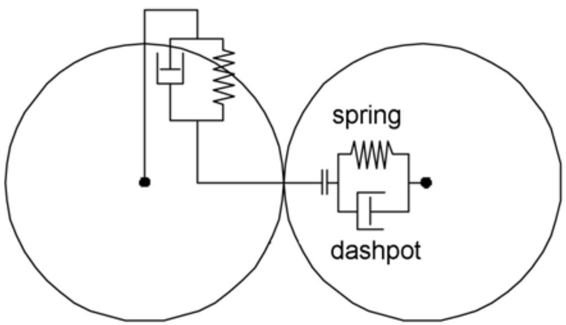


$$\vec{F}^{coll}_{ab,n} = \underbrace{-k}_{\text{spring constant}}\,\delta\,\vec{n}_{ab} - \underbrace{\eta}_{\text{damping coefficient}}\,\vec{v}_{ab,n}$$

- Electrostatic force $$\vec{F}^{el}_{ab} = -\frac{q^2}{4\pi\epsilon}\frac{\vec{n}_{ab}}{R^2_{ab}}$$

- Cohesive force $$\vec{F}^{coh}_{ab} = \frac{Ad}{6}\frac{\vec{n}_{ab}}{S^2_{ab}}$$

1A. Solid Phase Models: Soft-Sphere



$\vec{R}_a(t)\ ,\vec{V}_a(t)$

soft-sphere model

Coulomb force etc.

$\vec{F}_{ab}$

$$M\ddot{\vec{R}}_a = \sum_b \vec{F}_{ab}^{coll}$$

$\vec{R}_a(t+dt)$
$\vec{V}_a(t+dt)$

1B. Solid Phase Models: Hard-sphere

Simplified MD: hard-sphere model

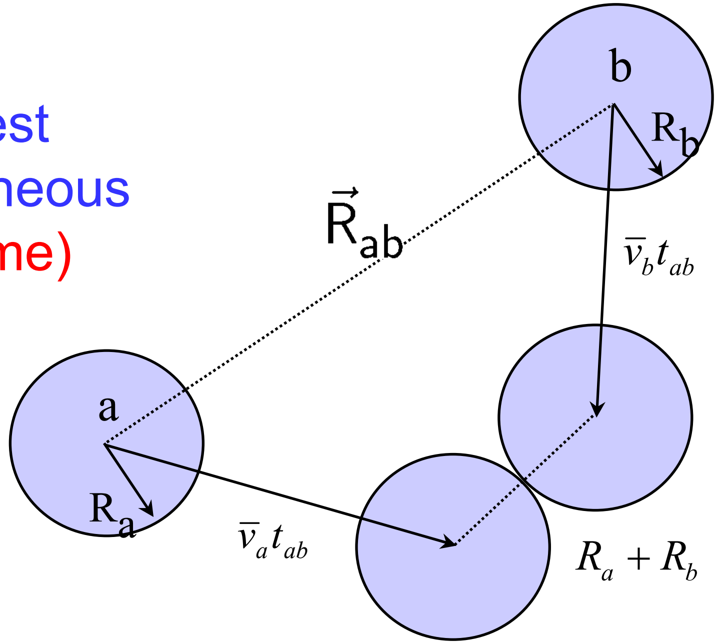
- Collision time between spheres can be calculated analytically:

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

- 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:

$$\Delta\vec{v}_a = \left(\frac{1+e}{2}\right)\frac{\vec{R}_{ab}\cdot\vec{v}_{ab}}{4R^2}\vec{R}_{ab}$$



1B. Solid Phase Models: Hard-Sphere

Advantages of hard-sphere over soft-sphere

- Much faster for dilute systems
- Soft potential often “too soft” to model e.g. glass spheres

Disadvantages of hard-sphere over soft-sphere

- HS breaks down for dense (close packed) systems
- Update not based on forces: more difficult to include other interactions

2. Models for the gas phase

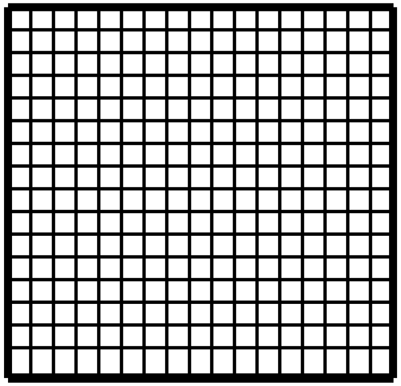
- Continuum description of the phase → Eulerian

- Time evolution governed by Navier-Stokes (NS) equation

- Two basic methods for solving the NS equations on a grid

  A. Computational Fluid Dynamics

  B. Lattice Boltzmann Method



2A. Gas Phase Models: Computational Fluid Dynamics (CFD)

Basic idea: solve the set of differential equations:

$$\partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0$$

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

by finite difference methods (CFD).

Closures for P and τ

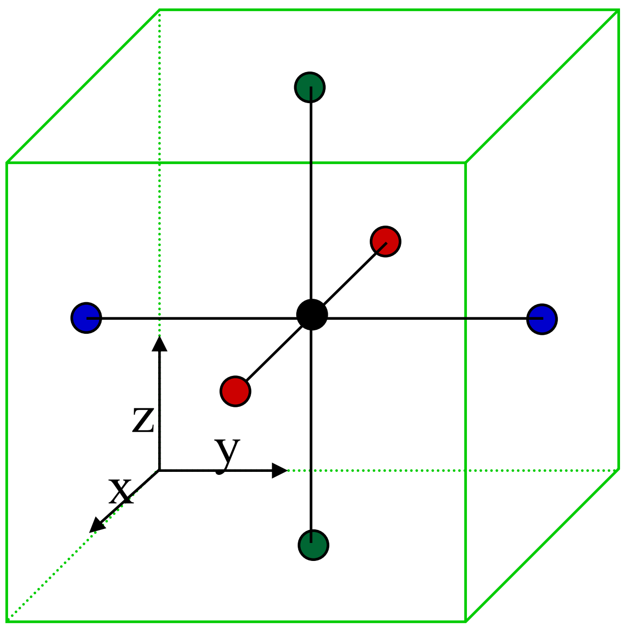
$$P = \frac{RT}{M}\rho$$

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

2A. Gas Phase Models: Computational Fluid Dynamics (CFD)

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 $P,\ \rho$
- 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

$$\rho^n_{\mathbf{i}}\ , \quad P^n_{\mathbf{i}}\ , \quad \mathbf{u}^n_{\mathbf{i}'} = \begin{pmatrix} u^n_{\mathbf{i}+h\mathbf{e}_x} \\ u^n_{\mathbf{i}+h\mathbf{e}_y} \\ u^n_{\mathbf{i}+h\mathbf{e}_z} \end{pmatrix}$$

with :
$$\mathbf{e}_x = (1,0,0) \qquad h = \frac{1}{2}$$
$$\mathbf{e}_y = (0,1,0)$$
$$\mathbf{e}_z = (0,0,1)$$

2A. Gas Phase Models: Computational Fluid Dynamics (CFD)

Finite difference of the mass continuity equation:

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

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

$$\boxed{\rho_{\mathbf{i}}^{n+1} - \rho_{\mathbf{i}}^{n} + \delta t \left[\vec{\nabla} \cdot \rho \mathbf{u}\right]_{\mathbf{i}}^{n+1} = 0}$$

$$\left[\vec{\nabla} \cdot \rho \mathbf{u}\right]_{\mathbf{i}}^{n+1} = \sum_{\alpha} \frac{[\rho \mathbf{u}]_{\mathbf{i}+h\mathbf{e}_\alpha}^{n+1} - [\rho \mathbf{u}]_{\mathbf{i}-h\mathbf{e}_\alpha}^{n+1}}{\delta l}$$

2A. Gas Phase Models: Computational Fluid Dynamics (CFD)

Finite difference of momentum continuity equation:

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

$$\frac{[\rho \mathbf{u}]_{\mathbf{i}'}^{n+1} - [\rho \mathbf{u}]_{\mathbf{i}'}^{n}}{\delta t} = -\left[\vec{\nabla} P\right]_{\mathbf{i}'}^{n+1} - \left[\vec{\nabla} \cdot \rho \mathbf{u}\mathbf{u} + \vec{\nabla} \cdot \overline{\overline{\tau}}\right]_{\mathbf{i}'}^{n}$$

$$[\rho \mathbf{u}]_{\mathbf{i}'}^{n+1} = -\delta t \left[\vec{\nabla} P\right]_{\mathbf{i}'}^{n+1} \underbrace{- \delta t \left[\vec{\nabla} \cdot \rho \mathbf{u}\mathbf{u} + \vec{\nabla} \cdot \overline{\overline{\tau}}\right]_{\mathbf{i}'}^{n} + [\rho \mathbf{u}]_{\mathbf{i}'}^{n}}$$

$$[\rho \mathbf{u}]_{\mathbf{i}'}^{n+1} = -\delta t \left[\vec{\nabla} P\right]_{\mathbf{i}'}^{n+1} + A_{\mathbf{i}'}^{n}$$

$$\boxed{\mathbf{u}_{\mathbf{i}'}^{n+1} = \frac{-\delta t \left[\vec{\nabla} P\right]_{\mathbf{i}'}^{n+1} + A_{\mathbf{i}'}^{n}}{\rho_{\mathbf{i}'}^{n+1}}}$$

Solution procedure to calculate variables at time $n+1$

First guess:

$$P_{\mathbf{i}}^{n+1}$$

$$\left[\vec{\nabla} P\right]_{\mathbf{i}',\alpha}^{n+1} = \frac{\left(P_{\mathrm{i}+\mathrm{e}_\alpha}^{n+1} - P_{\mathrm{i}}^{n+1}\right)}{\delta l}, \qquad \rho_{\mathbf{i}}^{n+1} = \frac{M P_{\mathrm{i}}^{n+1}}{RT}$$

$$\mathbf{u}_{\mathbf{i}'}^{n+1} = \frac{-\delta t \left[\vec{\nabla} P\right]_{\mathbf{i}'}^{n+1} + A_{\mathbf{i}'}^{n}}{\rho_{\mathbf{i}'}^{n+1}}$$

Test if $\rho_{\mathbf{i}}^{n+1}$ and $\mathbf{u}_{\mathbf{i}'}^{n+1}$ satisfy conservation of mass eq.

$$\rho_{\mathbf{i}}^{n+1} - \rho_{\mathbf{i}}^{n} + \delta t \left[\vec{\nabla} \cdot \rho \mathbf{u}\right]_{\mathbf{i}}^{n+1} = 0$$

?

no — try new $P_{\mathbf{i}}^{n+1}$

(Newton-Raphson procedure)

yes — go to $n+2$

2B. Gas Phase Models: Lattice Boltzmann Method (LBM)

Hydrodynamic variables for the gas phase: $\rho(\mathbf{r})$ and $\mathbf{u}(\mathbf{r})$

These 4 variables can be captured by 1 variable: $\mathsf{f}(\mathbf{r},\mathbf{c})$

$$\begin{aligned}\int d\mathbf{c}\; \mathsf{f}(\mathbf{r},\mathbf{c}) &= \rho(\mathbf{r}) \\ \int d\mathbf{c}\; \mathbf{c}\; \mathsf{f}(\mathbf{r},\mathbf{c}) &= \rho(\mathbf{r})\mathbf{u}(\mathbf{r})\end{aligned}$$

Time evolution of $\mathsf{f}(\mathbf{r},\mathbf{c})$: the Boltzmann Equation (BE)

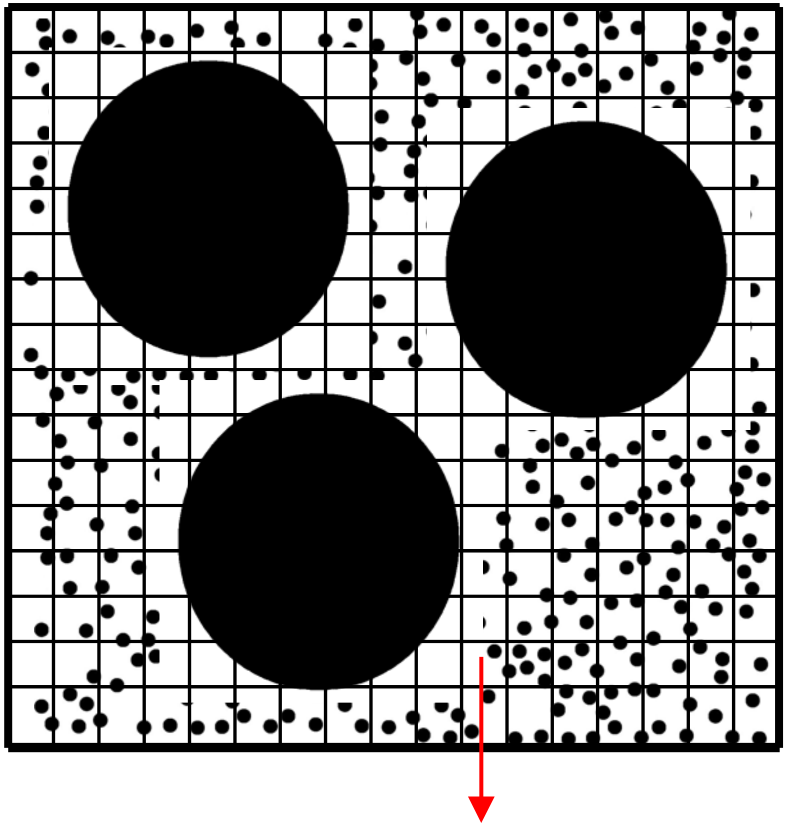
$$\boxed{\partial_t \mathsf{f} + \mathbf{c}\cdot\nabla \mathsf{f} = \mathcal{C}(\mathsf{f})} \qquad \mathcal{C}(\mathsf{f}) = -\frac{\mathsf{f}-\mathsf{f}_{eq}(\rho,\mathbf{u})}{\tau}$$

$$\int d\mathbf{c}\; \boxed{} \Rightarrow \quad \partial_t \rho + \nabla\cdot(\rho\mathbf{u}) = 0$$

$$\int d\mathbf{c}\; \mathbf{c}\; \boxed{} \Rightarrow \quad \partial_t (\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla \mathsf{p} - \nabla\cdot\tau$$

3. Modeling the gas-particle interaction

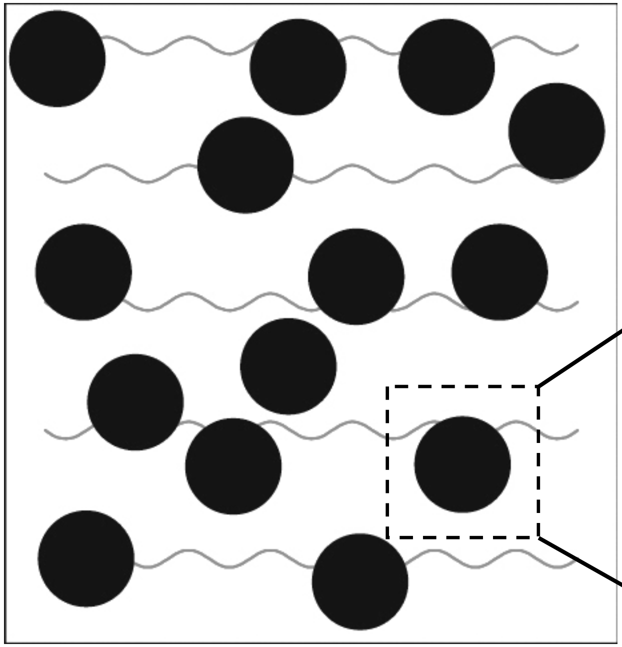
Introducing solid particles into an *Eulerian* model for the gas phase:



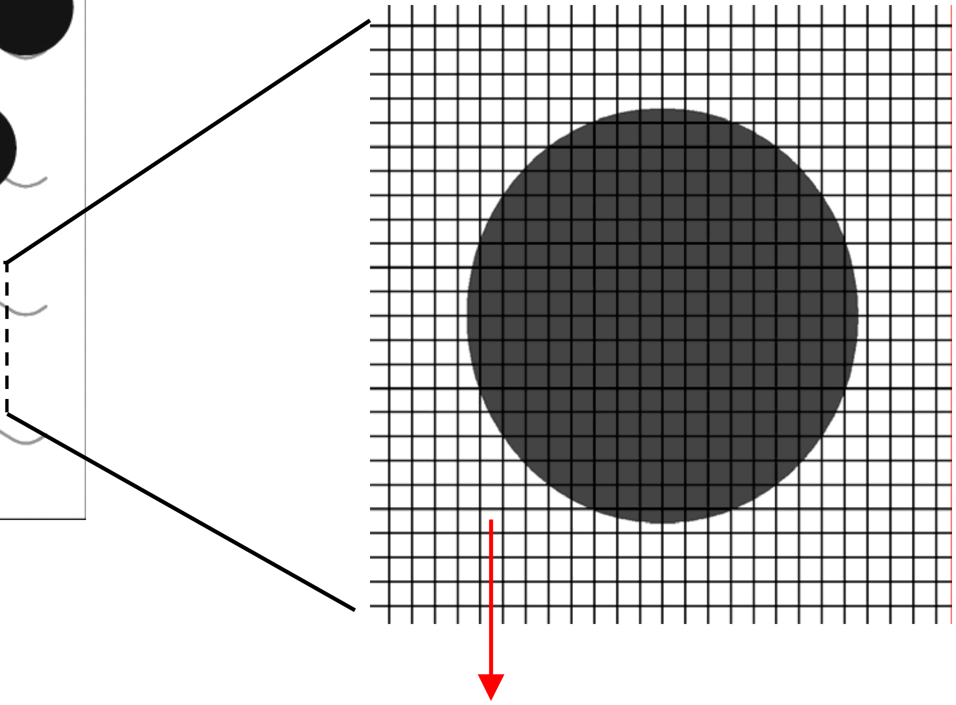
CDF or LBM

Resolved
Discrete Particle
Model

3A. Gas-Particle Interaction: Fully Resolved



Interaction between solid and gas: stick boundary condition at surface

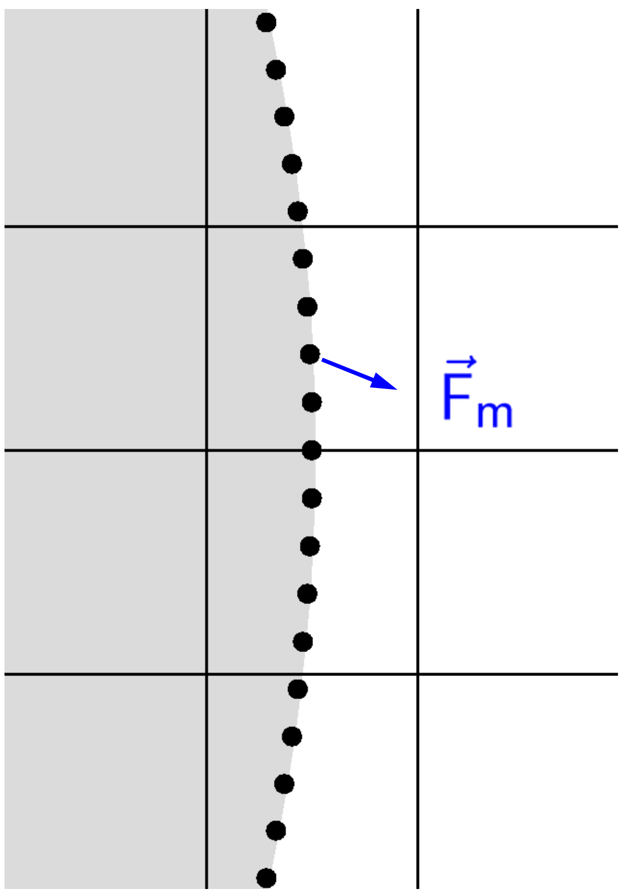


CFD or LB

3A. Gas-Particle Interaction: Fully Resolved (CFD)

Resolved flow with CFD: Immersed Boundary Method

Define Lagrangian force points on the surface of the particle:



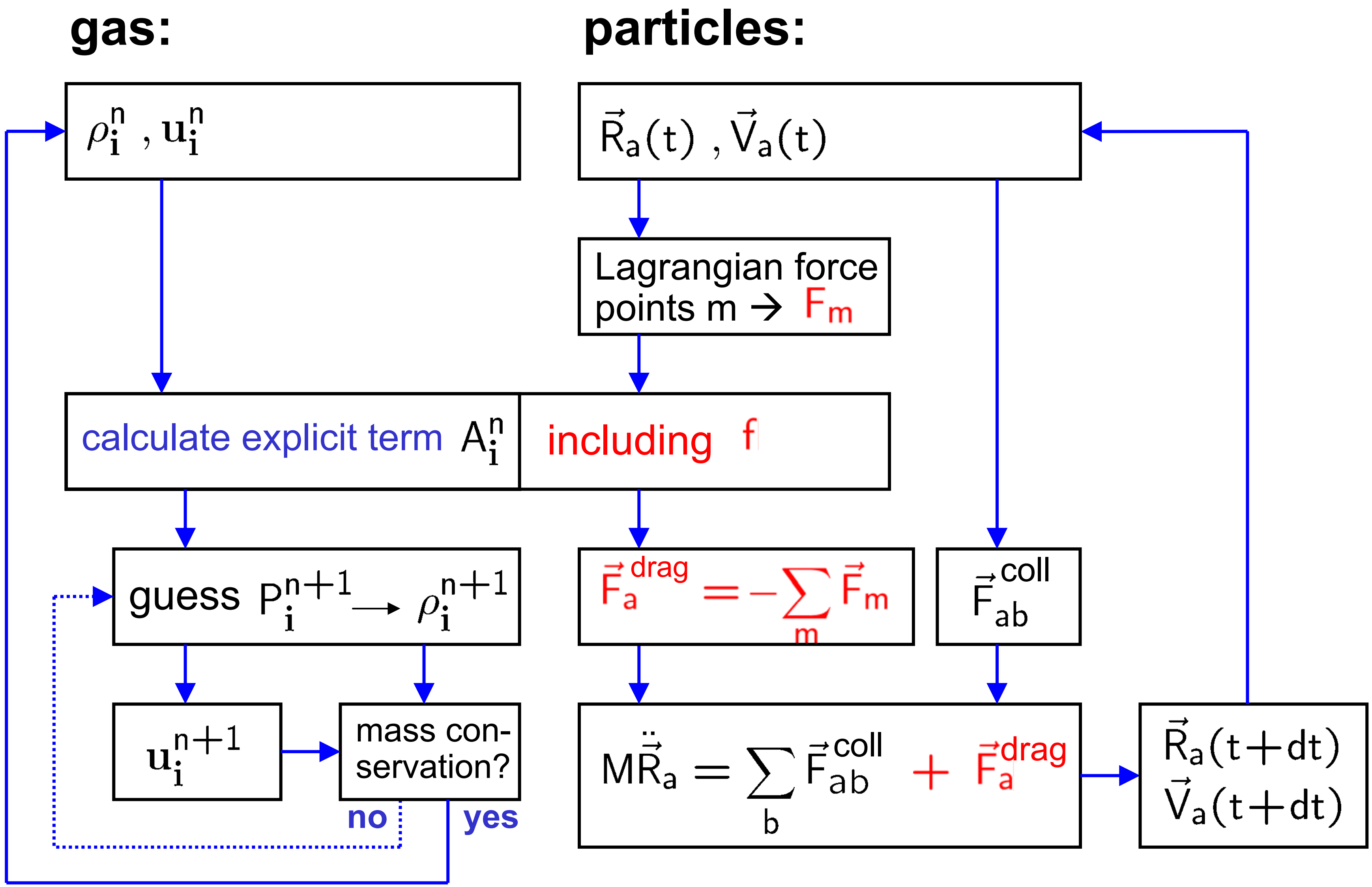
Each force point m applies a force $\vec{F}_m$ on the fluid, such that the local velocity of the fluid is equal to the local surface velocity

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

The momentum equation then becomes:

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

3A. Gas-Particle Interaction: Fully Resolved (CFD)



3A. Gas-Particle Interaction: Fully Resolved (CFD/LBM)

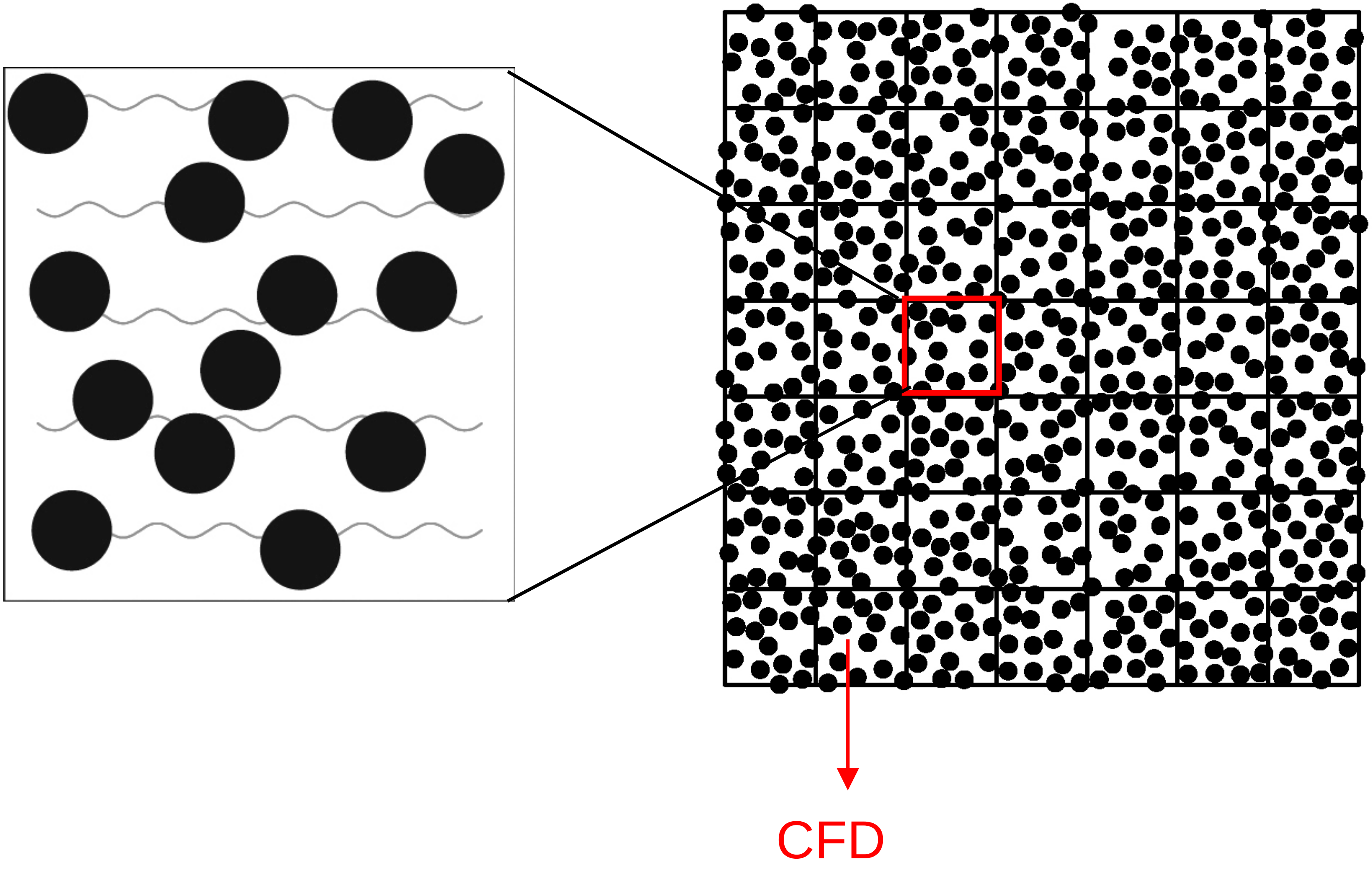
Results from fully resolved flow simulations

1. Sedimentation of 6144 particles using the LBM-BB method (A.J.C. Ladd, see http://ladd.che.ufl.edu)
2. Fluidized bed simulation with 3600 particles using the CFD-IB method (J.A.M. Kuipers, 2008)

Conclusion

Fully resolved methods provide the most detailed level of modeling gas-particle flow, yet number of particles are limited to O(10000)

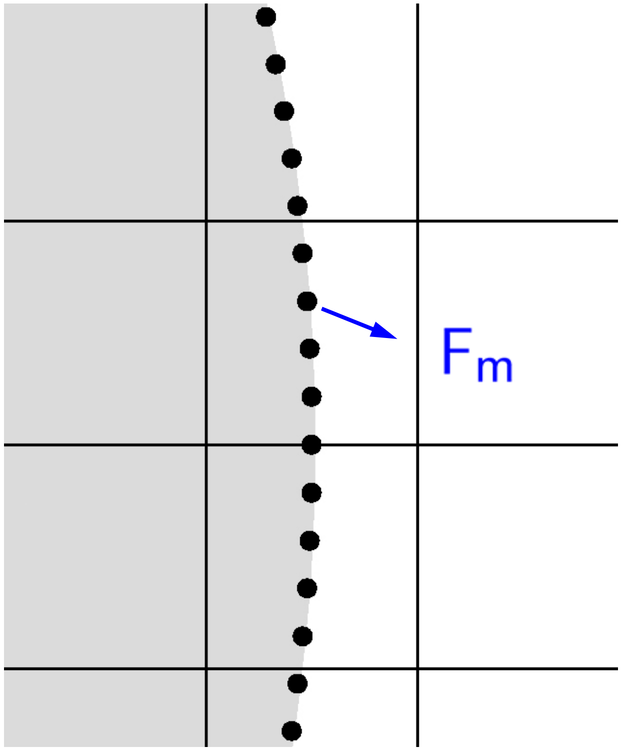
3A. Gas-Particle Interaction: Unresolved (CFD)

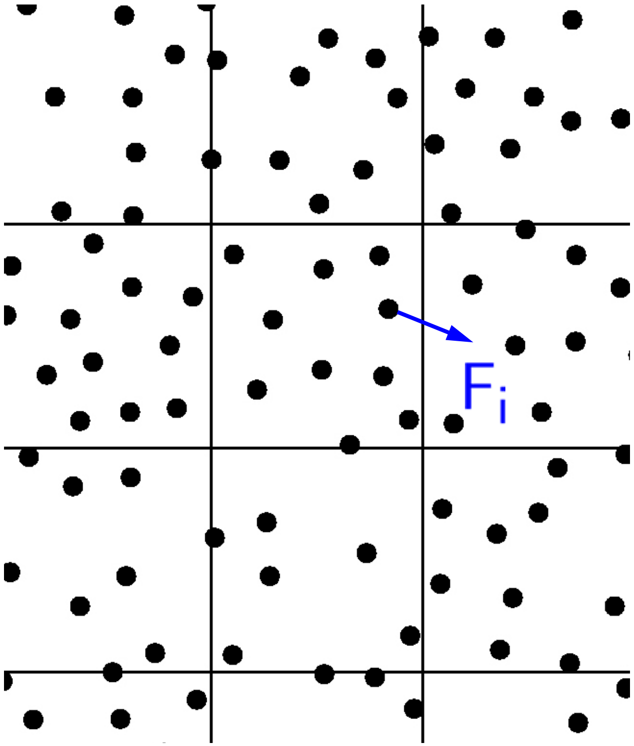


3A. Gas-Particle Interaction: Unresolved (CFD)

Unresolved flow with CFD: implementation similar to resolved flow

Resolved flow





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

3A. Gas-Particle Interaction: Unresolved (CFD)

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

Gas phase:

$$\partial_t \varepsilon\rho\vec{u} + \vec{\nabla}\cdot\varepsilon\rho\vec{u}\vec{u} = -\vec{\nabla}P - \vec{\nabla}\cdot\,\varepsilon\bar{\bar{\tau}} + \vec{f} + (1-\varepsilon)\vec{\nabla}P$$

Solid phase:

pressure force

$$\frac{d}{dt}m\vec{v}_i = \sum_j \vec{F}_{ij} - \vec{F}_i + V_i\vec{\nabla}P$$

Required: correlations for β

4. Examples of the effect of air on granular systems

Vibrated beds of small particles (< 0.5 mm)

A. Density segregation in deep beds

Christiaan Zeilstra, Hans Kuipers

B. Heaping in vibrated shallow beds

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

4A. Density segregation in deep beds: simulations

Vibrated bed of <u>equal-sized</u> bronze and glass spheres (100 μm)

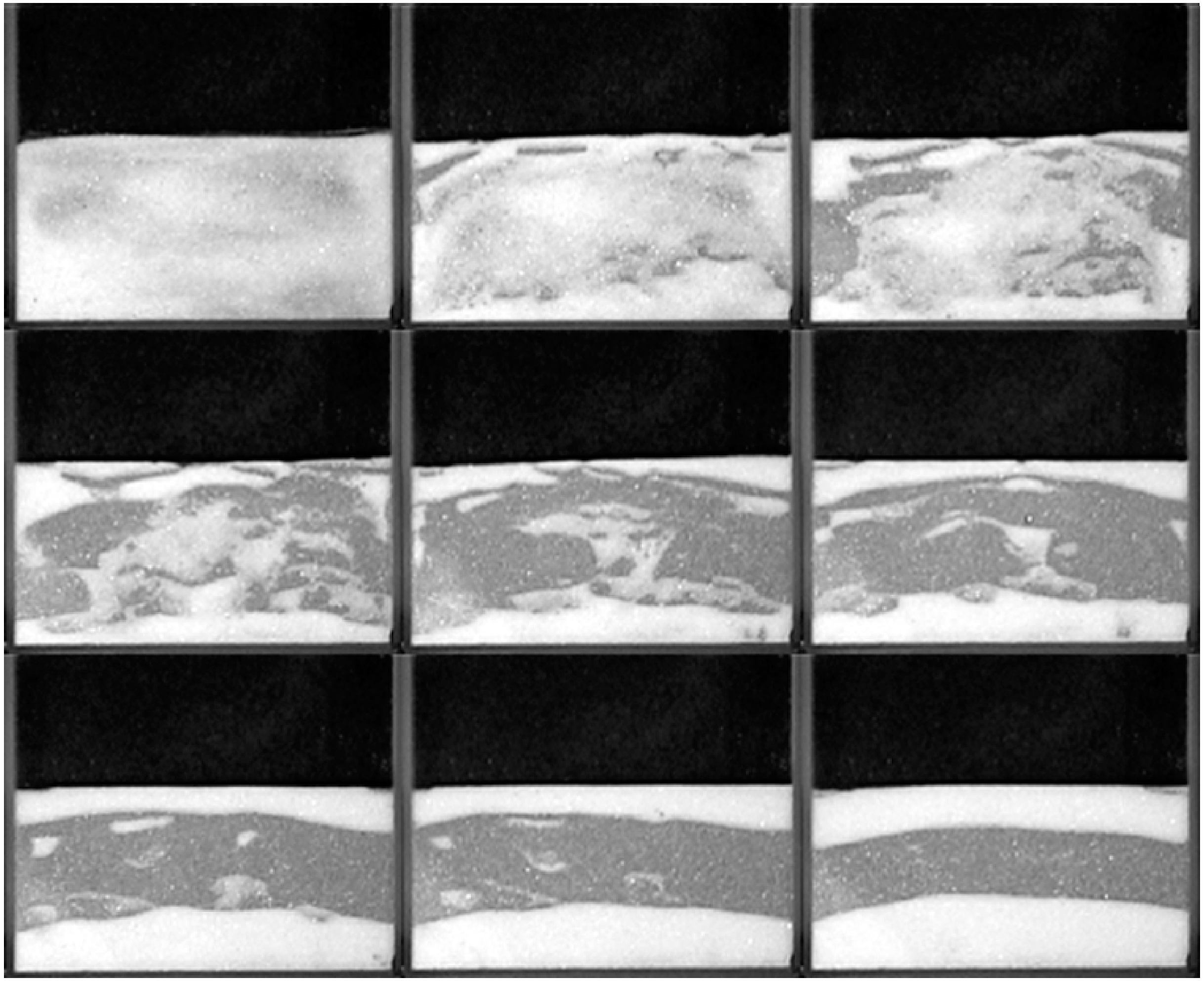
Experiments by Burtally, King and Swift (Science 2002)

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 x H x D = 8 x 6 x 0.6 mm^3
- Parameters: f = 55 Hz, A = 1 mm $\Rightarrow$ $\Gamma = \dfrac{A(2\pi f)^2}{g} = 12$

No air ▶ **Air** ▶

4A. Density segregation in deep beds: experiments



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

f = 50 Hz

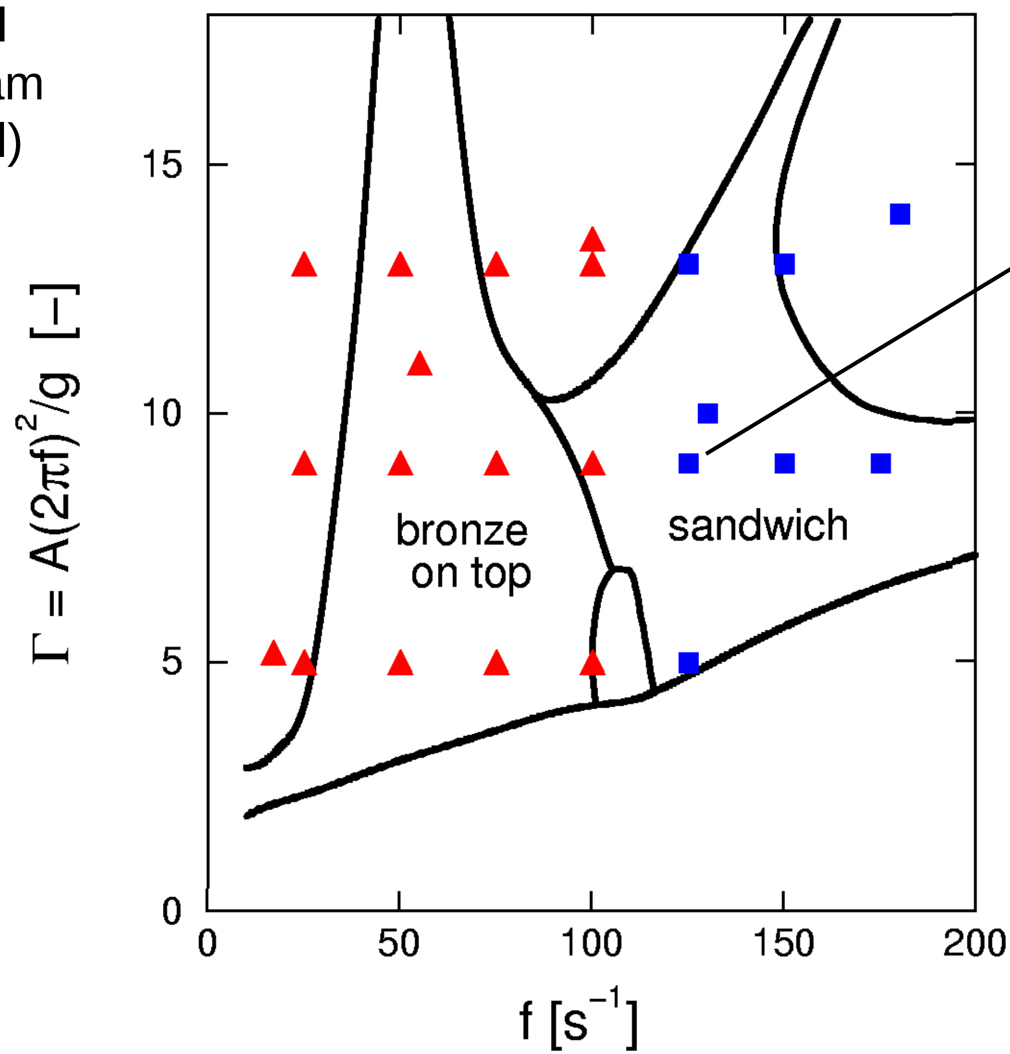
f = 130 Hz

A = 1 mm

A = 0.07mm

4A. Density segregation in deep beds: exp. and sim.

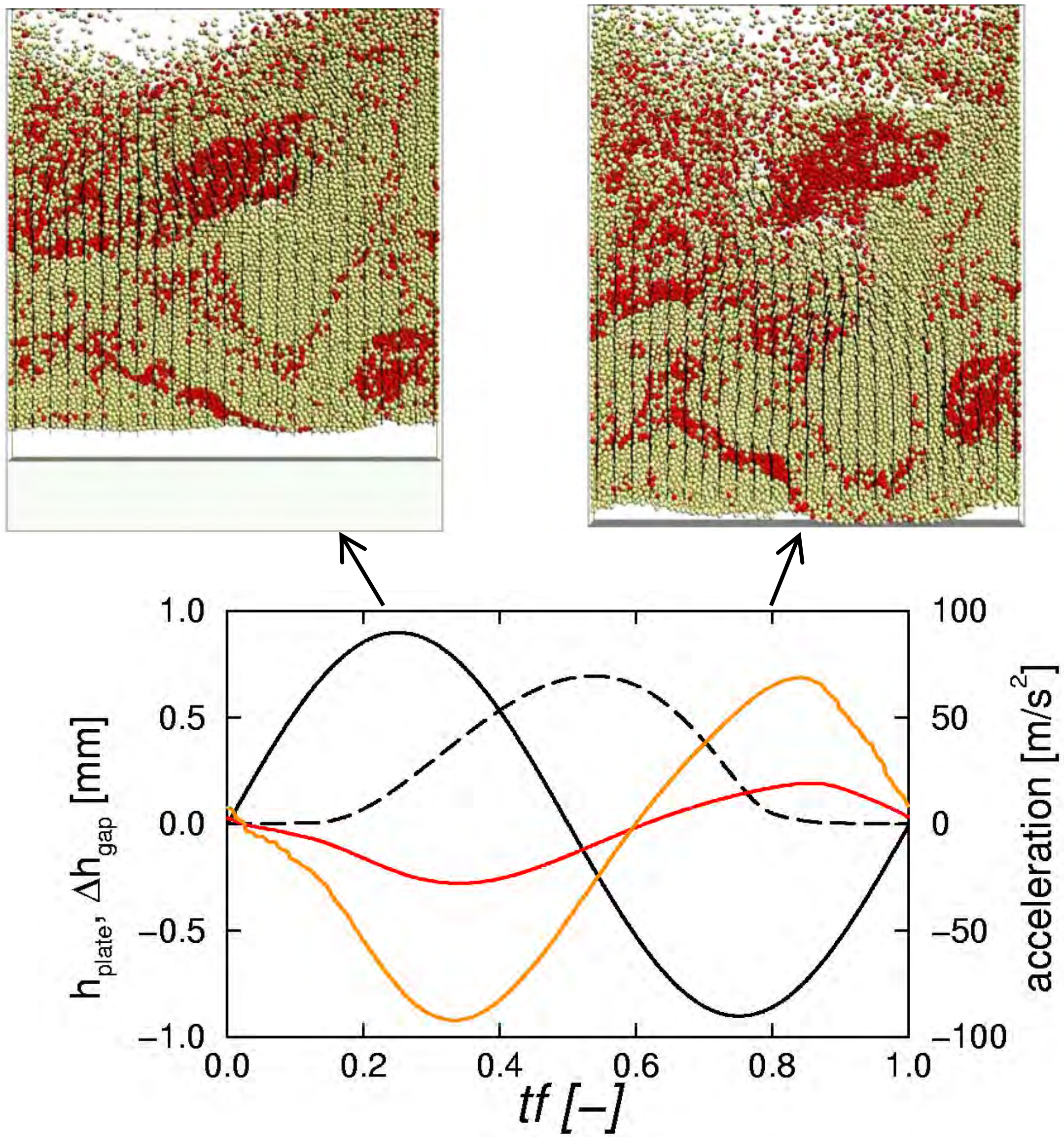
Experimental phase diagram (Burtally et al)



$f = 125$ Hz
$\Gamma = 9$

4A. Density segregation in deep beds: explanation

Why do the light particles sink to the bottom?



4A. Density segregation in deep beds: sandwich formation

Sandwich formation:

- Convection plays an important role

- Sensitive of the particle-particle and partice wall friction:

$\mu_{pp} \downarrow$ $\mu_{pw} \rightarrow$	0.0	0.1	0.4
0.0	Bottom	Bottom	Bottom
0.1	Middle (40 s)	**Middle** (10 s)	Top
0.4	Middle (20 s)	Middle (10 s)	Top

4B. Heaping in shallow beds

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: $N_p = 14\ 000$, $W \times H \times D = 100 \times 50 \times 2.1\ \text{mm}^3$
- Parameters: f = 6.25 Hz, A = 10 mm $\Rightarrow \quad \Gamma = \frac{A(2\pi f)^2}{g} = 1.6$

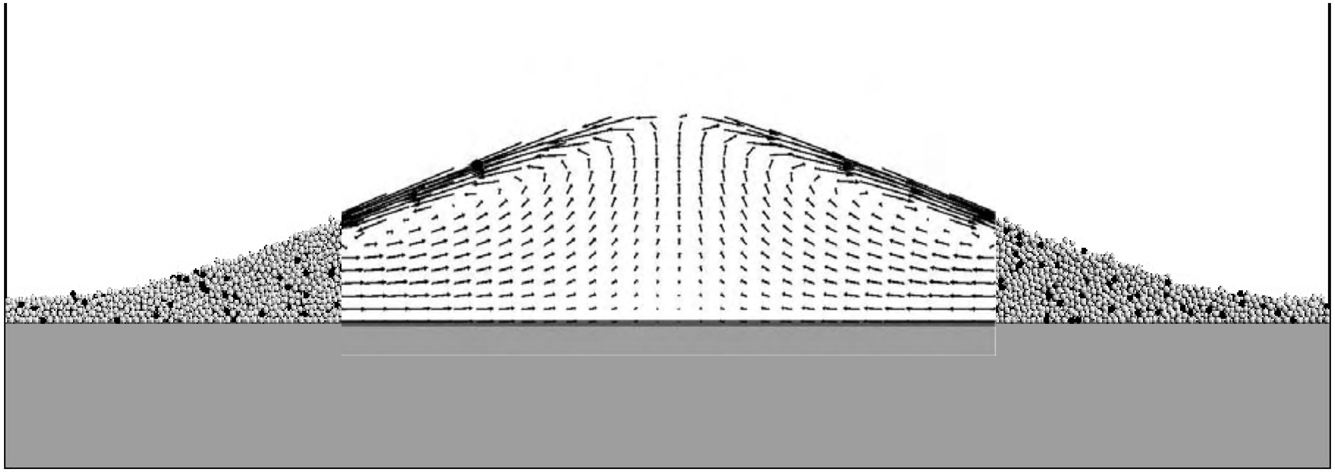
No air **Air**

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

4B. Heaping in shallow beds: mechanism

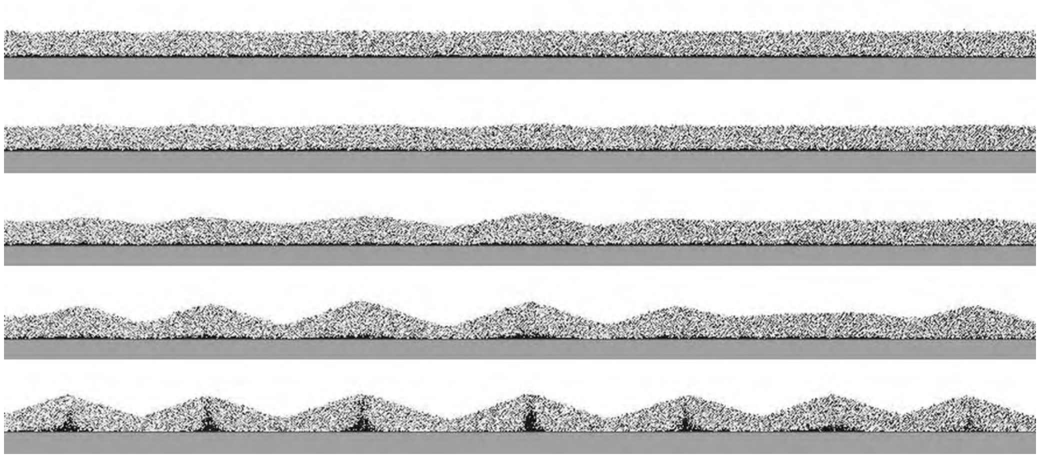
Three rivaling mechanisms for steady state heap

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])



4B. Heaping in shallow beds: instability

How does the heap come into existence?



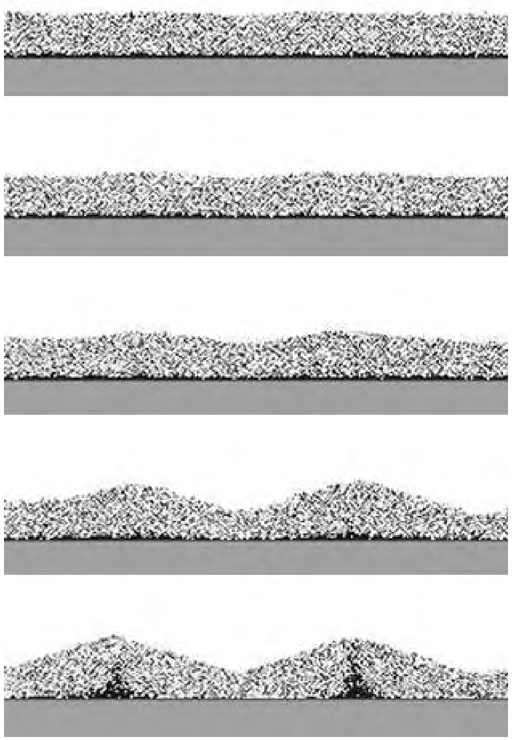
Two stages:

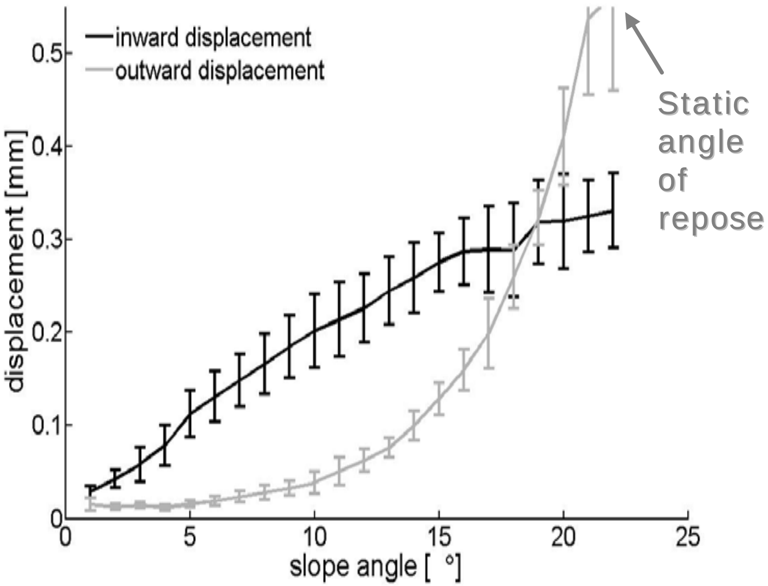
1. Fast initial stage where heaps are formed from a flat surface

2. Slow second stage where heaps merge:

4B. Heaping in shallow beds: initial stage

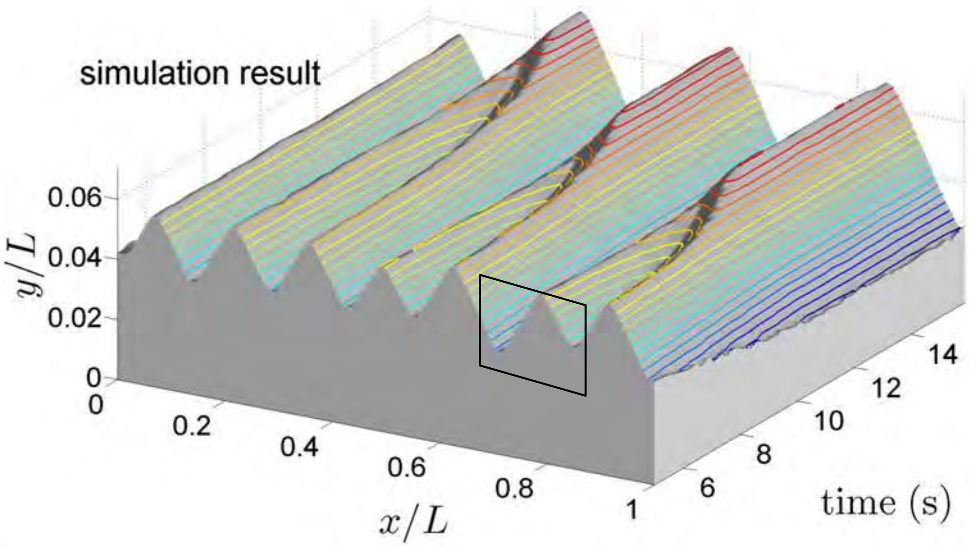
1. Fast initial stage where heaps are formed from a flat surface

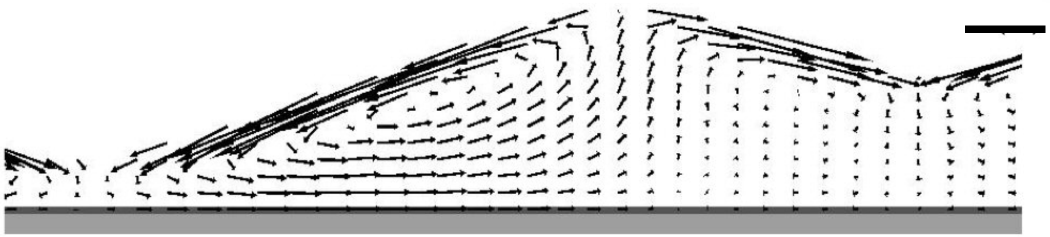




4B. Heaping in shallow beds: coarsening stage

2. Slow second stage where heaps merge:





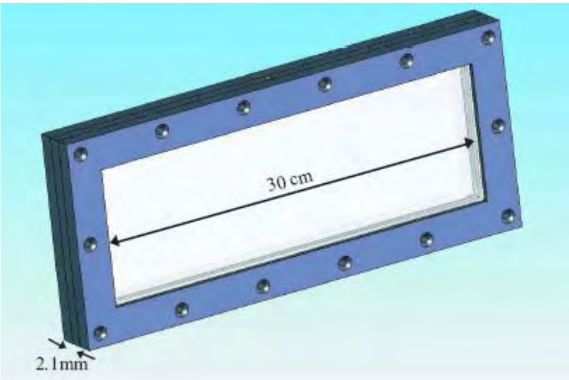
What is the functional form of the life-time T_N of the N-heap state?

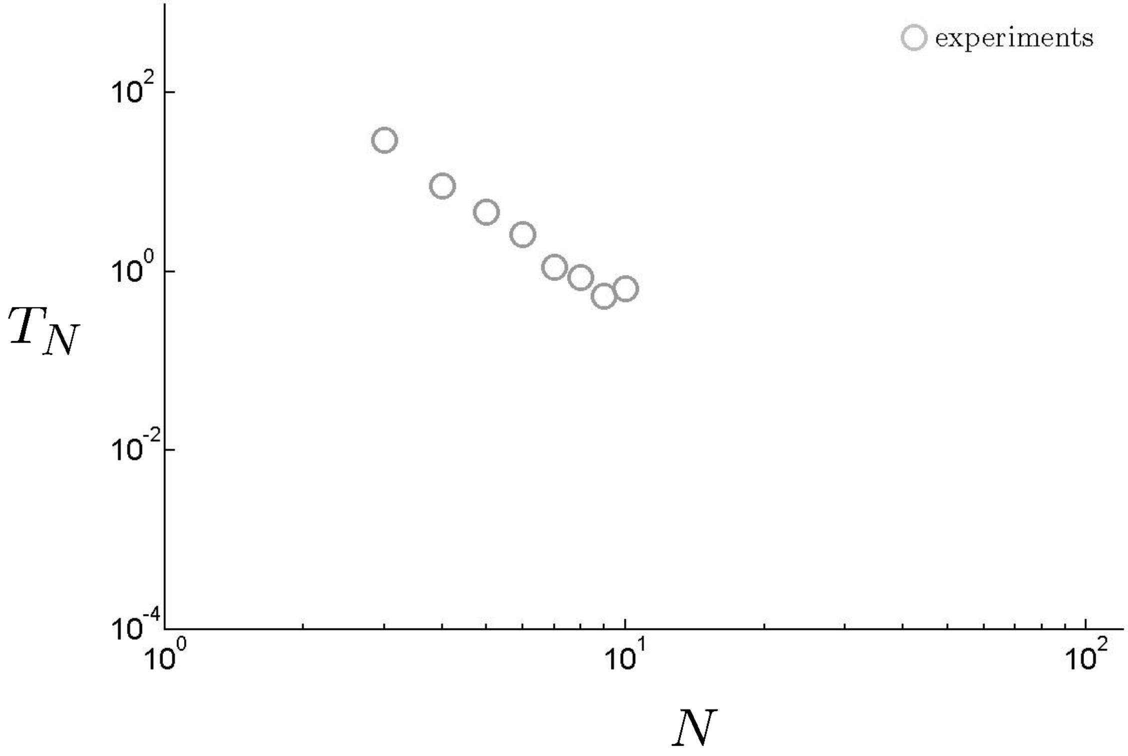
$$T_N \sim N^{-\alpha} \quad ?$$

$$T_N \sim e^{-\alpha N} \quad ?$$

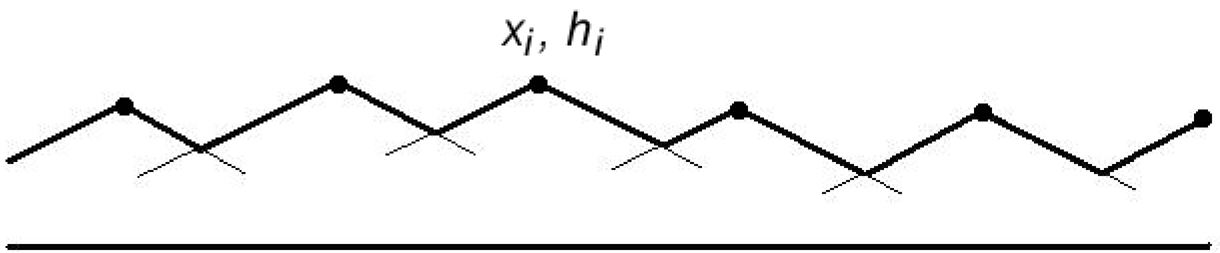
4B. Heaping in shallow beds: experiments

Experiment





4B. Heaping in shallow beds: a simple model

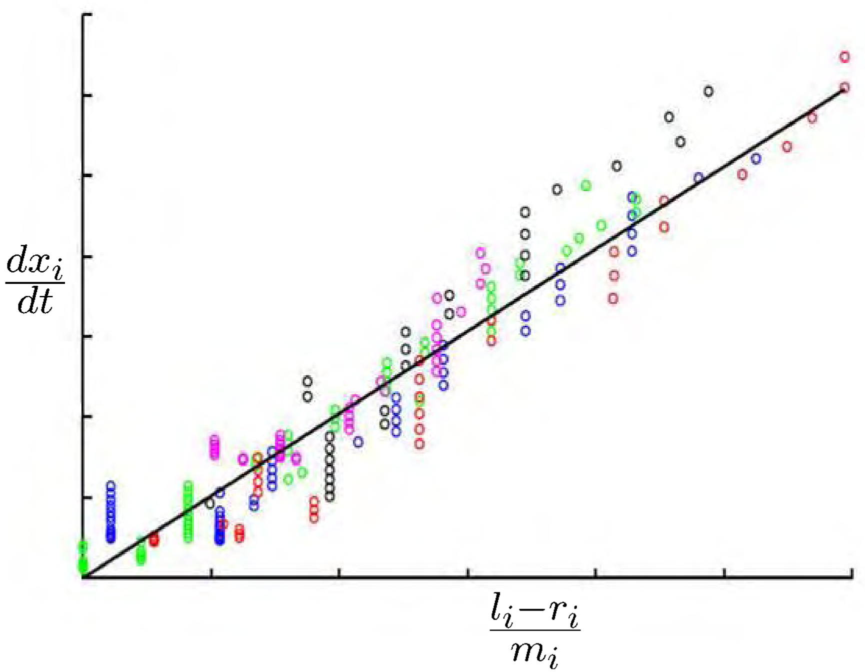


$$m_i \frac{dx_i}{dt} = C(l_i - r_i)$$

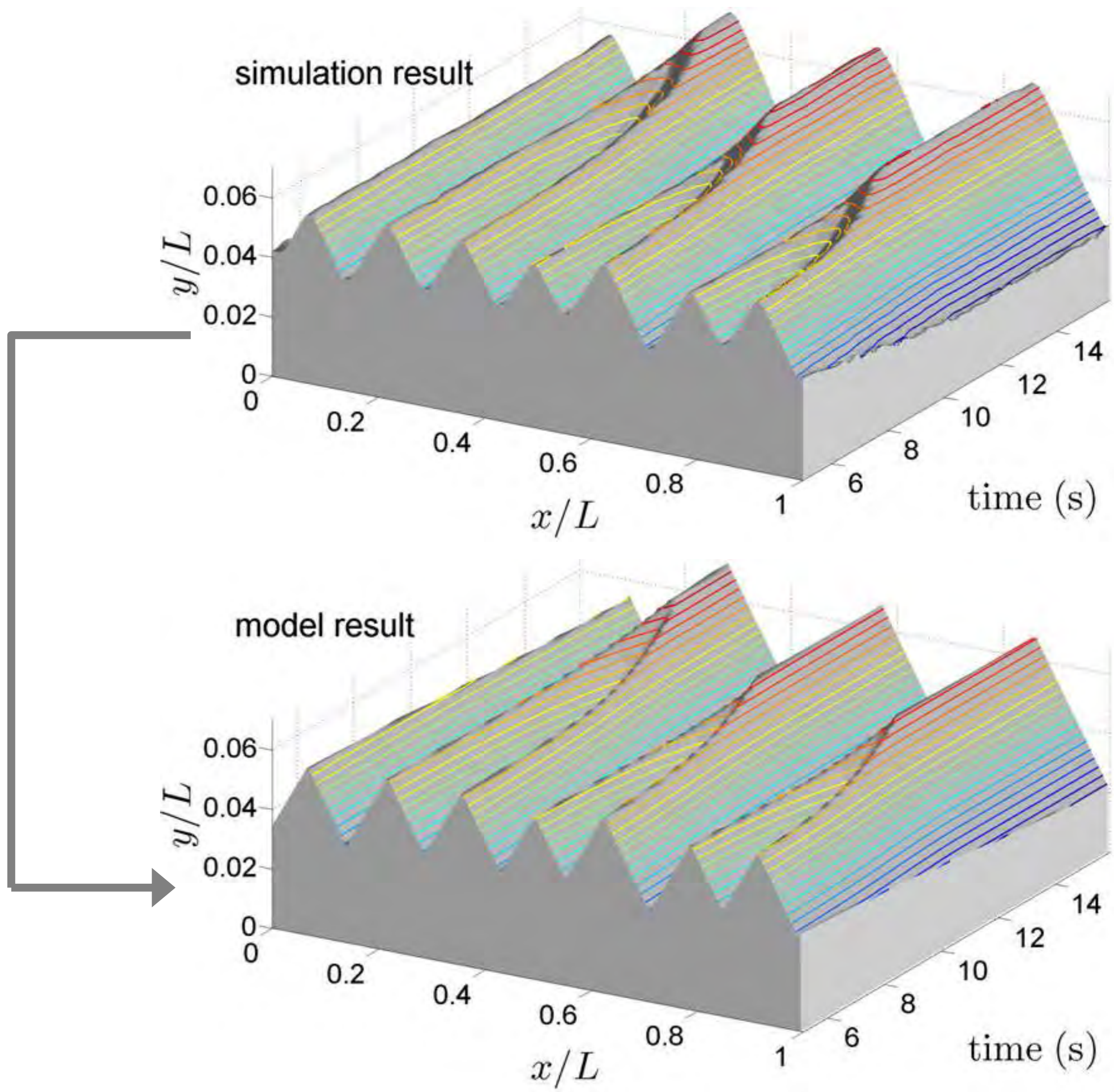
~ area under heap

determined from simulation data

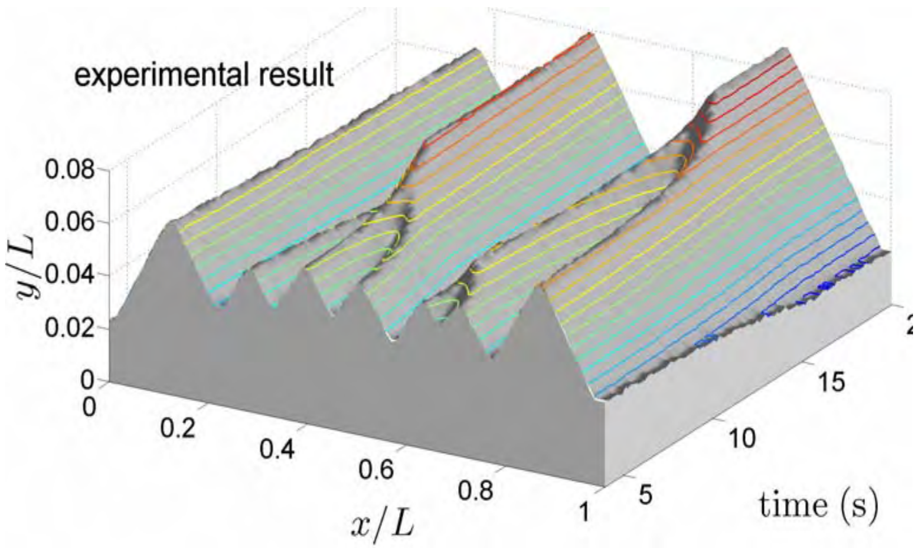
h_i is modified such that m_i is preserved

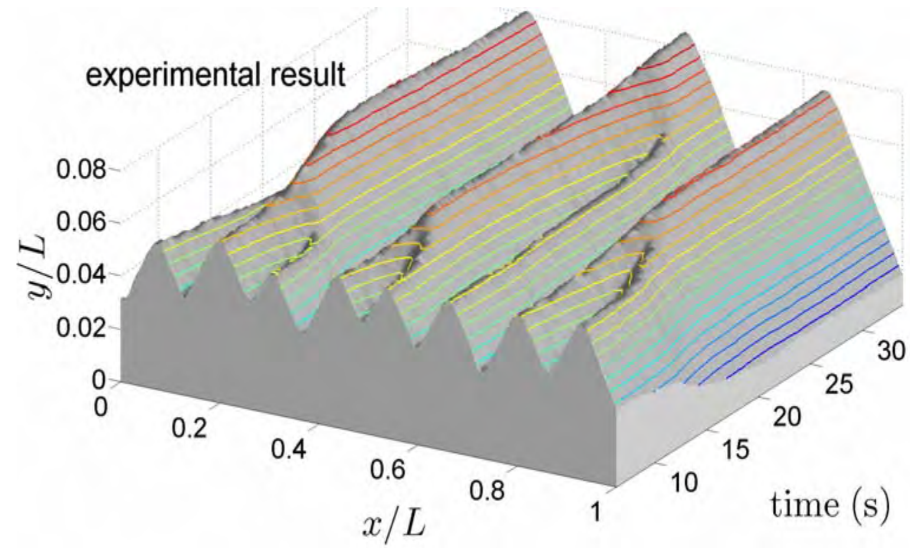


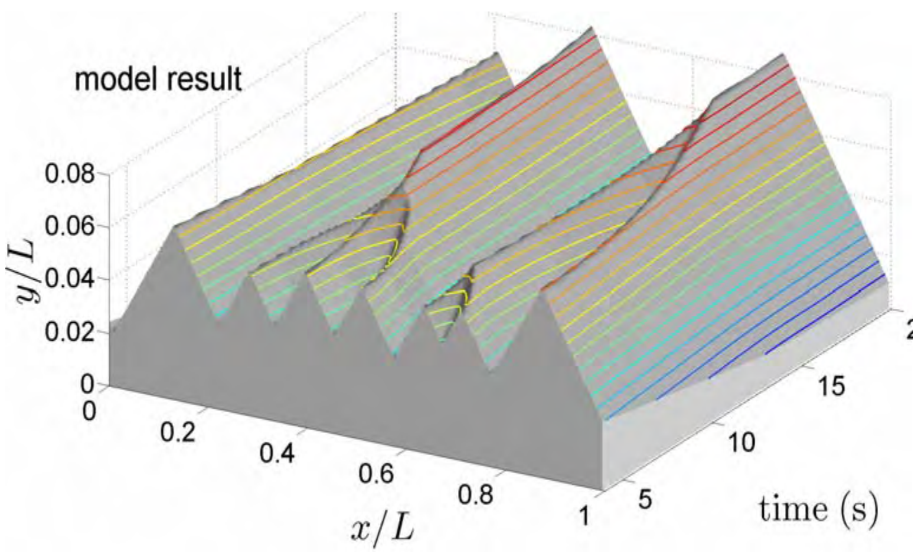
4B. Heaping in shallow beds: model result

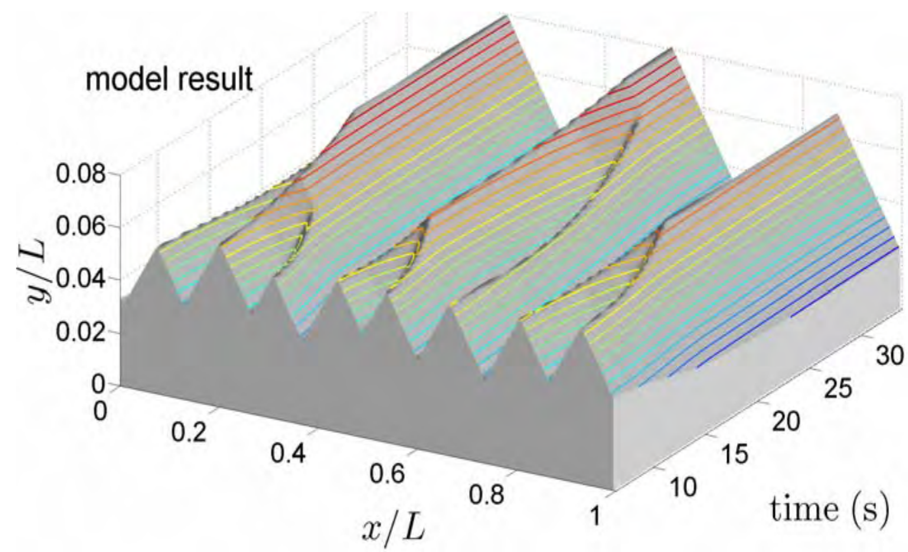


4B. Heaping in shallow beds: model result

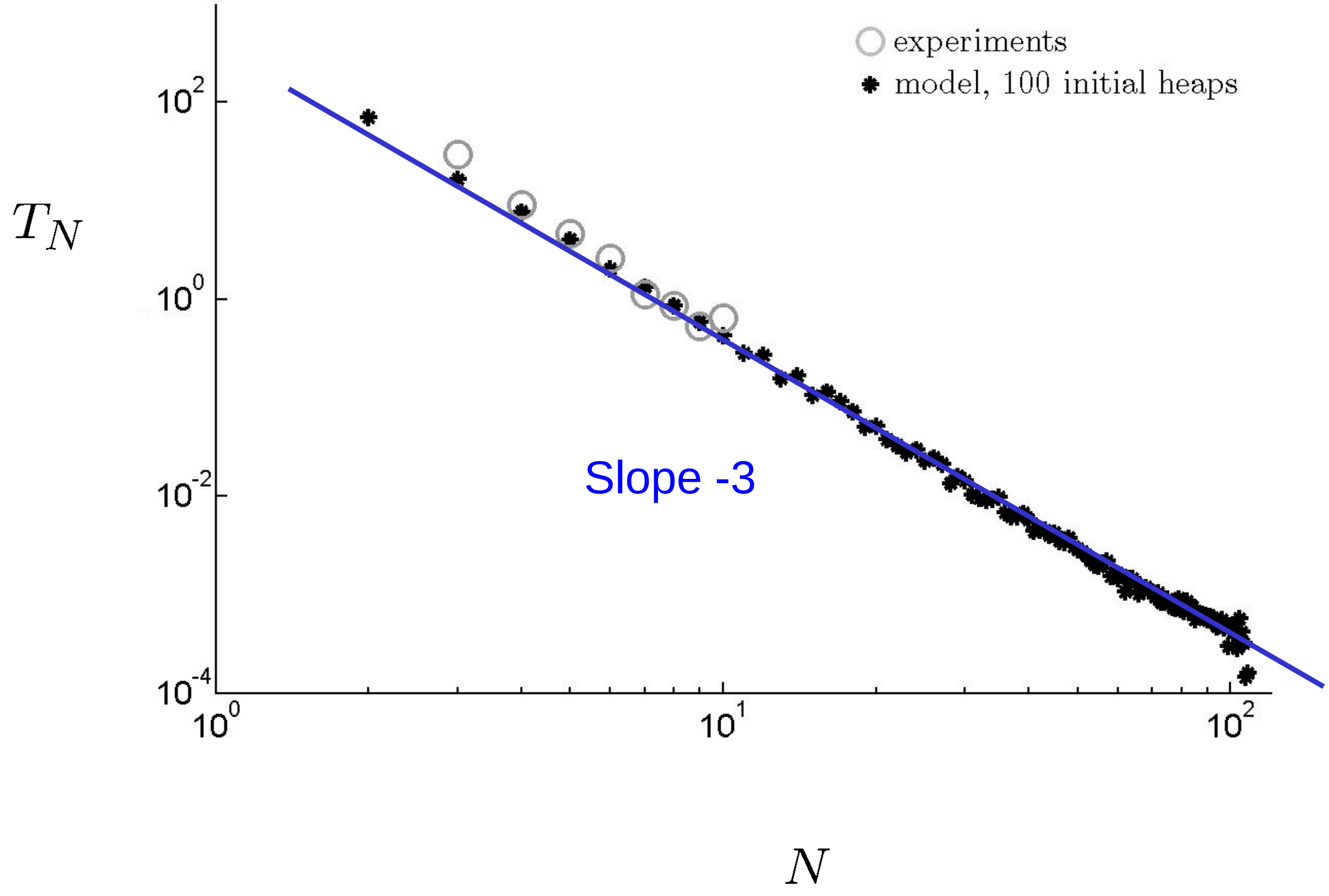






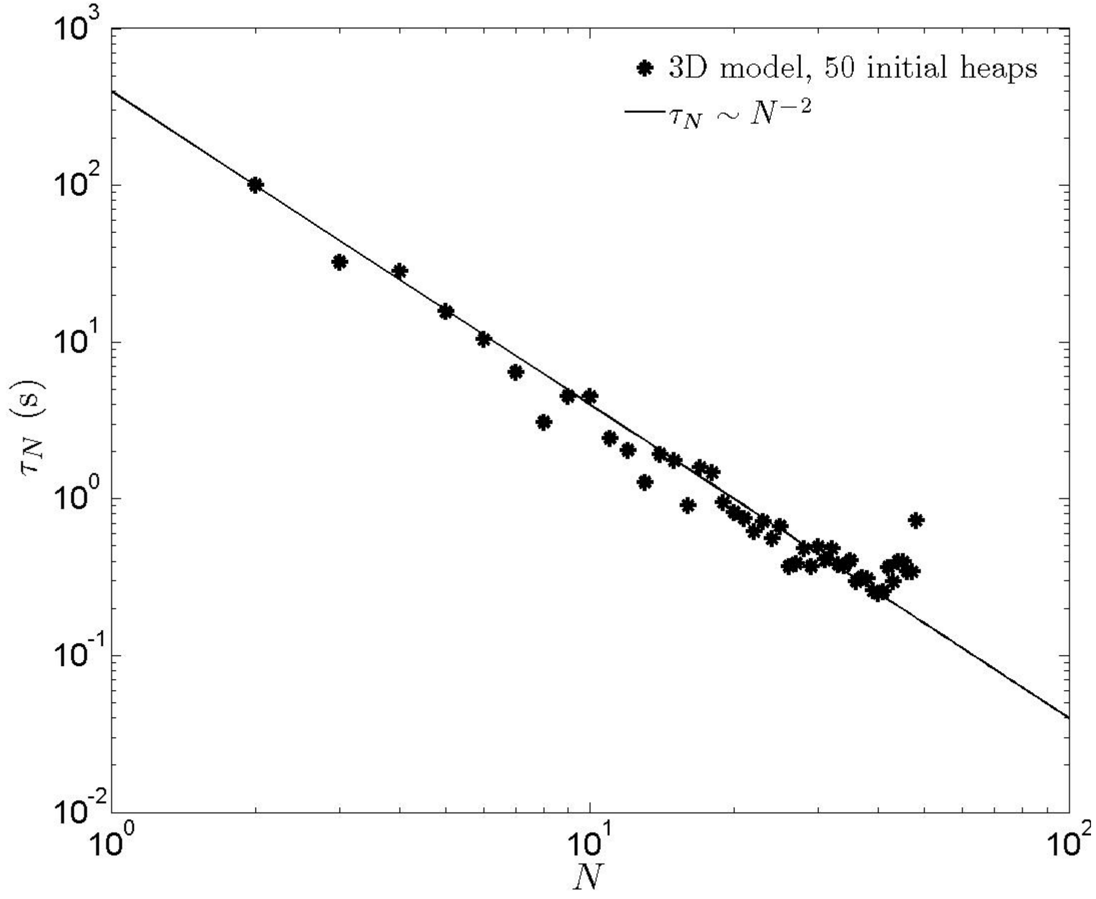


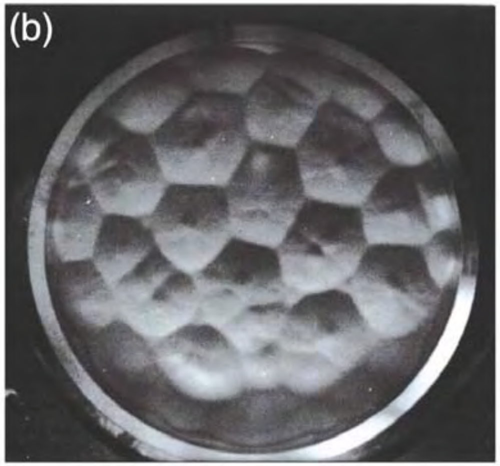
4B. Heaping in shallow beds: model result



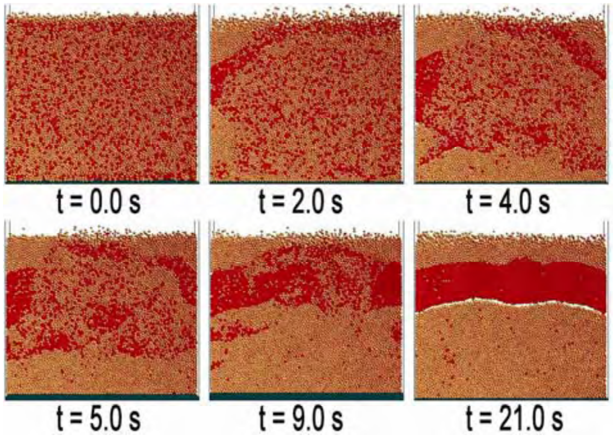
4B. Heaping in shallow beds: model result in 3-D

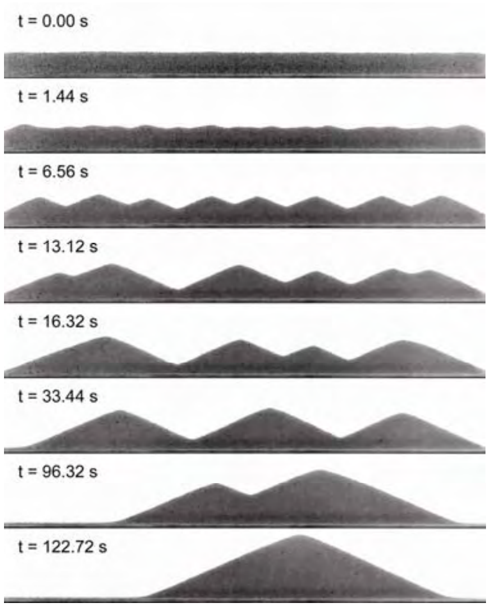
Model in 3-D



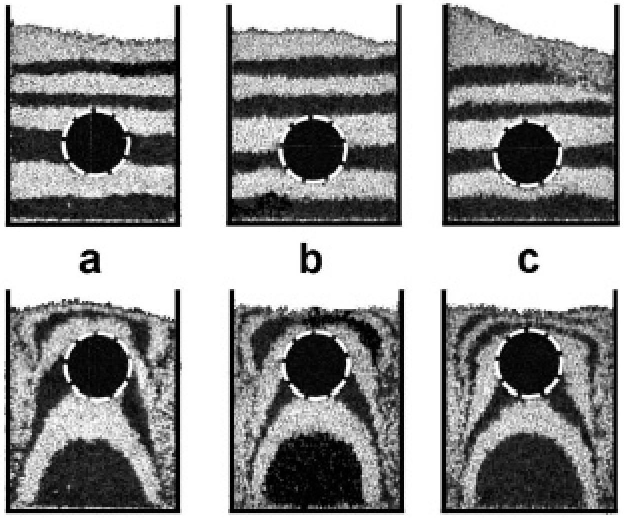


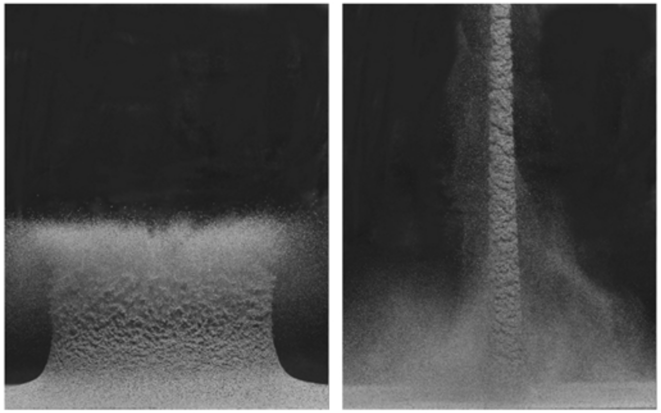
Recapt.I: Two examples of the effect of air in granular matter:





There are many more .....

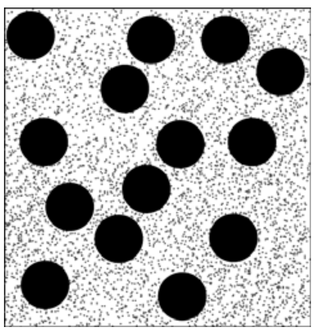




Air effects **must** be included for d < 1 mm

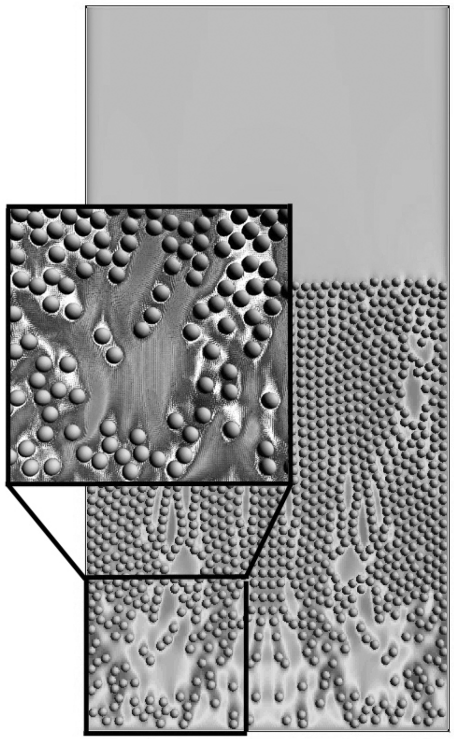
Recapt.II: Modeling gas-solid flow

SRD



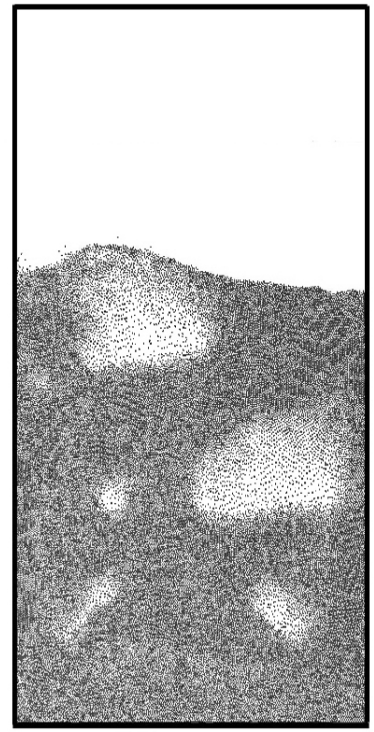
Lagrange
Lagrange

DNS



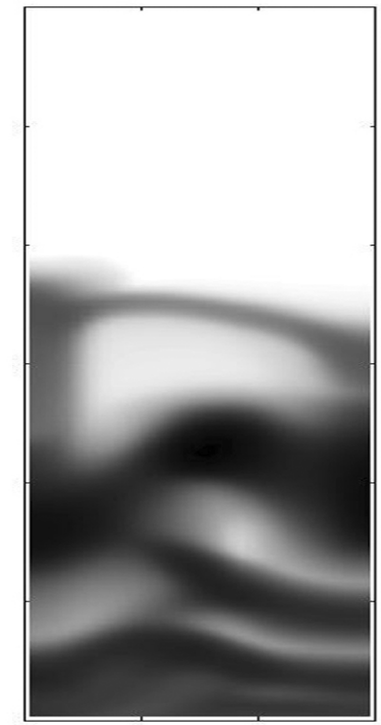
Euler
Lagrange

DEM



Euler
Lagrange

TFM



Euler
Euler