Multiphase flows

Lecture 4

Multiscale Modelling of Multiphase Flows:

Lagrangian Particle Tracking (LPT)

Goals

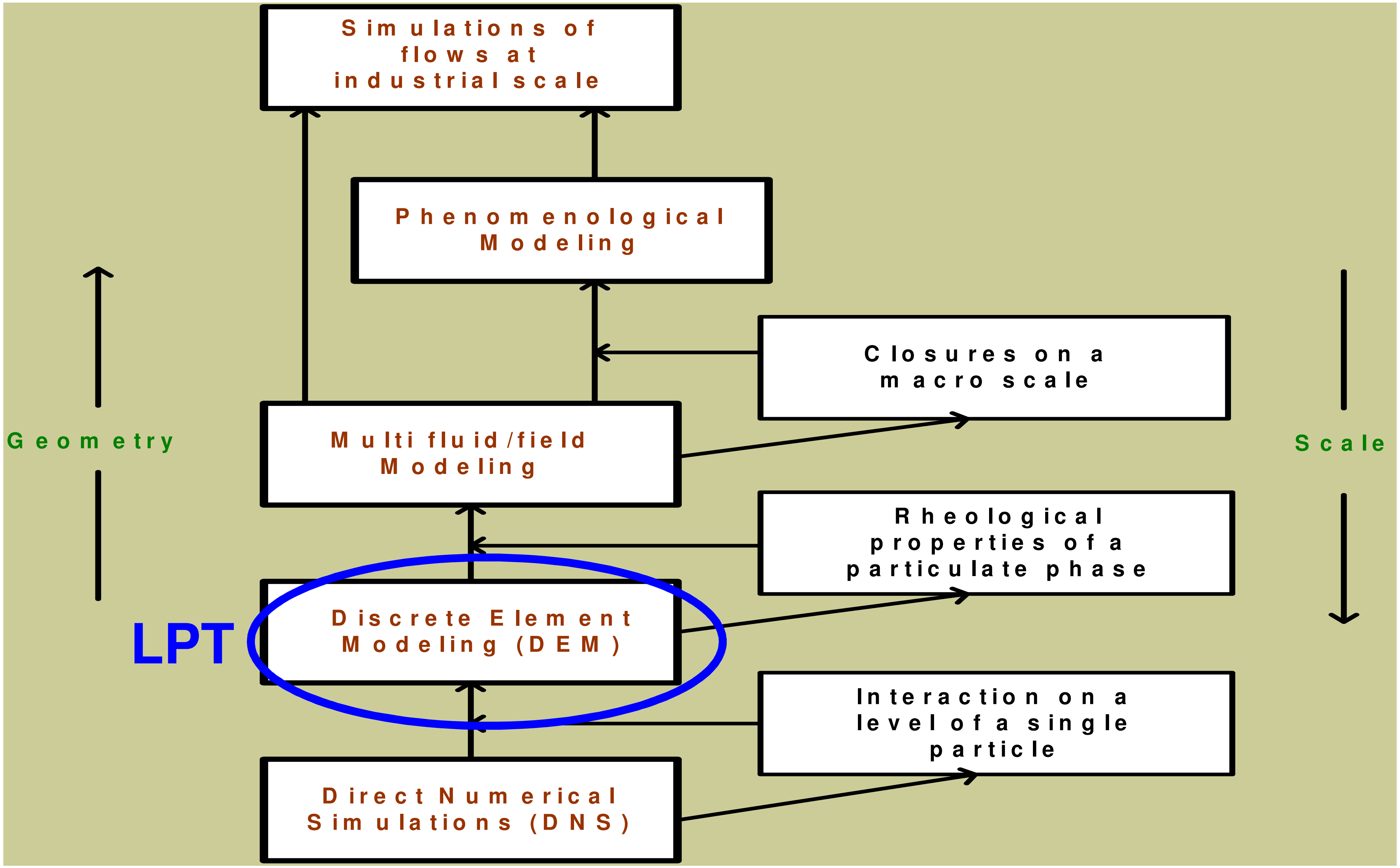
1. To make sure that a modelling approach be as general as possible
2. To put the approach studied into the general perspective of modelling procedures
3. To obtain the governing equations using rigorous mathematical procedures
4. To emphasize abilities, disadvantages and costs of the procedure studied

Fundamental questions

1. How much is LPT framework ***ab initio*** (from the beginning, from first principles in a mathematical sense) methods?

2. If not, why? Can this be changed in the future?

3. Can LPT be used as ***predictive*** and ***design*** procedures instead of experiments?

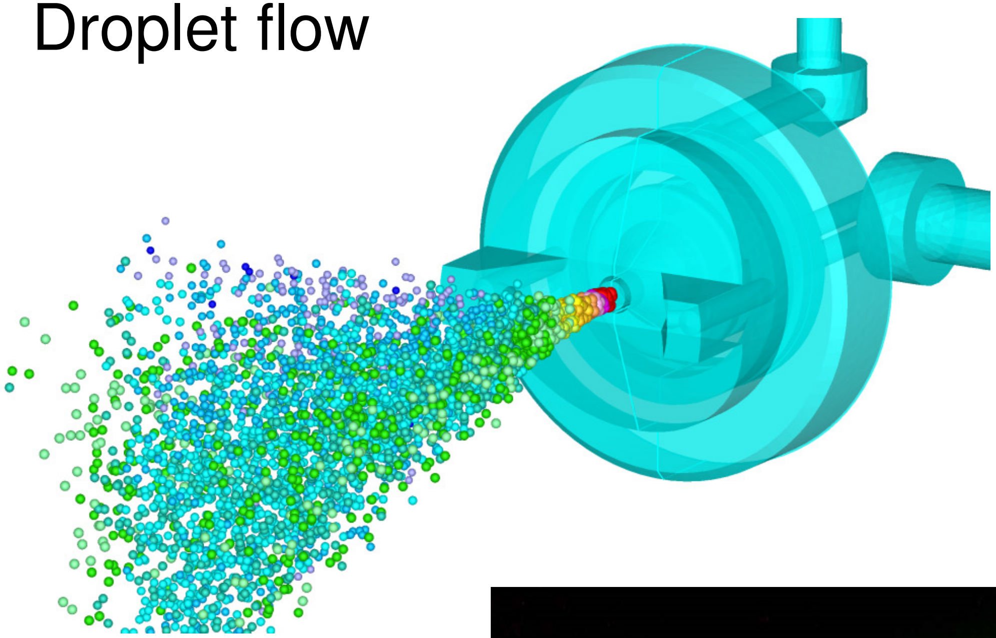

Simulations of flows at industrial scale
Phenomenological Modeling
Closures on a macro scale
Multi fluid/field Modeling
Rheological properties of a particulate phase
Discrete Element Modeling (DEM)
Interaction on a level of a single particle
Direct Numerical Simulations (DNS)
Geometry
Scale
LPT

A child of many names…

- Eulerian-Lagrangian particle tracking
- Lagrangian particle tracking (LPT)
- Discrete phase model (DPM)
- Discrete particle model (DPM)
- Discrete element model (DEM)

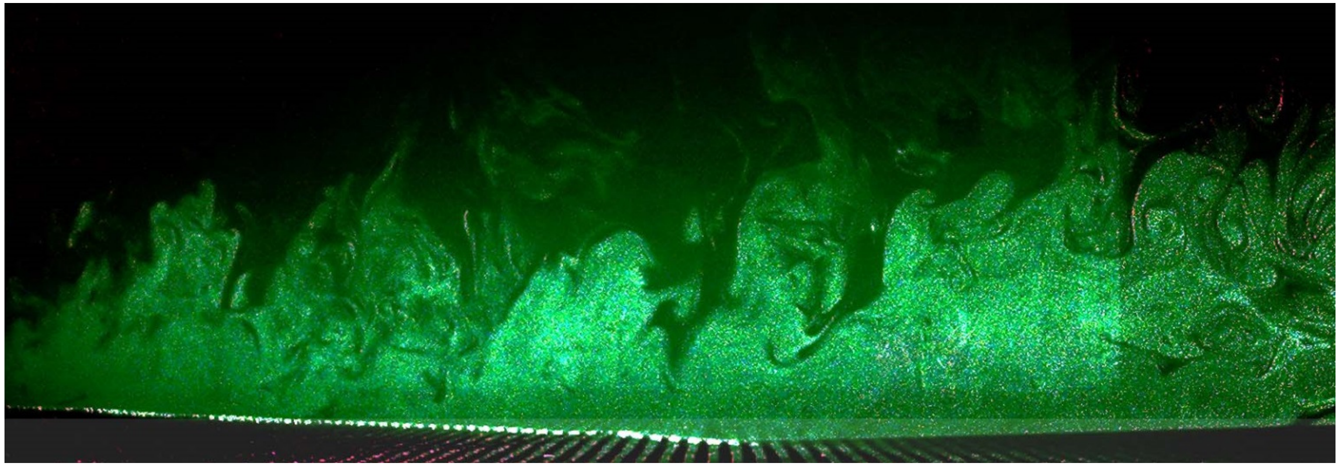
Dispersed multiphase flows

Droplet flow



Dispersed bubble flow

Particle-laden flow



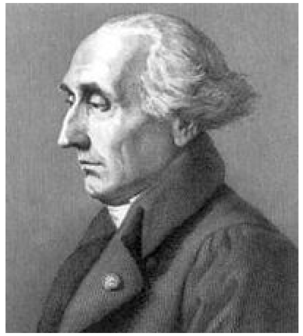
”Classical” challenges that are handled well

- Polydispersity
- Heat and mass transfer
- Chemical reactions
- Detailed information for individual particles

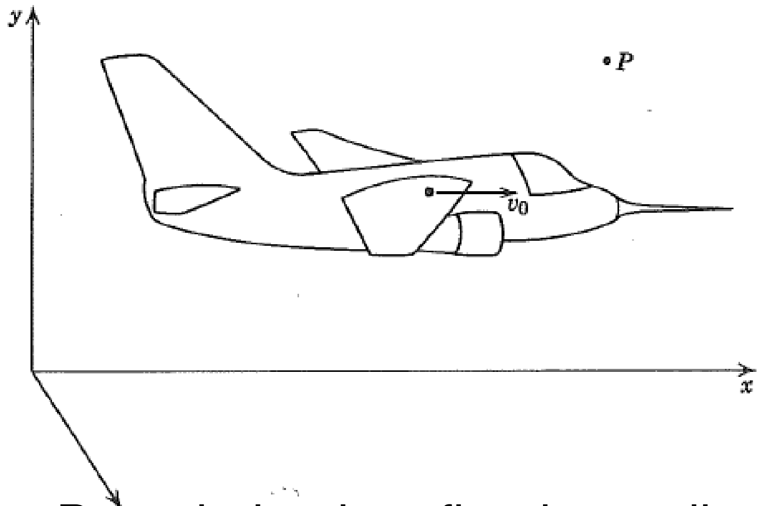
”Classical” applications

- Solid particle transport
  - Transport and/or deposition of a dilute suspension of inertial particles (e.g. aerosols/dust particles)
  - Solid fuel combustion
  - Fluidized beds (?)
- Sprays
  - Heat & mass transfer and/or chemical reactions in a spray
  - Spray dryers
  - Liquid fuel combustion
- Behavior of small bubbles

Eulerian-Lagrangian modelling

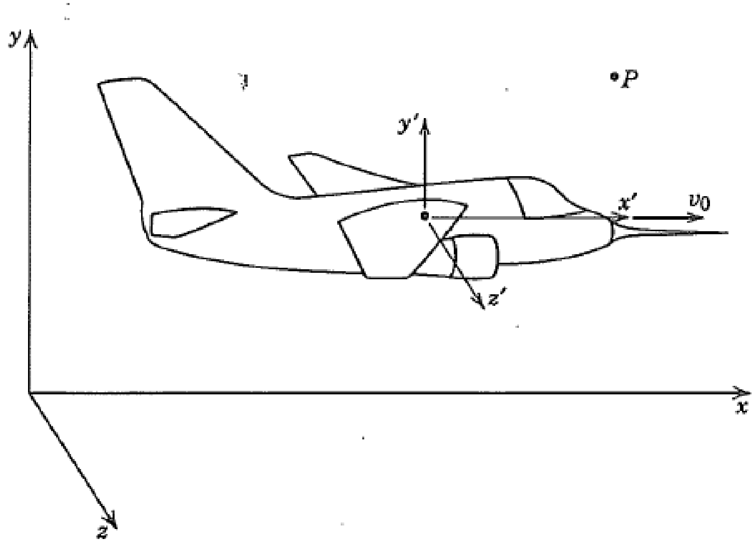


Eulerian reference frame



- Description in a fixed coordinate system
- For investigations in a certain point in space
- Dominates single-phase fluid dynamics (?)

Lagrangian reference frame



- Description that follows a system (i.e. fluid element or particle)
- Common for rigid body mechanics or for particles in a flow field

Eulerian reference frame

$$\boldsymbol{v}(\boldsymbol{x}, t)$$

$$p(\boldsymbol{x}, t)$$

- Velocity ***v*** and pressure *p at* location ***x*** and time *t*

Lagrangian reference frame

$$\boldsymbol{X}(\boldsymbol{a}, t)$$

- Position ***X*** of an element ***a*** at time *t*

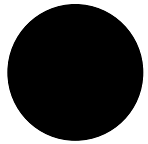
$$\boldsymbol{v}(\boldsymbol{X}(\boldsymbol{a}, t), t) = \frac{\partial \boldsymbol{X}}{\partial t}(\boldsymbol{a}, t)$$

Relation between the Eulerian and the Lagrangian descriptions

Newton's second law

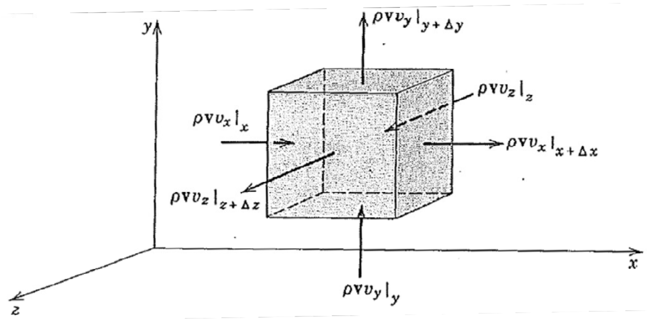
Newton's second law
for an isolated system

$$\sum \mathbf{F} = m\mathbf{a} = \frac{d}{dt}(m\mathbf{V})$$



Newton's second law
for a control volume

$$\sum \mathbf{F} = \frac{d}{dt}\left(\int_{CV} \mathbf{V}\rho d\mathcal{V}\right) + \int_{CS} \mathbf{V}\rho(\mathbf{V}\cdot\mathbf{n})\, dA$$



Differential form

$$-\nabla p + \nabla\cdot\boldsymbol{\tau} + \rho\mathbf{g} = \rho\frac{D\mathbf{V}}{Dt}$$

Lagrangian particle tracking

Fluid flow calculation in an Eulerian reference frame (e.g. using DNS, LES, RANS…)

(2) Changes to the continuous phase

(3) Additional processes

Calculation of particle motion in a Lagrangian reference frame (accounting for all relevant forces on the particles)

(1) Particle motion

Modelling of elementary processes like:
- turbulent dispersion
- particle-wall interactions
- particle-particle interactions

Fundamental principles

1. The state vector (location, velocity, acceleration,…) of each individual particle is computed
2. Study of particle interactions on a single particle level
3. Interactions between particles are typically treated on a particle-particle pair basis
4. Particles: real or stochastic

Why do we use LPT?

- The system is small (enough)
- A part of the system is representative for the entire system
- To study specific physical phenomena
- To obtain information for modelling of processes on a larger scale (i.e. to obtain closure laws)
- …

How many particles *at present*?

- Example: a vessel of 1m^3 with solid particles

d_p= 500 μm and volume fraction of ~ 50 %.

$$N_P \frac{1}{6} \pi \left(500 \cdot 10^{-6}\right) = 0.5 \Longrightarrow N_P \approx 1 \cdot 10^{10}$$

How many particles *in the foreseeable future*?

- Moore's law: computer power doubles every 18 months
- For efficient algorithms, the computers cost scales with *N log N*
- At present, one solves ~100 000 particles

$$N \log N = 5 \cdot 10^{5} \cdot 2^{\frac{y}{1.5}}$$

y	**N**
5	**850 000**
10	$\mathbf{5 \cdot 10^{6}}$
50	$\mathbf{3.6 \cdot 10^{13}}$

About particle-particle interactions

Why study individual particle-particle interactions?

When do we need to know details about particle-particle interactions?

What types of forces (effects) exist with particle-particle interactions?

Particle-particle interactions – **Why?**

- Particle properties often change due to interactions (attrition, agglomeration,…)
- Particle interactions affect the fluid particle contact (drag, coating, …)
- Particle interaction generally have a big effect on the rheology of the flow

Particle-particle interactions – **When?**

- In any multiphase flow application when the local volume fraction is over 1%
- When wall effects are of importance
- …

Particle-particle forces (effects) – **What?**

- Hydrodynamic forces
- Cohesive forces
- Friction between particles
- …

Coupling between the dispersed and the carrier phase

- **One way**
  - Particles do not affect the continuous phase
  - Particles do not “see” each other
  - Equations for the continuous phase solved first, particles are tracked afterwards

- **Two way**
  - Continuous phase affected by particles through momentum transfer and/or volume fraction
  - Particles do not “see” each other
  - Particles in the continuous phase as “point sources” (or DNS)

- **Four way**
  - Continuous phase affected by particles
  - Particle-particle interactions taken into account
  - Particles in the continuous phase as “point sources” (or DNS)

Modelling approaches

- Tracking particles as *point-sources*
- Tracking *computational parcels*
- Tracking *real particles*

Terminology

Computational parcel: A cloud consisting of a number of particles

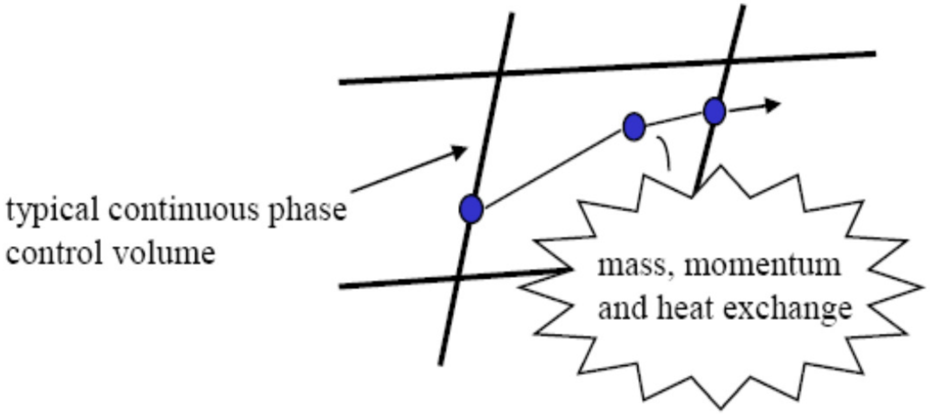
Particles as point-source(s): *particles have mass* ***but no*** *volume*

Real particles: *particles have mass* ***and*** *volume*

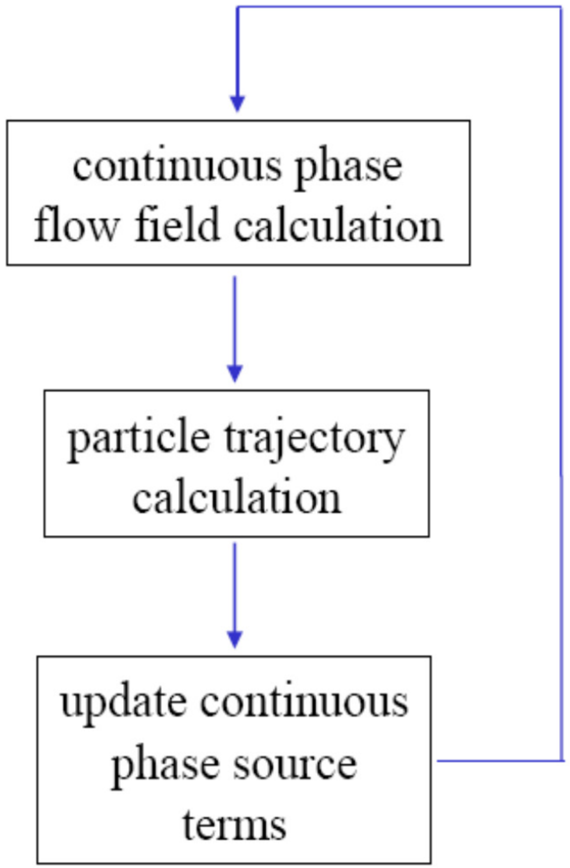
Tracking parcels

- Particles can exchange momentum, heat, mass with the carrier phases
- Volume fraction less than 10 % (no limitations in mass loading)
- No particle-particle interaction (?)
- Turbulent dispersion easily modelled
- Modelling of spray drying, combustion (liquid, coal), particle separation, boiling, …

Tracking parcels



General algorithm



Equations of motion for each individual *parcel*

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}_P$$

$$\frac{d\mathbf{u}_P}{dt} = \mathbf{g} - \frac{grad\ P_f}{\rho_{\mathrm{P}}} + \frac{\beta_P}{\rho_{\mathrm{P}}}\left(\mathbf{u}_f - \mathbf{u}_P\right) + \frac{1}{m_P}\mathbf{F}_{c,P}$$

$$I_P \frac{d\boldsymbol{\omega}_P}{dt} = \mathbf{T}_P$$

To be modelled ⇐ Net contact force due to collisions of parcel *p* with other parcels and walls

Alternatively:

Solids pressure

$$\frac{d\mathbf{u}_P}{dt} = \mathbf{g} - \frac{grad\ P_f}{\rho_{\mathrm{P}}} + \frac{\beta_P}{\rho_{\mathrm{P}}}\left(\mathbf{u}_f - \mathbf{u}_P\right) - \frac{grad\ P_s}{\rho_{\mathrm{P}}\alpha_P}$$

Normal stress acting on each parcel (with the purpose to avoid exceeding of maximum packing

$$P_s = \begin{cases} P^* f\left(\alpha_P, \alpha_{P,\max}\right) & \alpha_P < \alpha_{P,\max} \\ P_s^{old} & \alpha_P \geq \alpha_{P,\max} \end{cases}$$

Assumptions:

- All particles within a parcel have the same velocity as the parcel (thus: “particle” velocity and “parcel” velocity may be used interchangeably)

- Typically (but not always!), the **parcel density** is equal to the material density of an **individual particle** (no void within a computational parcel)

- Then, d_{eq} (equivalent parcel diameter):

$$d_{eq} = \left(6 n_{particle} V_{particle} / \pi\right)^{1/3} = n_{particle}^{1/3} d_{particle}$$

Mass of the parcel:

or particle

$$m_{parcel} = \rho_{parcel} d_{eq}^3 \pi / 6$$

Volume of the parcel:

$$V_{parcel} = n_{particle} V_{particle} = d_{eq}^3 \pi / 6$$

Source term - transfer of momentum between the continuous phase and each parcel

Volume of parcel

$$S_{parcel} = \frac{1}{V_{cell}} \int_{V_{cell}} \sum_{i=0}^{N_P} \frac{V_i \beta}{\alpha_p} \left(\mathbf{u_f} - \mathbf{u_P}\right) \delta\left(\mathrm{x} - \mathrm{x}_{\mathrm{P}}\right) dV$$

Interphase momentum exchange coefficient

Turbulent dispersion of parcels (particles): dispersion of particles due to turbulence of the carrier phase

Two things of fundamental importance

1) No dispersion by a mean field (flow)
2) Engineering CFD simulations result in mean fields

Discrete Random Walk model: stochastic tracking

Decomposition of velocity field

$$u_i = U_i + u_i^{'}$$

$$\tau_l = C_l \frac{k}{\varepsilon}$$

Life-time of an eddy

The fluctuating part is modelled:

$$u_i^{'} = \zeta \sqrt{\frac{2k}{3}}$$

Random number (with normal distribution)

Stochastic tracking – important to have in mind

- Can be used in complex geometries
- A large number of tries are required in order to achieve a statistically significant sampling
- Possible convergence problems
- Isotropy assumed

Tracking of *real (individual)* particles

The continuum-phase governing equations

stress tensor

$$\frac{\partial}{\partial t}\left(\underline{\alpha_f}\rho_f\right)+\nabla\cdot\left(\alpha_f\rho_f\,\mathbf{u_f}\right)=S_{mass}$$

$$\frac{\partial}{\partial t}\left(\alpha_f\rho_f\boldsymbol{u_f}\right)+\nabla\cdot\left(\alpha_f\rho_f\,\boldsymbol{u_f}\boldsymbol{u_f}\right)=-\alpha_f\nabla p_f-\nabla\cdot\left(\alpha_f\underline{\boldsymbol{\tau}_f}\right)-S_P+\alpha_f\rho_f\boldsymbol{g}$$

Instantaneous velocity field (?)

Source term – coupling between the phases

Source term - transfer of momentum between the continuous phase and each individual particle

Volume of particle

$$S_P = \frac{1}{V_{cell}} \int_{V_{cell}} \sum_{i=0}^{N_P} \frac{V_i \beta}{\alpha_p} \left(\boldsymbol{u}_f - \boldsymbol{u}_P \right) \delta \left(x - x_P \right) dV$$

Coupling of the phases:

- volume fraction
- inter-phase momentum exchange

- **Modelling of drag force –** more info and some recapitulation

1. Drag force in an infinite fluid
2. Drag force averaged in a cell containing one particle
3. Drag force averaged in a cell with many particles

Drag force – a single particle

$$F_D = C_D \frac{d_P^2 \pi}{4} \frac{\rho_f v_{rel}^2}{2}$$

Drag force – presence of other particles

$$F_D = C_D \frac{d_P^2 \pi}{4} \frac{\rho_f v_{rel}^2}{2} f(\alpha)$$

Drag force – examples of correlations

$$F_{Ergun} = \beta \frac{d_P^2}{\mu} = 150 \frac{\alpha_p^2}{\alpha_f} + 1.75\, \alpha_p Re$$

$$F_{WenYu} = \beta \frac{d_P^2}{\mu} = \frac{3}{4} C_D\; Re\, \alpha_p \alpha_f^{-2.65}$$

from pressure drop measurements in fixed or settling beds

$$F_{KochHill} = \beta \frac{d_P^2}{\mu} = A \frac{\alpha_p^2}{\alpha_g} + B\, \alpha_p Re$$

from lattice-Boltzmann simulations

$$A = \begin{cases} 180 \\ \dfrac{18\alpha_f^3}{\alpha_p} \dfrac{1 + \frac{3}{\sqrt{2}}\sqrt{\alpha_p} + \frac{135}{64}\alpha_p \ln \alpha_p + 16.1\, \alpha_p}{1 + 0.681\, \alpha_p - 8.48\, \alpha_p{}^2 + 8.16\, \alpha_p{}^3} \end{cases}$$

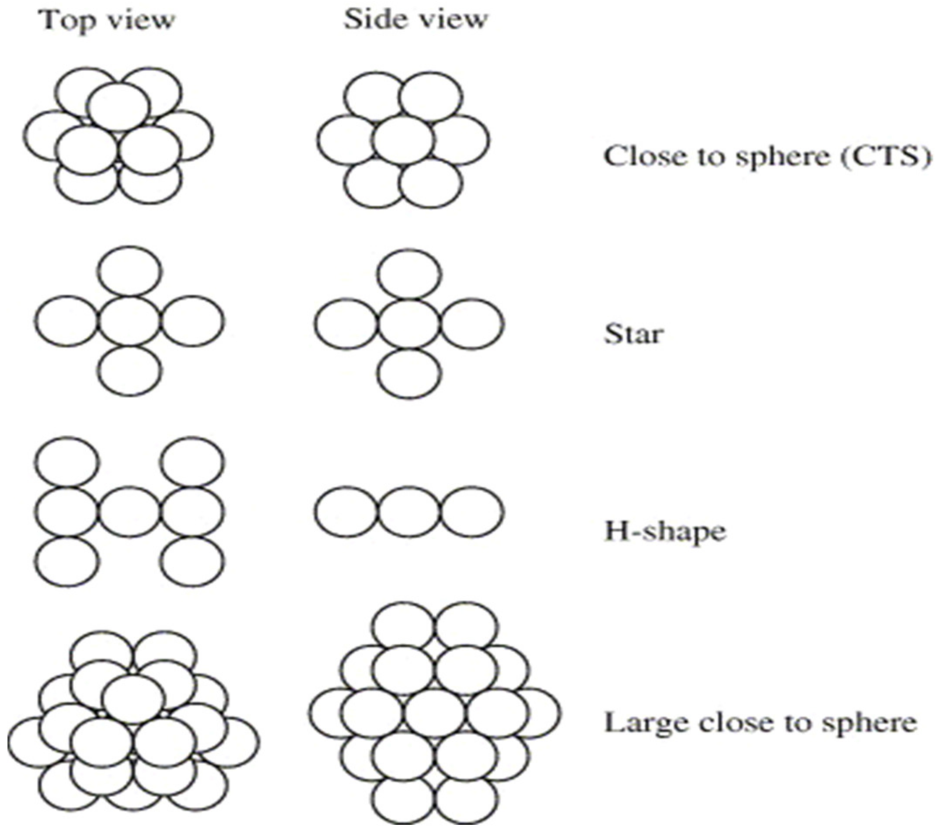
$$B = 0.6057\, \alpha_f^2 + 1.908\, \alpha_p\, \alpha_f^2 + \\ + 0.209\, \alpha_f^3$$

dense flows

Drag force – irregularly shaped particles

$$C_D = \frac{24}{Re}\frac{d_A}{d_n}\left[1+\frac{0.15}{\sqrt{c}}\left(\frac{d_A}{d_n}Re\right)^{0.687}\right]+$$

$$+\frac{0.42\left(\dfrac{d_A}{d_n}\right)^2}{\sqrt{c}\left[1+4.2\times10^4\left(\left(\dfrac{d_A}{d_n}\right)Re\right)^{-1.16}\right]}$$



Drag force – effect of polydispersity (a possible solution

$$F_i = F\left(\alpha_f, \langle Re \rangle\right)\left(\alpha_f \; p_i + \left(1 - \alpha_f\right) p_i^2\right)$$

$$F_i = F\left(\alpha_f, \langle Re \rangle\right)\left(\alpha_f \; p_i + \left(1 - \alpha_f\right) p_i^2 + 0.06\, \alpha_f \; p_i^3\right)$$

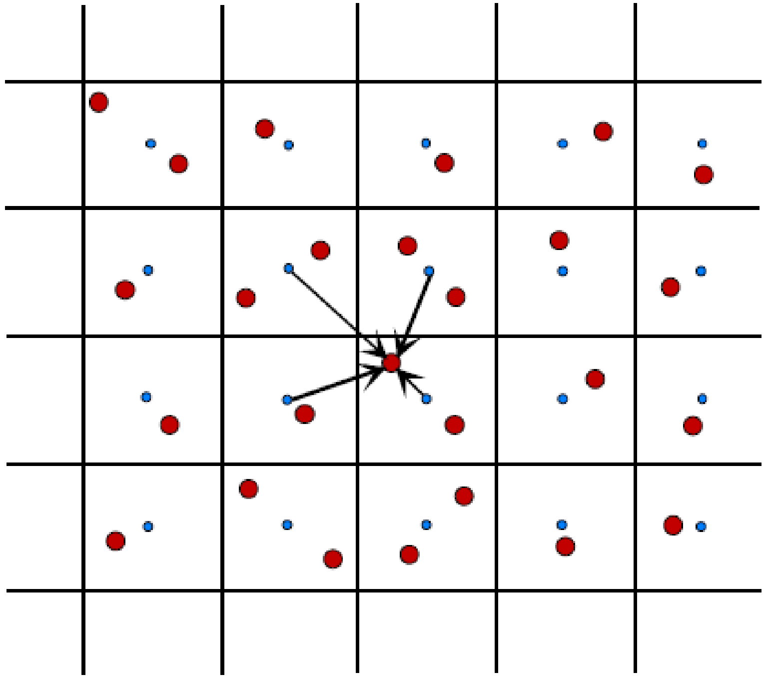
mass fraction of species *i* $\quad \chi_i = \dfrac{N_i \, d_i^3}{\sum\limits_{\mathrm{i}} N_i \, d_i^3} \qquad p_i = \dfrac{d_i}{\langle d \rangle}$

average diameter $\quad \dfrac{1}{\langle d \rangle} = \sum\limits_i \dfrac{\chi_i}{d_i} \qquad \langle Re \rangle = \dfrac{\rho_f \, U \, \langle d \rangle}{\mu_f}$

Particle-particle interaction

Why are collisions important?

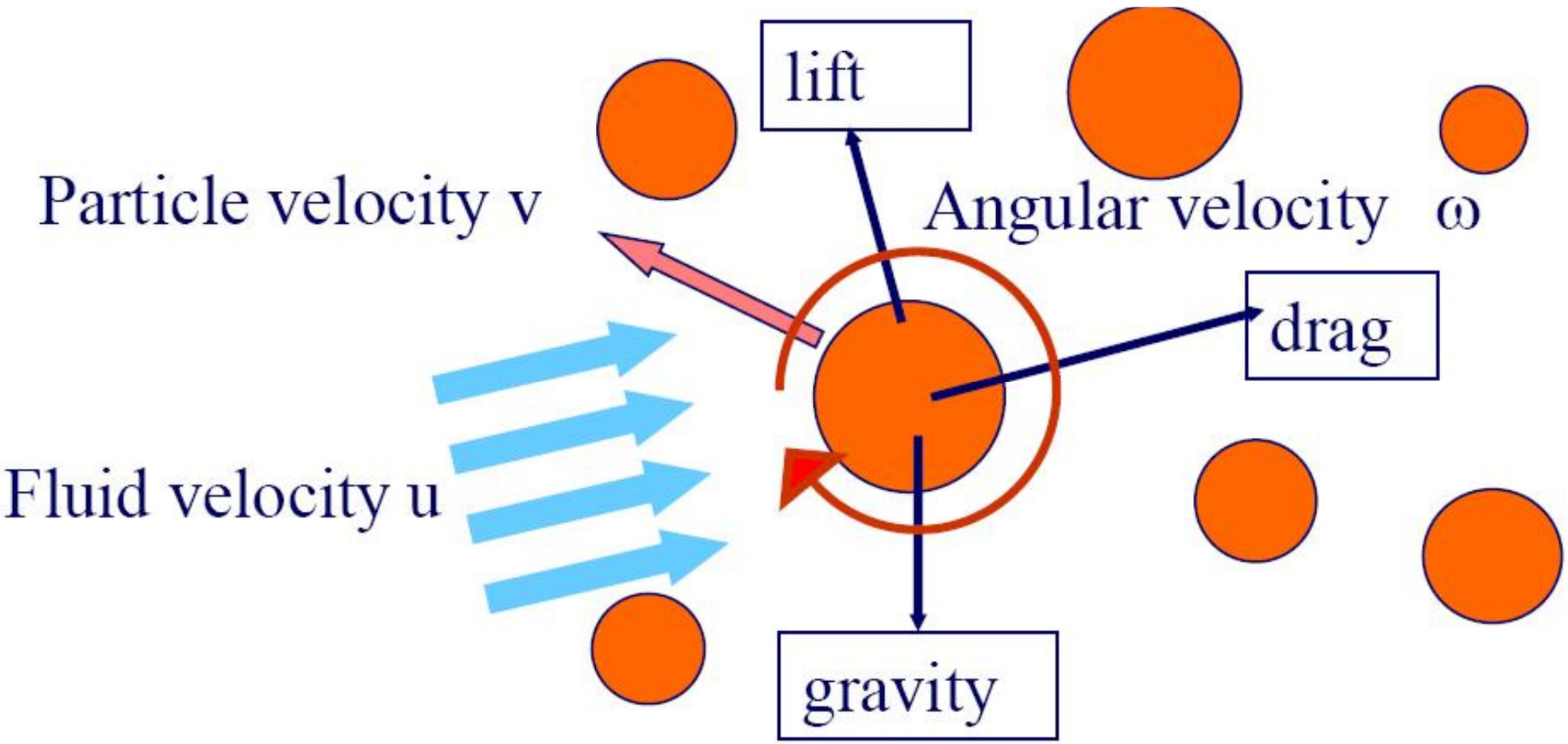
- what about maximum packing of particles in a cell?



Particle-particle interaction

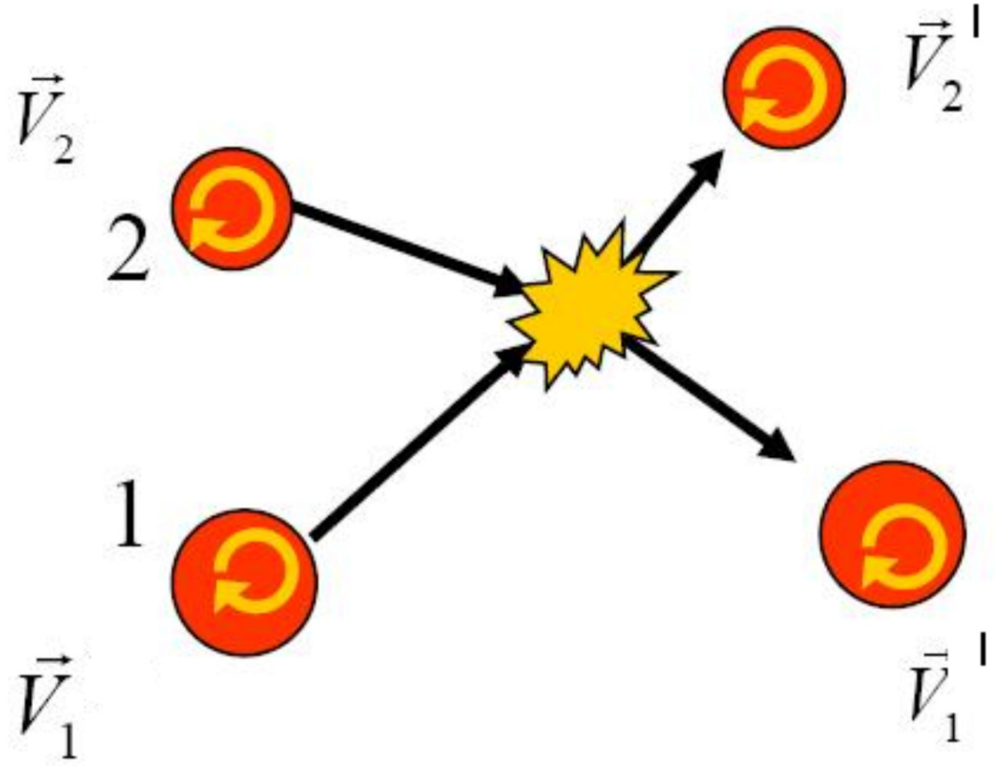
- **Hard sphere** approach (**collision-dominated** flows)
- **Soft sphere** approach (**contact- dominated** flows)

Collision **dominated** flows – forces on particles



Hard-sphere approach – main concept

before collision after collision



First solve the equation of motion between collisions

trajectory $\mathbf{x}_i(t) = \mathbf{x}_i(0) + \mathbf{v}_i(0)t + \frac{1}{2}\mathbf{g}t^2$

contact $\|\Delta\mathbf{x}_{ij}\| = \|\mathbf{x}_i(t) - \mathbf{x}_j(t)\| = r_1 + r_2$

$$\left(\Delta\mathbf{x}_{ij}(0) + \Delta\mathbf{v}_{ij}(0)t\right)^2 = (r_1 + r_2)^2$$

$$\underbrace{\Delta\mathbf{x}_{ij}^{\ 2} - (r_1 + r_2)^2}_{c} + \underbrace{\Delta\mathbf{x}_{ij} \cdot \Delta\mathbf{v}_{ij}}_{b}\, t + \underbrace{\Delta\mathbf{v}_{ij}^{\ 2}}_{a}\, t^2 = 0$$

event-time

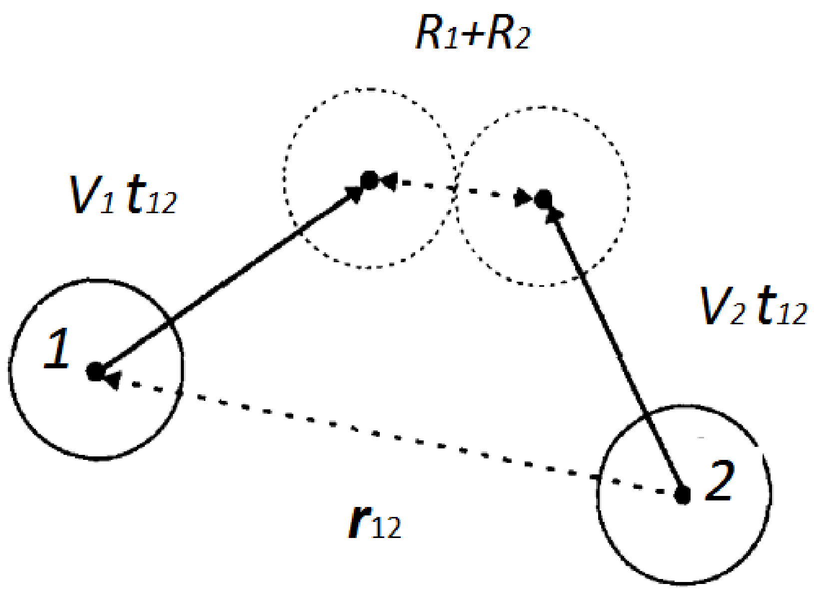
$$t_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Hard-sphere approach - general picture

Collision time (see the previous slide)

$$t_{coll} = \frac{-\mathrm{r}_{12} \cdot \mathrm{v}_{12} + \sqrt{(\mathrm{r}_{12} \cdot \mathrm{v}_{12})^2 - \mathrm{v}_{12}{}^2 \left[-r_{12}{}^2 - (R_1 + R_2)^2 \right]}}{\mathrm{v}_{12}{}^2}$$

v



Hard-sphere approach – determination of relevant parameters

- Velocities before and after collision

$$m_1\left(v_1^{'}-v_1\right)=-m_2\left(v_2^{'}-v_2\right)=J$$

J: *impulse*

$$\frac{I_1}{R_1}\left(\omega_1^{'}-\omega_1\right)=-\frac{I_2}{R_2}\left(\omega_2^{'}-\omega_2\right)=-n\times J$$

- Relative velocity at the point of contact

$$v_{12}=\left(v_1-v_2\right)-\left(R_1\omega_1+R_2\omega_2\right)\times n$$

Hard-sphere approach – determination of relevant parameters

Normal coefficient of restitution (**incomplete** restitution of the normal component of $\boldsymbol{v_{12}}$)

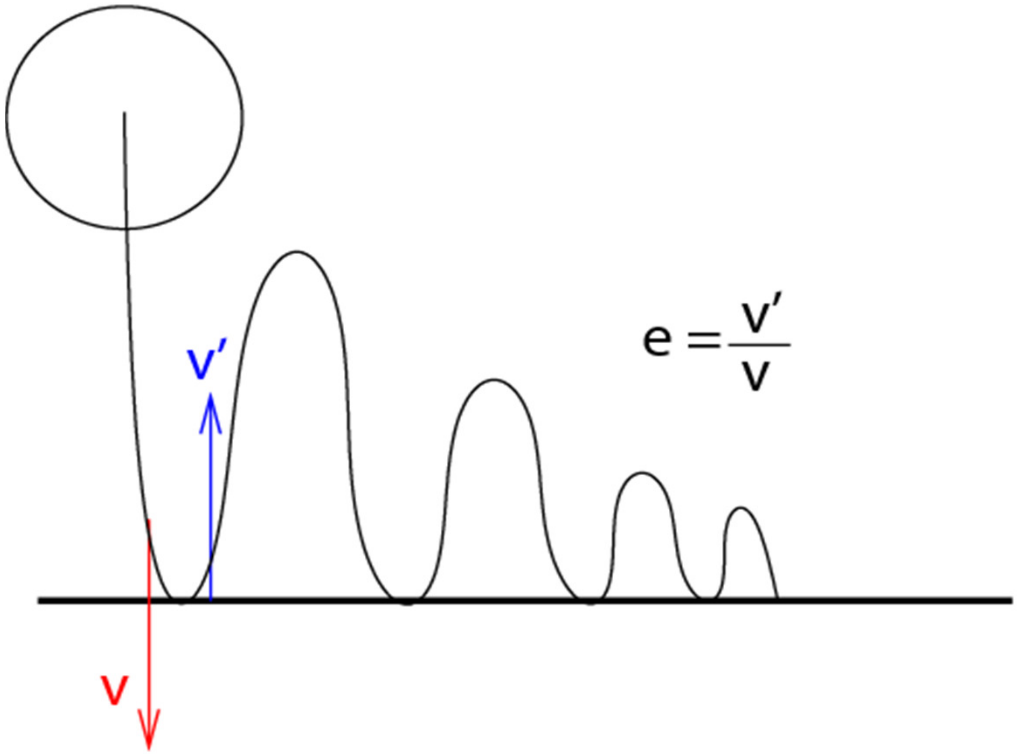
$$\boldsymbol{n} \cdot \boldsymbol{v}'_{12} = -e\, \boldsymbol{n} \cdot \boldsymbol{v}_{12}$$

Tangential coefficient of restitution (**incomplete** restitution of the tangential component of $\boldsymbol{v_{12}}$)

$$\boldsymbol{n} \times \boldsymbol{v}'_{12} = -\zeta\, \boldsymbol{n} \times \boldsymbol{v}_{12}$$

Hard-sphere approach – determination of relevant parameters

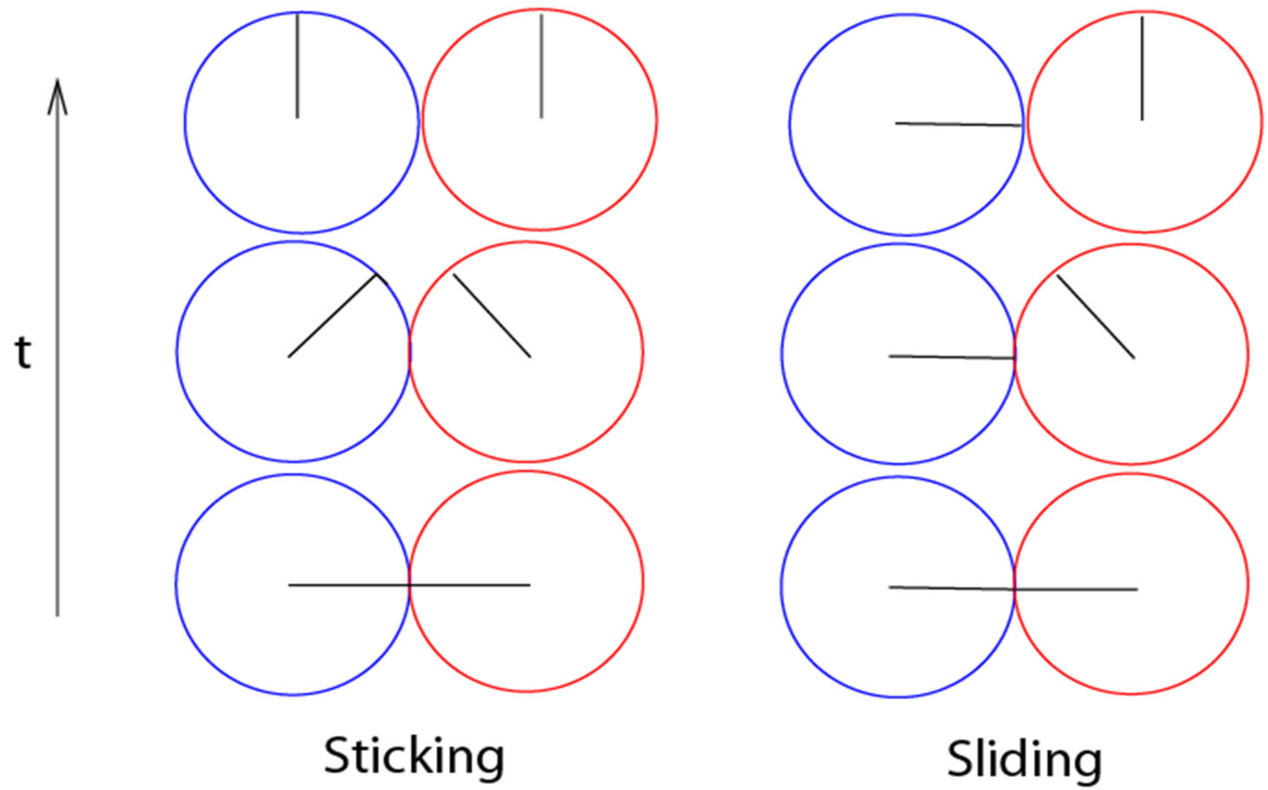
Coefficient of **normal restitution**



$$e = \frac{v'}{v}$$

Hard-sphere approach – determination of relevant parameters

Sticking or sliding



Sliding

Sliding resisted by Coulomb friction μ

Relation between the normal and the tangential components of the impulse

$$\left| n \times J \right| = \mu \left(n \cdot J \right)$$

Expression for impulse

$$J^{(1)} = \frac{(1+e)(v_{12} \cdot n)n + \mu(1+e)\cot\chi \left[v_{12} - n(v_{12} \cdot n) \right]}{\left(\frac{1}{m_1} + \frac{1}{m_2} \right)}$$

Sticking

Restitution in the tangential direction

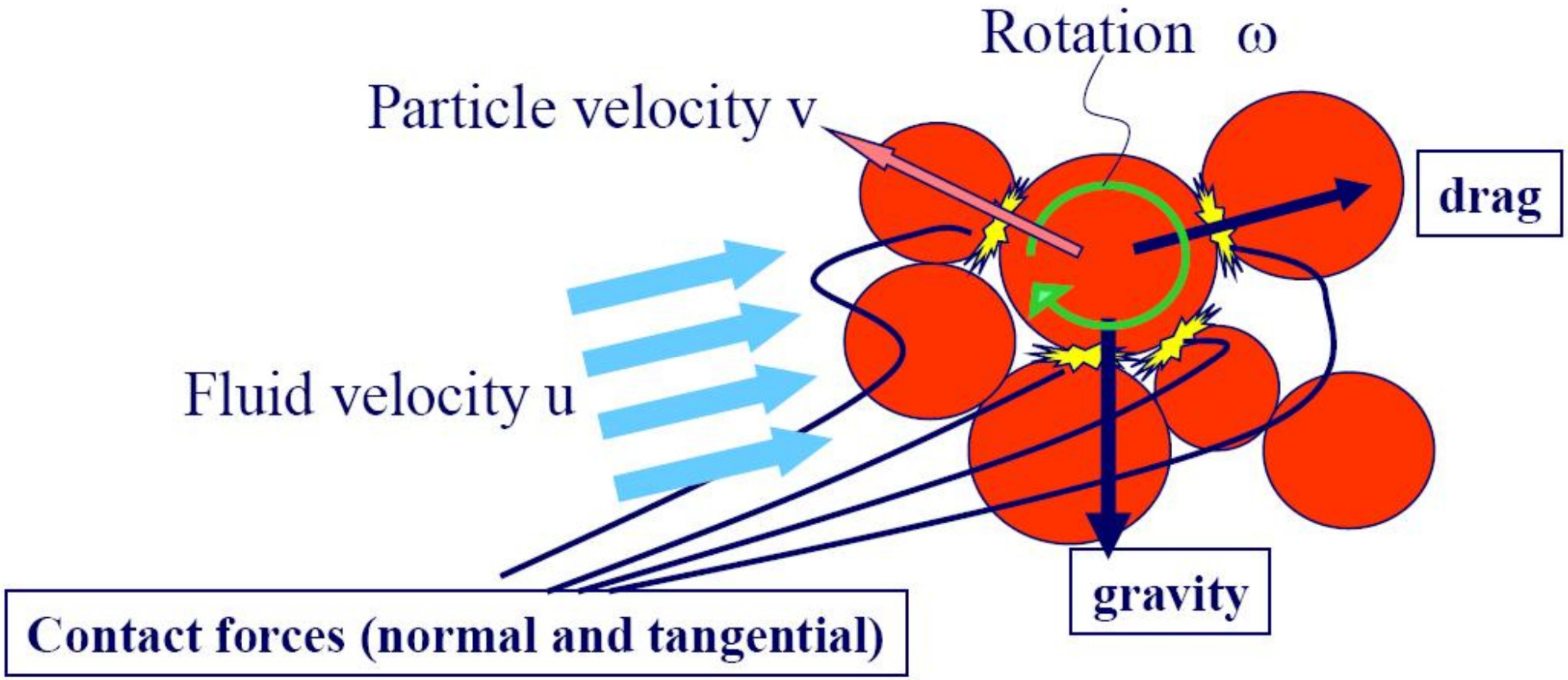
$$\boldsymbol{n} \times \boldsymbol{v}'_{12} = -\zeta\, \boldsymbol{n} \times \boldsymbol{v}_{12}$$

Expression for impulse

$$J^{(2)} = \frac{(1+e)(v_{12} \cdot n)n + \frac{2}{7}(1+\zeta)[v_{12} - n(v_{12} \cdot n)]}{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$$

Soft-sphere approach - general picture

contact dominated flows – forces on particles



Soft-sphere approach - general picture

Mechanisms for dissipation

- ✓ Plastic deformation (parameters – strength of the sphere(s), Young’s modulus of elasticity, Poisson’s ratio)
- ✓ Viscoelasticity of the material
- ✓ Elastic waves (excited by the impact)
- ✓ …

Soft-sphere approach - general algorithm

- ✓ A fixed time step is determined (**step 1**)

- ✓ Update particle locations with fixed time step (**step 2**)

- ✓ Overlap and relevant forces are determined (**step 3**)

- ✓ Back to step 2 (**step 4**)

Soft-sphere approach – Steps 1 and 2

Step 1 <u>Choosing</u> the time step

Caution: Time step *p – p* interaction must allow for a contact to last a number of time steps, but also to prevent an overlap to become too large

Step 2 (the updating step)

$$r_1(t+\Delta t) = r_1(t) + v_1(t)\,\Delta t + \frac{1}{2}a_1(t)\,\Delta t^2$$

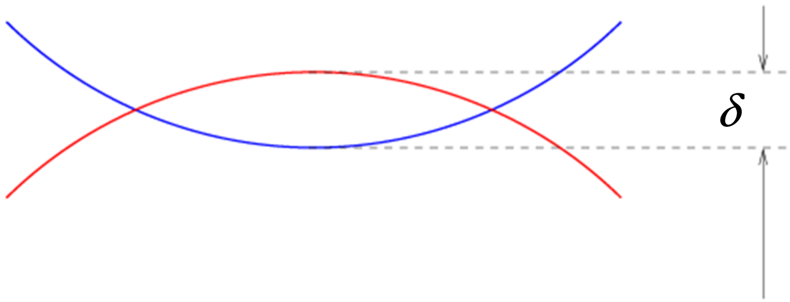
From collisional model

$$a_1(t) = g + \frac{F_D}{m_1} + \frac{F_O}{m_1}$$

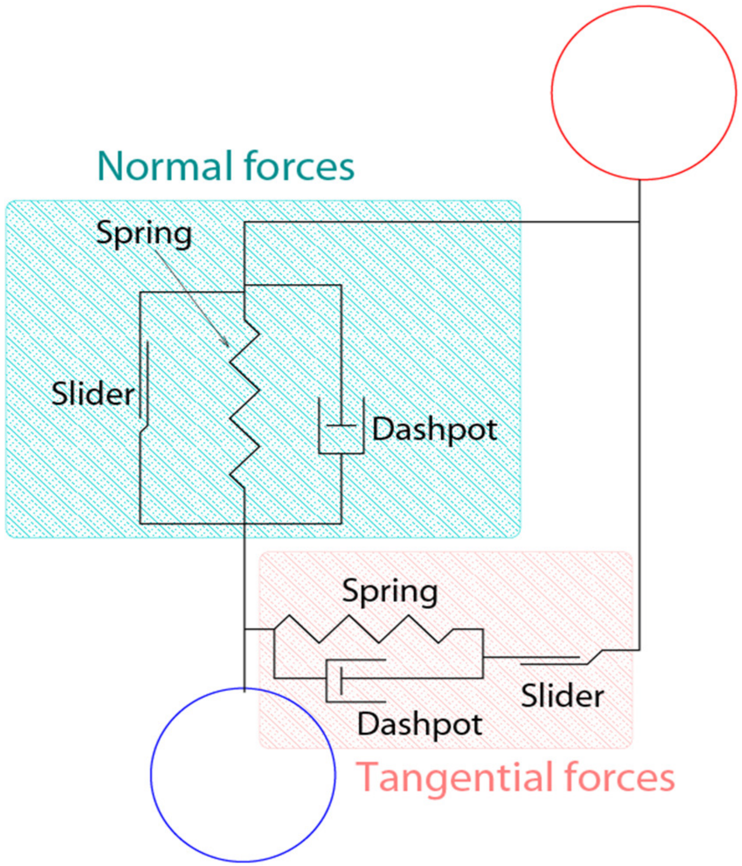
Step 3 - overlap

Overlap: local deformation of a particle

A maximum overlap has to be defined



Step 3 - models



Step 3 - models

Two main effects are to be considered: repulsion and dissipation (η)

1. Damped harmonic oscillator

$$F_n = -k_n \delta - \eta \dot{\delta}$$

Collision time

$$t_{coll} = \pi \left(\frac{k_n}{m_{eff}} - \left(\frac{\eta}{2m_{eff}} \right)^2 \right)^{-\frac{1}{2}}$$

Max overlap

$$\delta_{\max} \leq \frac{v_i \, t_{coll}}{\pi}$$

2. Hertz theory of elastic contact (without or with dissipation)

$$F_n = -\bar{k}_n \delta^{3/2} - \eta \dot{\delta}$$

$$t_{coll} = 3.21 \left(\frac{m_{eff}}{\bar{k}_n} \right)^{\frac{2}{5}} v_i^{\frac{1}{5}}$$

Relative velocity between the particles

Sliding or sticking?

$$|F_t| > f|F_n| \begin{cases} yes \rightarrow sliding & F_t = -f|F_n|\dfrac{v_{12}}{|v_{12}|} \\ no \rightarrow sticking & F_t = -k_t\delta_t - \eta_t v_{12t} \end{cases}$$

Collision models - summary

- **Hard sphere**

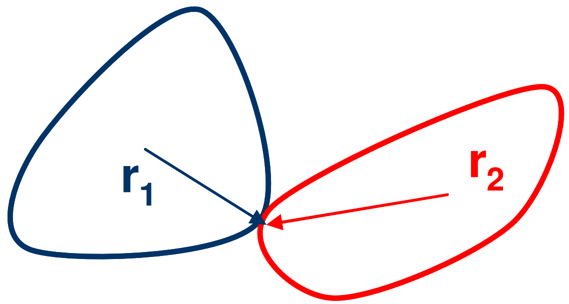
i. Physics up to a great deal straightforward and sound
ii. For dilute flows
iii. Problems when simulating more dense flows

- **Soft sphere**

i. Mostly for dense particulate flows
ii. Physics are less straightforward
iii. A very small time step is needed

Non-spherical particles

i. Arbitrary shapes, approximations needed (polynomial bodies, gluing small spherical particles together…)
ii. Stochastic models



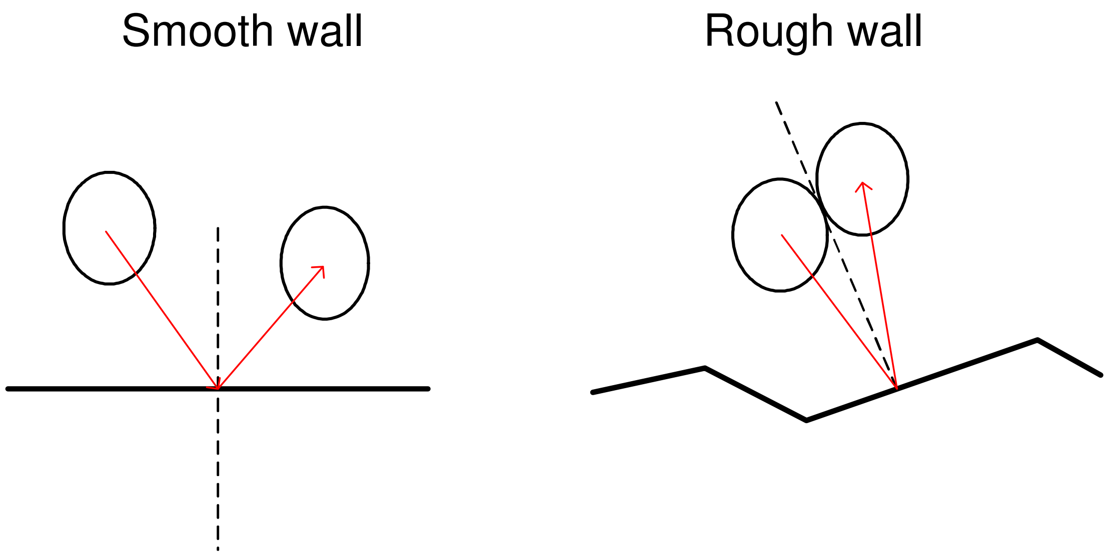
Other issues of relevance - Walls

i. Walls as chains of fixed particles
ii. Walls as particles with zero diameter, zero velocity, zero rotational velocity and infinite mass
iii. Walls with different coefficients o restitution and friction
iv. Walls as rough and smooth surfaces

Other issues of relevance - Walls

✓ No difficulties in treating rough walls

✓ Rough walls are modelled by adding random components to the normal. The size of the components depends on the roughness of the wall



Heat and mass transfer (only basic remarks)

Heat and mass transfer

- Each particle is assigned **a single** temperature and **a single** mass fraction of each species

→ Approach only valid if the thermal and mass transfer Biot numbers are small!

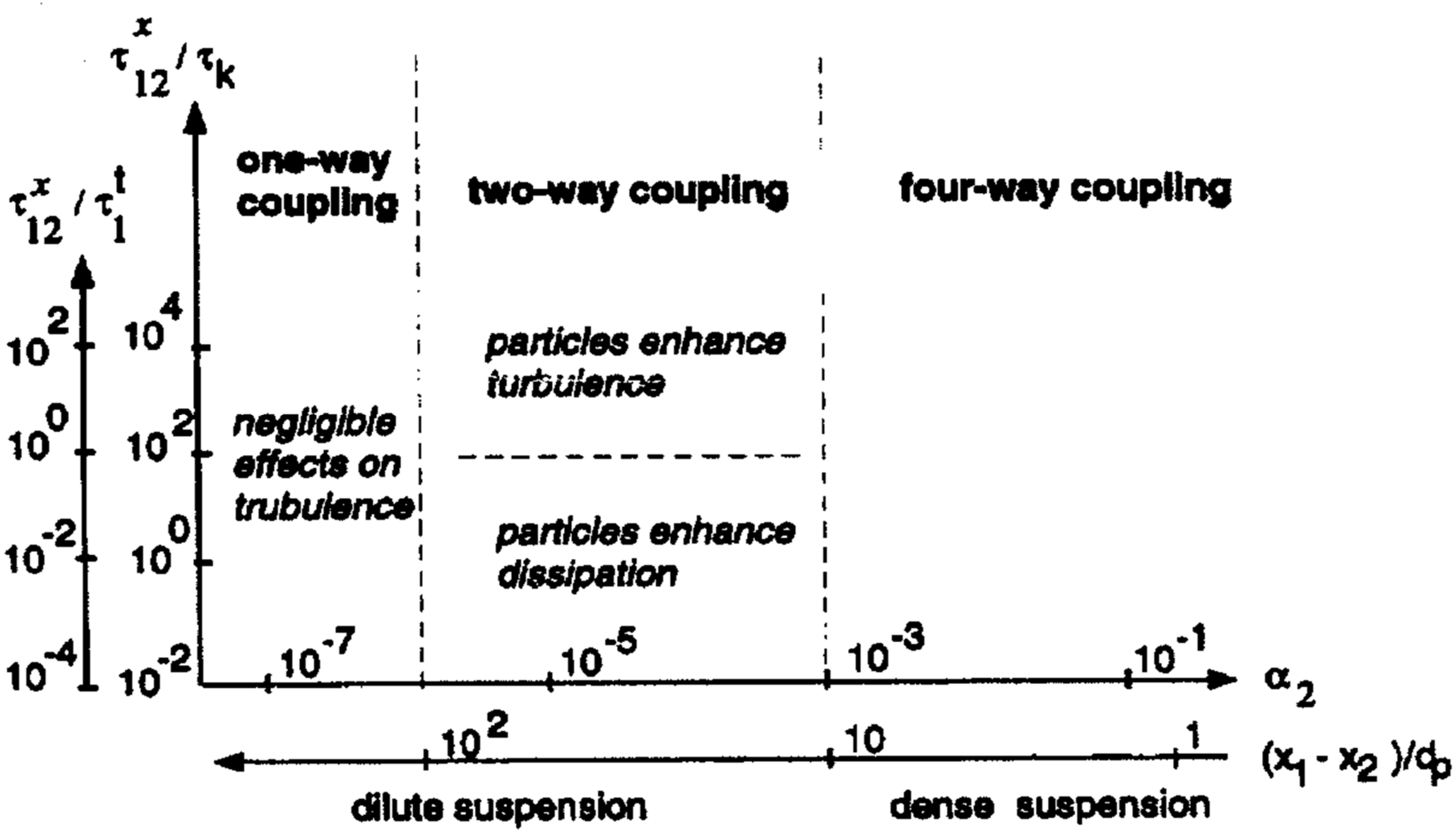
$$\mathrm{Bi} = \frac{hL_C}{k_b}$$

h - convective heat transfer coefficient

k - conductive heat transfer coefficient

Coupling between the phases

Elgobashi (1983)



Status of LPT model development

Status of model development	mainly solved	should be improved	open issues
Particle transport/dispersion by turbulence			
Non-spherical particle transport ⇨ forces			
Droplet/bubble deformation ⇨ trajectory			
Droplet and bubble break-up ⇨ fragments			
Particle-wall collisions with roughness			
Droplet and bubble wall collisions			
Inter-particle collisions (restitution, friction)			
Collisions of non-spherical particles			
Agglomeration of particles (structure model)			
Coalescence of droplets and bubbles			
Bubble-particle interactions (three-phase)			

Summary - LPT

- Pros:
  - Theoretically ”straightforward”
  - Very versatile and flexible
  - Well suited for polydisperse systems
  - Mathematically robust and relatively efficient
  - Easy to implement
- Cons:
  - Combination of several models masks theoretical inconsistencies
  - Quality and efficiency may be dubious for dense systems

Best practice guidelines (1/2)

1. Establish a good starting point by identifying a representative single-phase setup

2. Determine size distribution, physical properties and volume fraction(s) of interest

3. Establish which forces are important

Best practice guidelines (2/2)

4. Turbulence-particle interactions are size-dependent – make sure not to overlook effects of polydispersity.
5. Perform validation simulations for a similar system to establish the degree of accuracy that you may expect
6. Do not forget that many sub-models (e.g. bubble/droplet breakup & collisions) are not yet accurate enough for general use