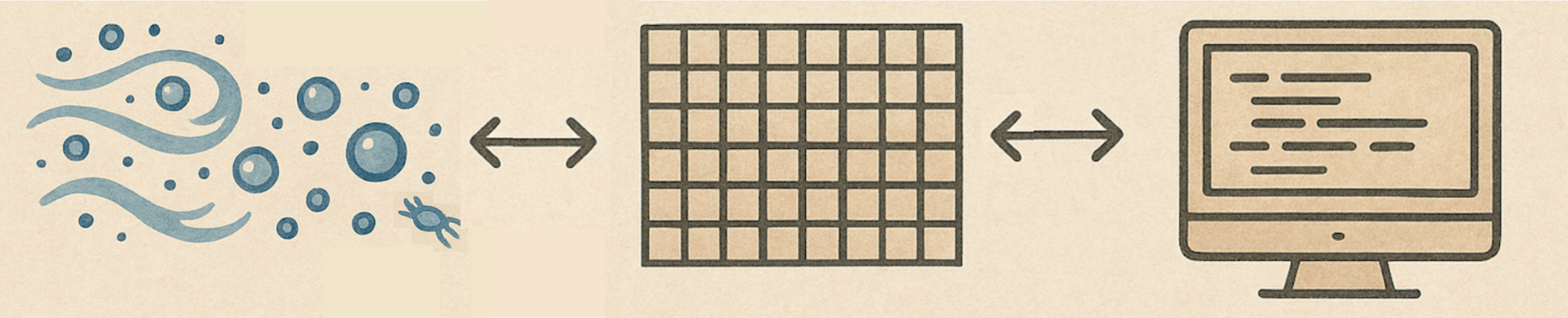

What simulations reveal about particle dynamics in turbulent flows

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CoPartCoFlow

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Outline

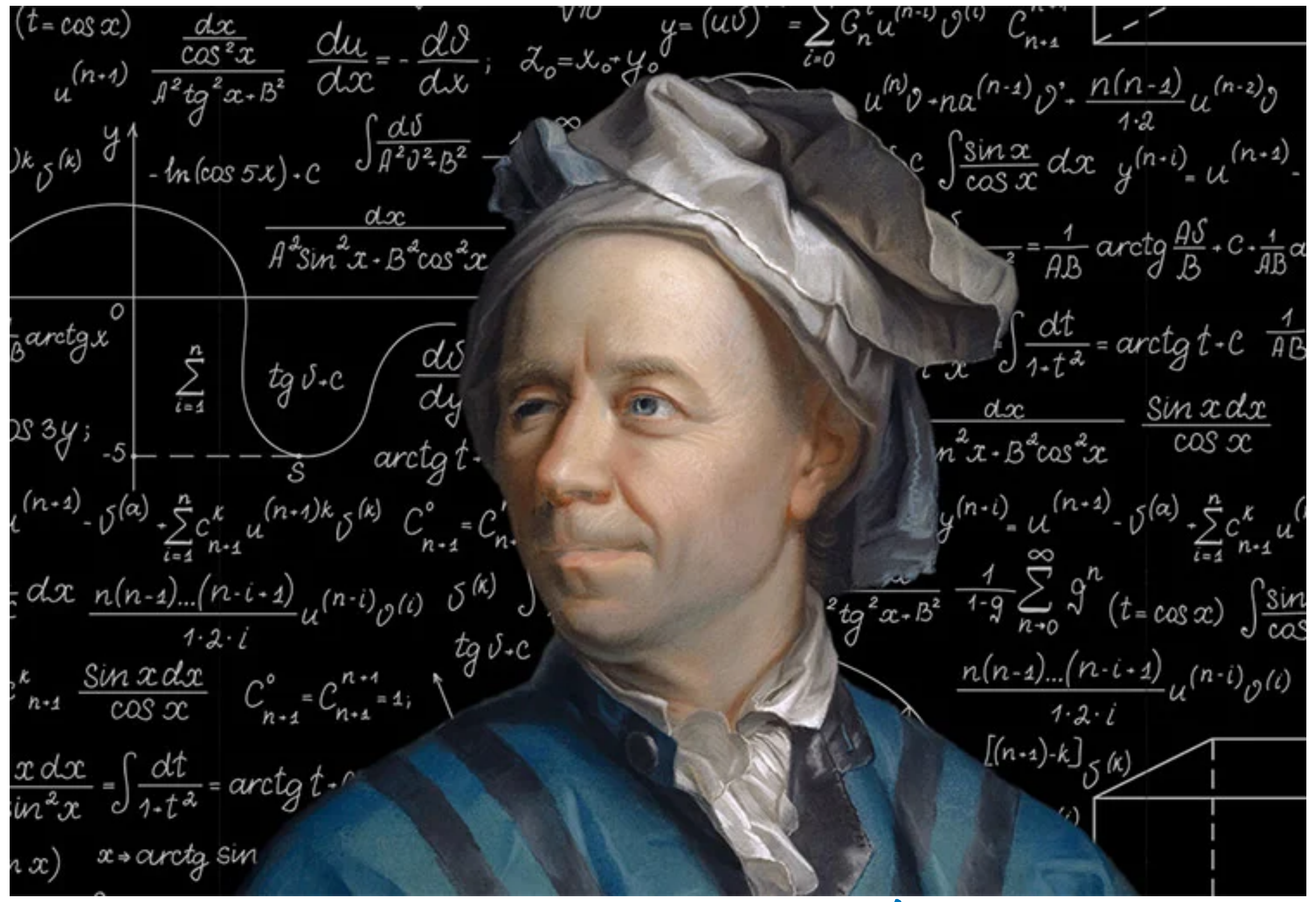
1. **Models** of material particles transported by a fluid
2. **Methods** for simulating the particle motion in a fluid
3. **Hands on:** CFD of particle centrifugation by vortices

Part 1

Models

How to describe the motion of a fluid

Two point of views



Euler

a.k.a. spatial or field description

$\mathbf{u}(\mathbf{x}, t) \qquad \rho(\mathbf{x}, t)$

Reynolds transport th. — Gauss th.

$$\frac{d}{dt}m = 0 \Rightarrow \frac{d}{dt}\int_{V(t)} \rho(\mathbf{x}, t)\ dV = 0 \Rightarrow \int_{V(t)} \partial_t \rho(\mathbf{x}, t)\ dV + \int_{S(t)} \rho\ \hat{\mathbf{n}} \cdot \mathbf{u}\ dS = 0 \Rightarrow \int_V \partial_t \rho + \nabla \cdot (\rho \mathbf{u})\ \ dV = 0$$

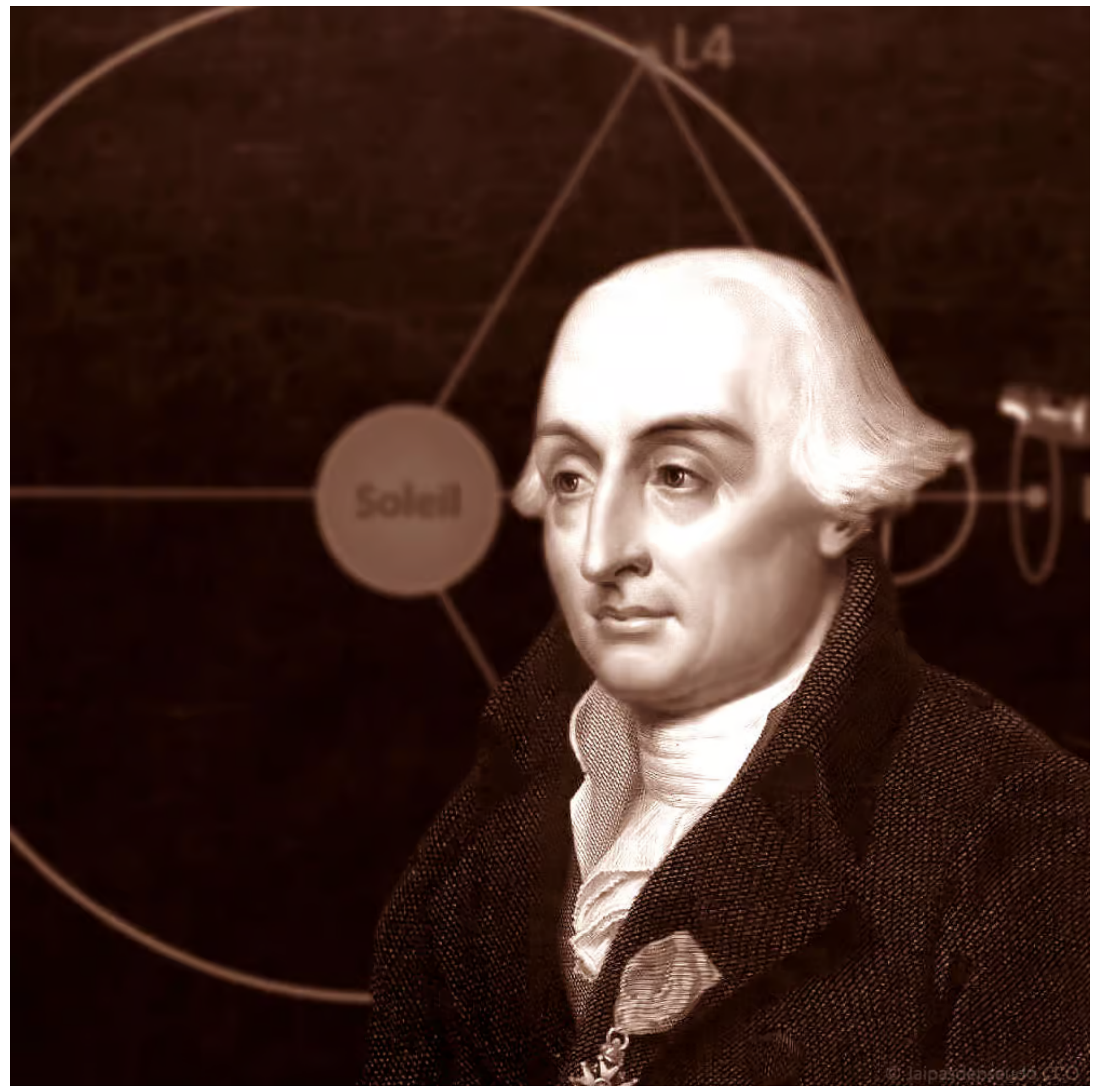
if $\rho = const. \Rightarrow$ $\boxed{\nabla \cdot \mathbf{u} = 0}$

$$\frac{d}{dt}(m\mathbf{U}) = \mathbf{F} \Rightarrow \int_V \rho\ \mathbf{a}\ dV = \int_V \nabla \cdot \sigma + \rho\ \mathbf{g}\ \ dV = 0 \Rightarrow \mathbf{a}(\mathbf{x}, t) = -\frac{\nabla p}{\rho_f} + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$

$$\boldsymbol{\sigma} = -\rho_f p \mathcal{I} + \mu_f (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\boxed{D_t \mathbf{u} = \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}}$$

How to describe the motion of a fluid



Two point of views

Lagrange

aka material or particle description

$$\mathbf{x}_f(t; \mathbf{x}_0, t_0)$$

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}(t), t)$$

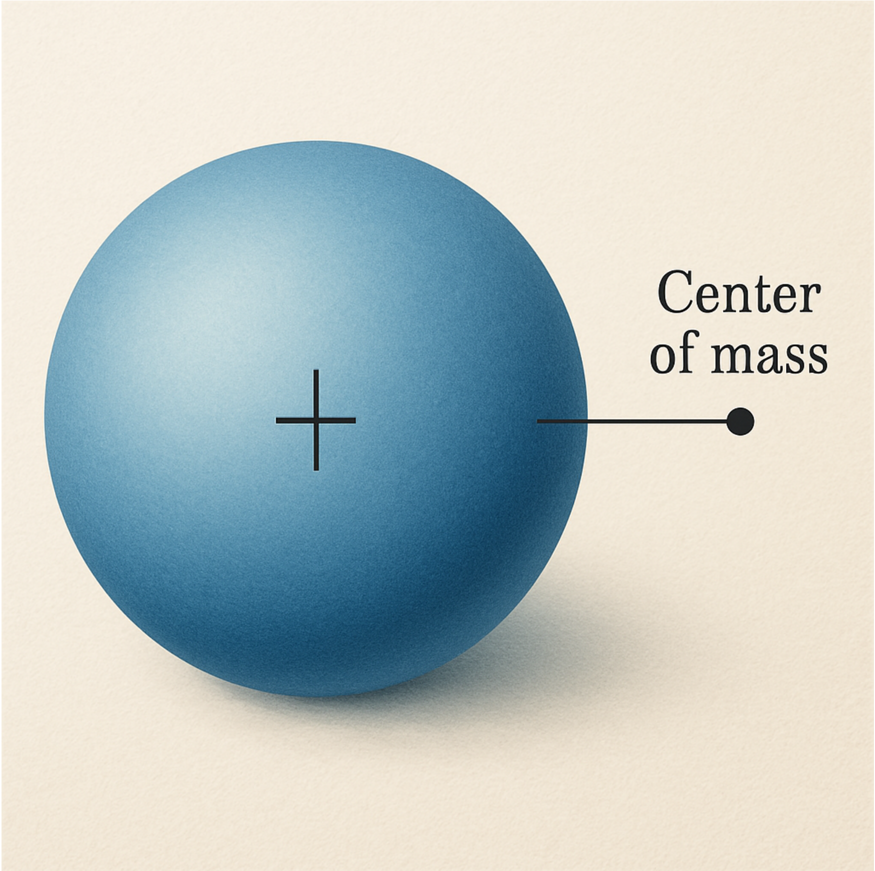
$\frac{d}{dt} m = 0$ ⇒ $N_p = const.$ and trajectories do not cross

$\frac{d}{dt}(m\mathbf{U}) = \mathbf{F}$ ⇒ $\ddot{\mathbf{x}} = D_t \mathbf{u}(\mathbf{x}(t))$

A particle does not go with the flow

$$\dot{\mathbf{x}}_p = \mathbf{v}(t) \neq \mathbf{u}(\mathbf{t})$$

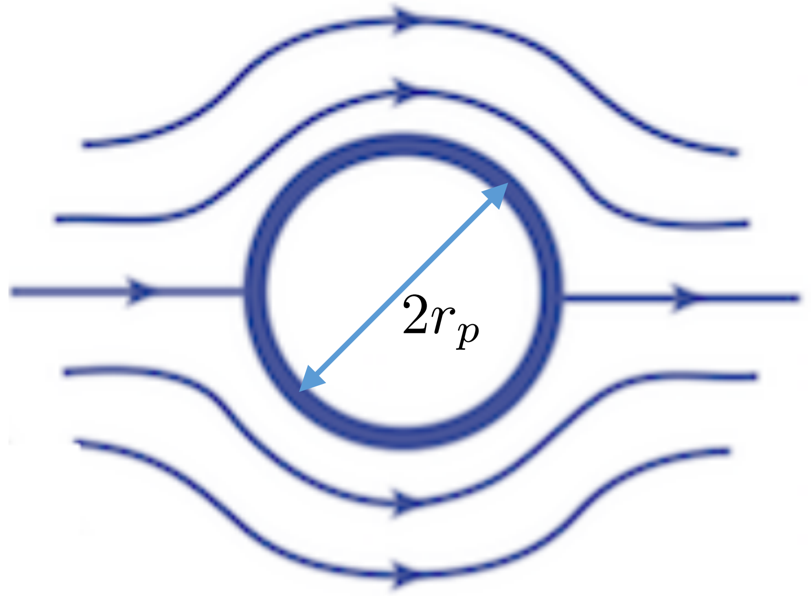
$$\ddot{\mathbf{x}}_p = \dot{\mathbf{v}} = \mathbf{f}_h(t)$$



$$\frac{d\mathbf{x_p}}{dt} = \mathbf{v}(t)$$

$$m_p \frac{d\mathbf{v}}{dt} = 6\pi\mu r_p(\mathbf{u} - \mathbf{v})$$

drag



$$Re_p = \frac{||\mathbf{u} - \mathbf{v}||(2r_p)}{\nu} \ll 1$$

Stokes (1851)

Used by Einstein (1905) in his famous article on Brownian motion

Hydrodynamic forces on a particle

Small inertial particles, *an equation with many authors and many names*

Stokes (1851)

Boussinesq (1885), Basset (1888), Oseen (1927) -> BBO eq.

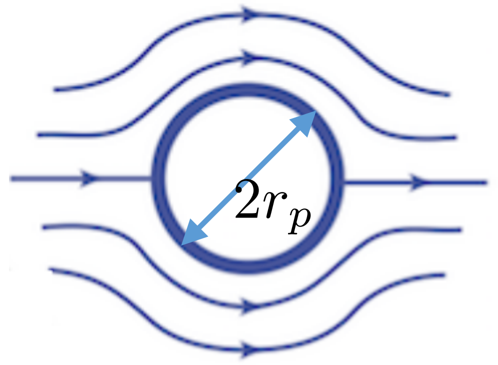
Tchen (1947), Corrsin-Lumley(1956)

Maxey-Riley (1983), Gatignol (1983) -> MRG eq. *extension to non-uniform creeping flows*

$$\frac{d\mathbf{x_p}}{dt} = \mathbf{v}(t)$$

$$m_p \frac{d\mathbf{v}}{dt} = 6\pi\mu r_p(\mathbf{u}-\mathbf{v}) + m_f \frac{D\mathbf{u}}{Dt} + \frac{m_f}{2}\frac{d(\mathbf{u}-\mathbf{v})}{dt} + 6r_p^2\sqrt{\pi\rho_f\mu}\int_0^t \frac{d(\mathbf{u}-\mathbf{v})}{d\tau}\frac{d\tau}{\sqrt{t-\tau}} + (m_p - m_f)\mathbf{g}$$

drag | fluid acceleration | added mass | history | buoyancy



$$Re_p = \frac{||\mathbf{u}-\mathbf{v}||(2r_p)}{\nu} \ll 1$$

$$Re_s = \frac{||\nabla\mathbf{u}||(2r_p)^2}{\nu} \ll 1$$

Small particles

Can we describe a particle with a field? Overdamped limit or equilibrium Eulerian approach

$$\frac{d\mathbf{v}}{dt} = \beta\frac{D\mathbf{u}}{Dt} + \frac{1}{\tau_p}(\mathbf{u}-\mathbf{v}) + (1-\beta)\mathbf{g} \qquad \beta = \frac{3\rho_f}{\rho_f + 2\rho_p} \qquad \tau_p = \frac{r_p^2}{3\nu\beta}$$

β-St model

1. Expand the velocity in a small parameter

$$\mathbf{v} \simeq \mathbf{u} + \tau_p\mathbf{v}_1 + \tau_p^2\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{u} - \mathbf{v} = -\tau_p\mathbf{v}_1 - \tau_p^2\mathbf{v}_2$$

2. Derivatives

$$\frac{D}{Dt}() = \frac{\partial}{\partial_t}() + \mathbf{u}\cdot\nabla()$$

$$\frac{d}{dt}() = \frac{\partial}{\partial_t}() + \mathbf{v}\cdot\nabla()$$

$$\Rightarrow \quad \frac{D}{Dt}() = \frac{d}{dt}() + (\mathbf{u}-\mathbf{v})\cdot\nabla() = \frac{d}{dt}() - (\tau_p\mathbf{v}_1 + \tau_p^2\mathbf{v}_2)\cdot\nabla()$$

Small particles

3. Rewrite the equation

$$\frac{d\mathbf{u}}{dt} + \tau_p \frac{d\mathbf{v}_1}{dt} + \tau_p^2 \frac{d\mathbf{v}_2}{dt} = \beta \frac{d\mathbf{u}}{dt} - \beta(\tau_p \mathbf{v}_1 + \tau_p^2 \mathbf{v}_2) \cdot \nabla \mathbf{u} - \mathbf{v}_1 - \tau_p \mathbf{v}_2 + (1-\beta)\mathbf{g}$$

4. Solve order by order

Order τ_p^0

$$\frac{d\mathbf{u}}{dt} = \beta \frac{d\mathbf{u}}{dt} - \mathbf{v}_1 + (1-\beta)\mathbf{g} \quad \Rightarrow \quad \mathbf{v}_1 = (1-\beta)\left(\mathbf{g} - \frac{d\mathbf{u}}{dt}\right)$$

Order τ_p

$$\frac{d\mathbf{v}_1}{dt} = -\beta\, \mathbf{v}_1 \cdot \nabla \mathbf{u} - \mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = (1-\beta)\frac{d^2\mathbf{u}}{dt^2} - \beta(1-\beta)\left(\mathbf{g} - \frac{d\mathbf{u}}{dt}\right) \cdot \nabla \mathbf{u}$$

Small particles

$$\mathbf{v} \simeq \mathbf{u} + \tau_p(1-\beta)\left(\mathbf{g} - \frac{d\mathbf{u}}{dt}\right) + \tau_p^2\left[(1-\beta)\frac{d^2\mathbf{u}}{dt^2} - \beta(1-\beta)\left(\mathbf{g} - \frac{d\mathbf{u}}{dt}\right)\cdot\nabla\mathbf{u}\right]$$

5. Express the result in terms of fluid quantities

$$\frac{D\mathbf{u}}{Dt} \simeq \frac{d\mathbf{u}}{dt} - \tau_p(1-\beta)\left(\mathbf{g} - \frac{d\mathbf{u}}{dt}\right)\nabla\mathbf{u} + \mathcal{O}(\tau_p^2)$$

$$\mathbf{v} \simeq \mathbf{u} + \tau_p(1-\beta)\left(\mathbf{g} - \frac{D\mathbf{u}}{Dt}\right) + \mathcal{O}(\tau_p^2)$$

$$\mathbf{v} \simeq \mathbf{u} + \tau_p(1-\beta)\left(\mathbf{g} - \frac{D\mathbf{u}}{Dt}\right) + \tau_p^2(1-\beta)\left[(1-2\beta)\left(\mathbf{g} - \frac{D\mathbf{u}}{Dt}\right)\cdot\nabla\mathbf{u} + \frac{D^2\mathbf{u}}{Dt^2}\right] + \mathcal{O}(\tau_p^3)$$

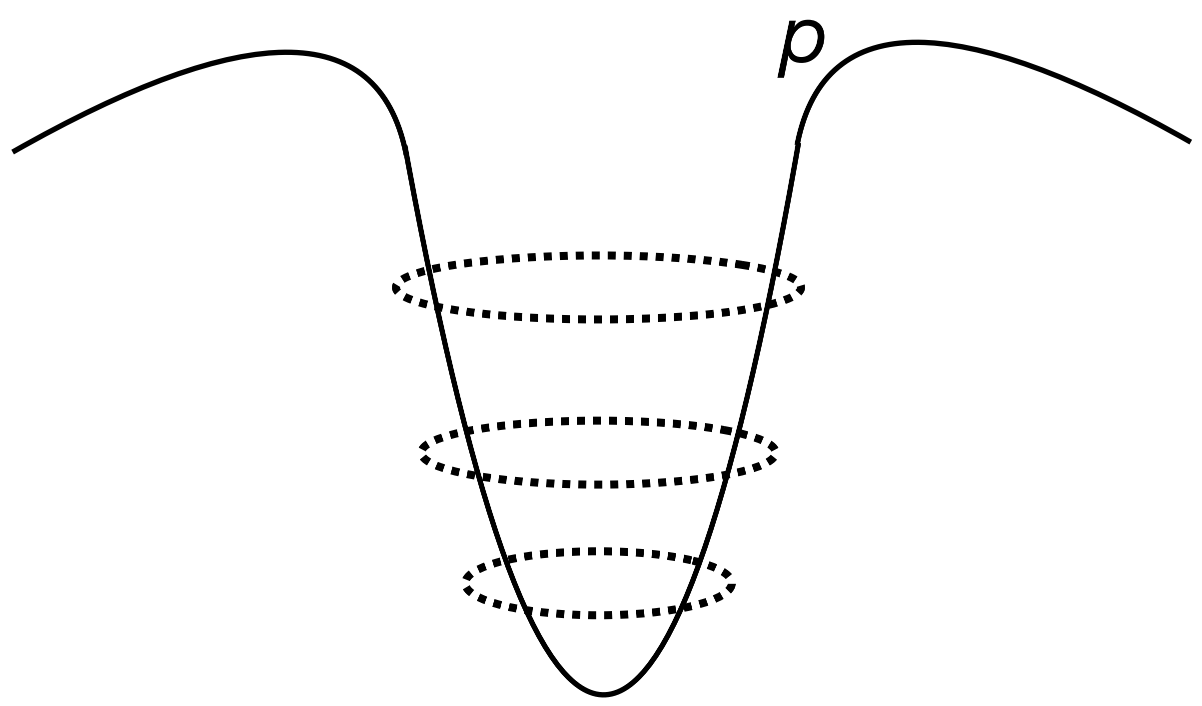
Small particle models

$$\mathbf{v} = \mathbf{u} + (1-\beta)\tau_p\,(\mathbf{g} - D_t\mathbf{u}) \quad \longleftarrow \quad \boxed{\mathbf{v} = \mathbf{u} + \mathbf{v}_{add}}$$

$n(\mathbf{x}, t)$ particle number density

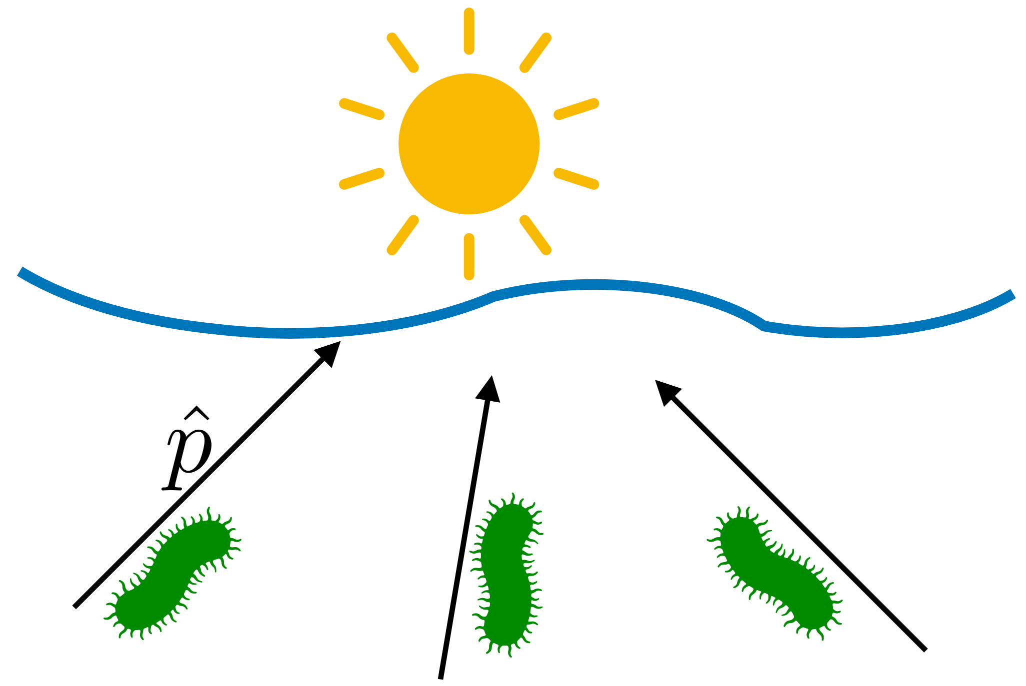
$$\partial_t n + \nabla\cdot(n\ \mathbf{v}) = 0 \quad \Rightarrow \quad \partial_t n + \mathbf{v}\cdot\nabla n = -n(\nabla\cdot\mathbf{v}_{add})$$

$$\mathbf{v} = \mathbf{u} + \mathbf{v}_{sink} = \mathbf{u} + (1-\beta)\tau_p\mathbf{g} \quad \Rightarrow \quad \partial_t n + \mathbf{v}\cdot\nabla n = 0$$



$$\mathbf{v} = \mathbf{u} + (1-\beta)\tau_p\,(\mathbf{g} - D_t\mathbf{u}) \quad \Rightarrow \quad \partial_t n + \mathbf{v}\cdot\nabla n = n\ \tau_p(1-\beta)(\nabla\cdot D_t\mathbf{u}) = n\ \tau_p(\beta-1)\Delta p$$

$$\mathbf{v} = \mathbf{u} + \mathbf{v}_{swim} = \mathbf{u} + v_{swim}\ \hat{\mathbf{p}} \quad \Rightarrow \quad \partial_t n + \mathbf{v}\cdot\nabla n = -n(\nabla\cdot\hat{\mathbf{p}})$$



(not so) small particles

Eulerian particle description breaks down

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS April 2007
EPL, **78** (2007) 14001 www.epljournal.org
doi: 10.1209/0295-5075/78/14001

The Eulerian description of dilute collisionless suspension

G. BOFFETTA[1], A. CELANI[2], F. DE LILLO[3] and S. MUSACCHIO[2]

Lagrangrangian-Eulerian particles

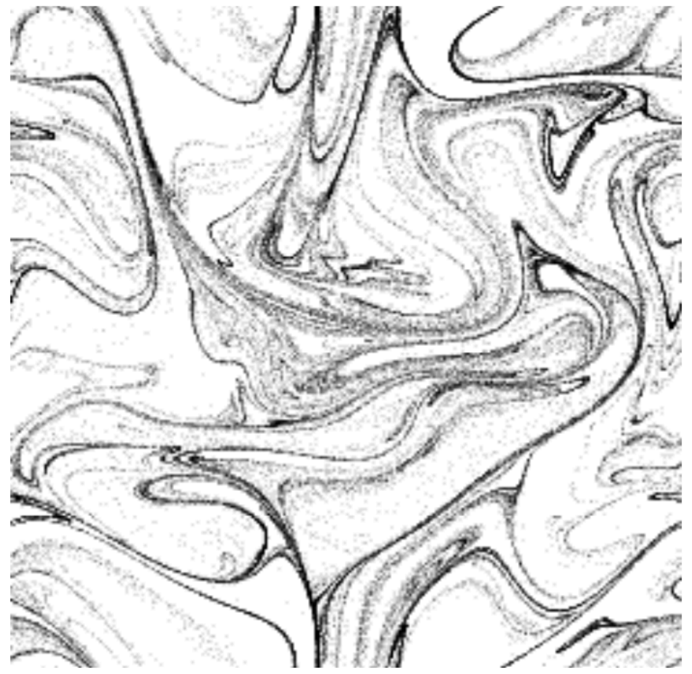
$$\dot{\mathbf{x}}_{ep} = \mathbf{V}(\mathbf{x}_{ep}, t)$$

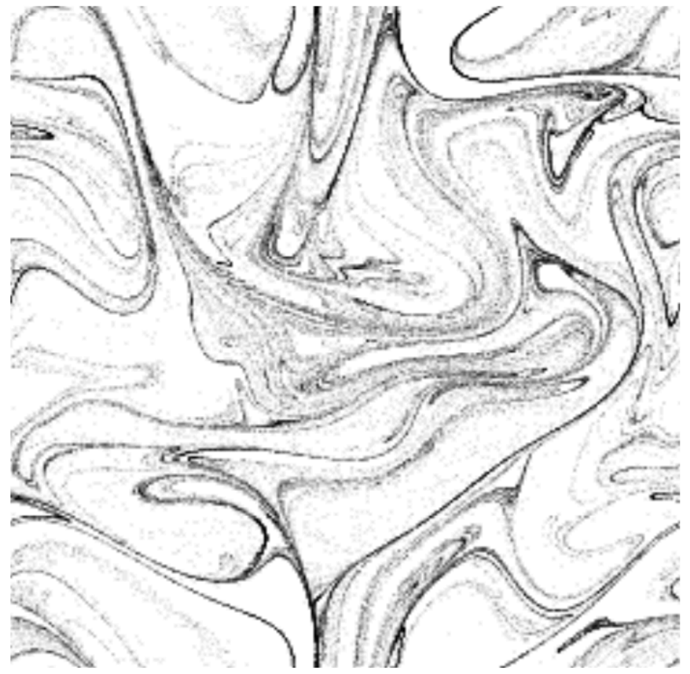
$$\partial_t \mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V} = \frac{\mathbf{u} - \mathbf{V}}{\tau_p}$$

Truly Lagrangian particles

$$\dot{\mathbf{x}}_p = \mathbf{v}(t)$$

$$\dot{\mathbf{v}} = \frac{\mathbf{u}(\mathbf{x_p}, t) - \mathbf{v}}{\tau_p}$$

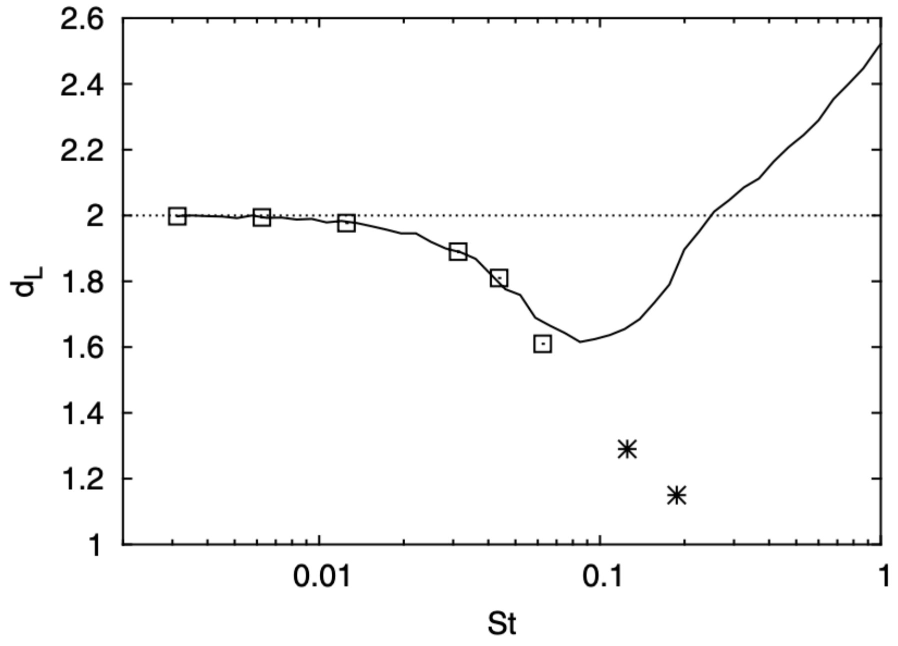


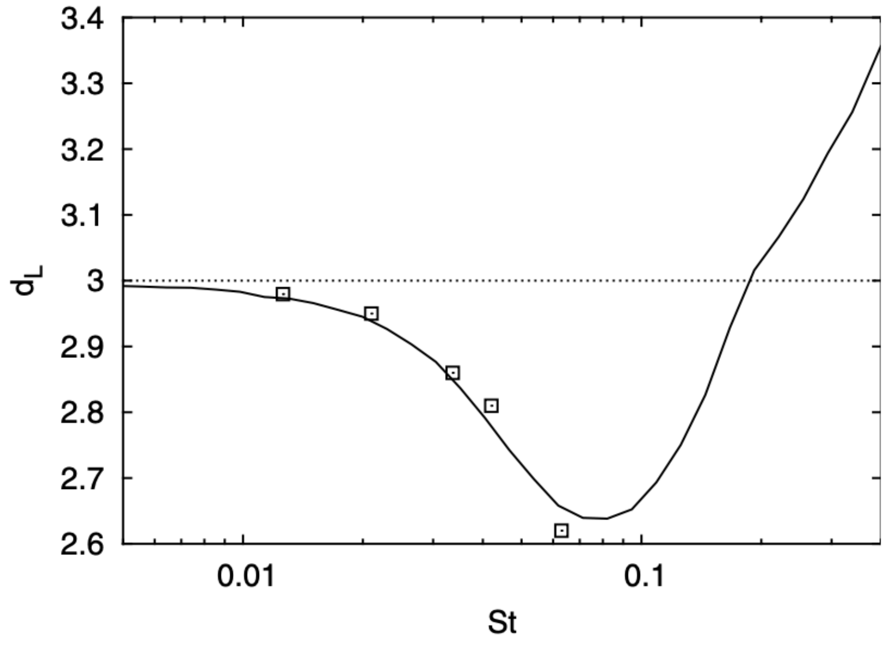


Different phase space of the two systems

Sling effect: crossing of trajectories

$$St = \frac{\tau_p}{\tau_\eta} \geq 1$$





Finite-sized particles

Corrections to the point-particle equation

$$\frac{d\mathbf{v}}{dt} = \beta\frac{D\mathbf{u}}{Dt} + \frac{1}{\tau_p}(\mathbf{u}-\mathbf{v}) + (1-\beta)\mathbf{g}$$

↓

$$\frac{d\mathbf{v}}{dt} = \beta\frac{D[\mathbf{u}]_V}{Dt} + \frac{1}{\tau_p}([\mathbf{u}]_S-\mathbf{v}) + (1-\beta)\mathbf{g}$$

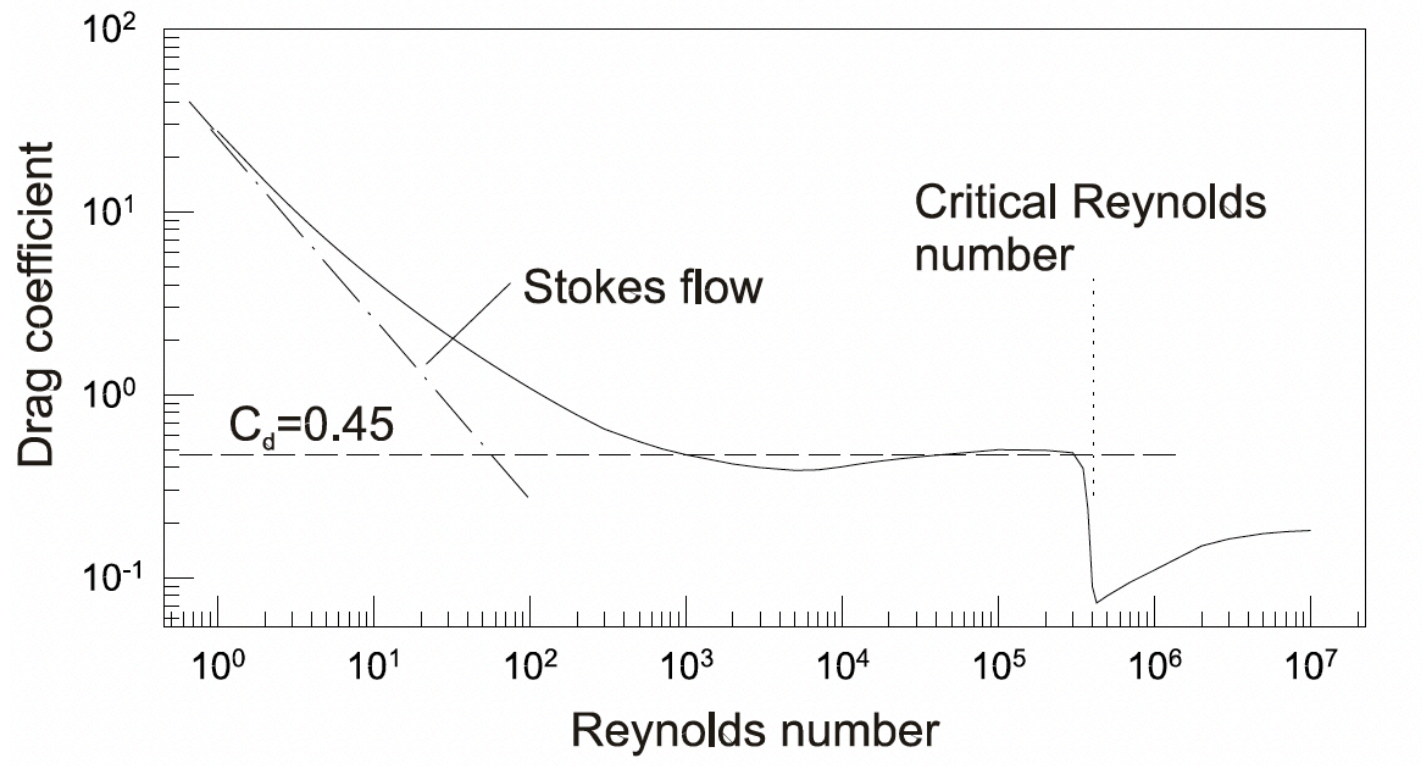
Finite-size effect (Faxén laws 1922)

$$\mathbf{u} \to [\mathbf{u}]_S \simeq \mathbf{u} + \frac{r_p^2}{6}\Delta\mathbf{u}$$

in drag , history

$$\mathbf{u} \to [\mathbf{u}]_V \simeq \mathbf{u} + \frac{r_p^2}{10}\Delta\mathbf{u}$$

in fluid acceleration , added mass



Finite-Reynolds effect (Shiller-Neumann 1935) wake drag empirical correlation

$$6\pi\mu r_p \to 6\pi\mu r_p(1+0.15Re_p^{0.687}) \qquad Re_p \lesssim 10^3$$

Lift force for light particles (Auton JFM 1987, inviscid calculation)

$$\mathbf{f}_{lift} = \frac{m_f}{2}(\mathbf{u}-\mathbf{v}) \times (\nabla \times \mathbf{u})$$

Different from Magnus lift

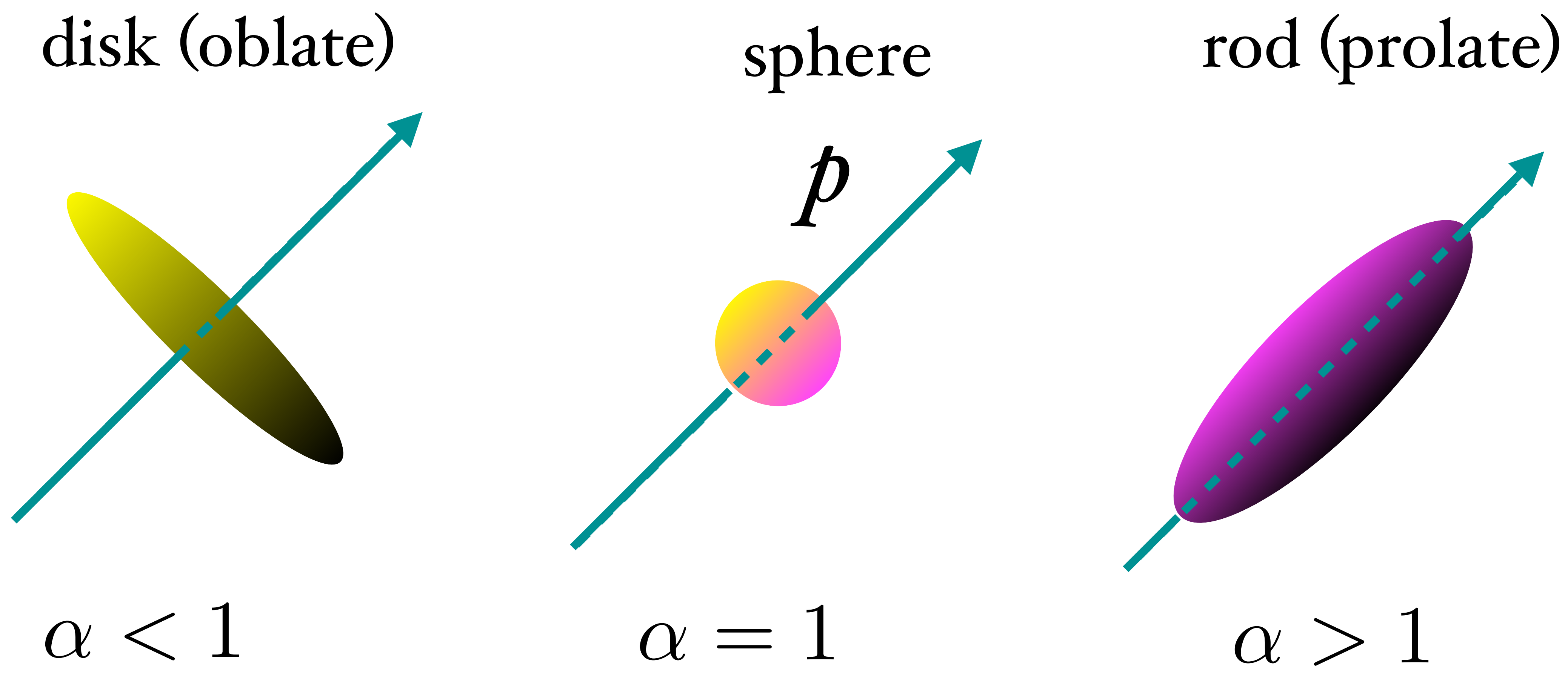
$$\mathbf{f}_{Magnus} \sim (\mathbf{u}-\mathbf{v}) \times \boldsymbol{\omega}_p$$

Particles with a shape

Spheroidal particles

aspect ratio

$$\alpha = \frac{l}{d}$$



fluid velocity gradient tensor

$$\nabla \mathbf{u} = \Omega + \mathcal{S}$$

rotation rate   strain rate

$$\dot{\boldsymbol{p}}(t) = \boldsymbol{\Omega} \cdot \boldsymbol{p} + \frac{\alpha^2 - 1}{\alpha^2 + 1} (\mathcal{I} - \boldsymbol{pp}) \cdot \mathcal{S}\boldsymbol{p}$$

Jeffery (1922) equation

Valid inertialess axisymmetric fore-aft sym. particles

Particles with a shape

rate of rotation tensor $\Omega_{ij} = -\frac{1}{2}\varepsilon_{ijk}\omega_k$ ← fluid vorticity

Other way of writing the same equation

$$\dot{\mathbf{p}} = \boldsymbol{\omega}_J \wedge \mathbf{p} \qquad \boldsymbol{\omega}_J = \frac{\boldsymbol{\omega}}{2} + \frac{\alpha^2-1}{\alpha^2+1}\mathbf{p} \wedge \mathcal{S}\mathbf{p}$$

B.Mehlig, K.Gustavsson, Byron

Particle angular velocity ($\boldsymbol{\omega}_J$)

$\dot{\boldsymbol{p}}$ tumbling rotation rate $\qquad (\boldsymbol{\omega}_J \cdot \boldsymbol{p})\boldsymbol{p}$ spinning rate

$$\dot{\mathbf{p}}(t) = \frac{\mathbf{q}(t)}{|\mathbf{q}(t)|} \qquad \dot{\mathbf{q}}(t) = \left(\boldsymbol{\Omega} + \frac{\alpha^2-1}{\alpha^2+1}\mathcal{S}\right)\mathbf{q}$$

A.Szeri
Phil. Trans. **A345**, 477-508, (1993)

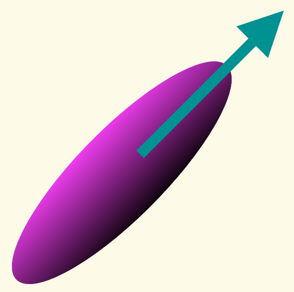
$$\Rightarrow \quad \mathbf{q}(t) = \mathbf{q}(0)e^{\int_0^t(\boldsymbol{\Omega}+\frac{\alpha^2-1}{\alpha^2+1}\mathcal{S})dt'}$$

Particles with a shape

$$\dot{\mathbf{q}}(t) = \left(\mathbf{\Omega} + \frac{\alpha^2 - 1}{\alpha^2 + 1}\mathcal{S}\right)\mathbf{q}$$

A.Szeri
Phil. Trans. **A345**, 477-508, (1993)

Rods $\alpha \to \infty$



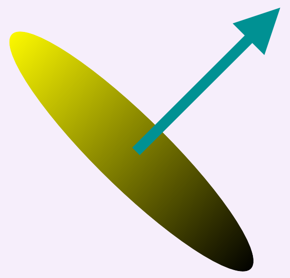
$$\dot{\mathbf{q}} = \nabla\mathbf{u} \cdot \mathbf{q}$$

Vorticity

$$\dot{\omega} = \nabla\mathbf{u} \cdot \omega + \nu\Delta\omega$$

Pumir & Wilkinson New J.Physics **13** 093030 (2011)

Disks $\alpha \to 0$



$$\dot{\mathbf{q}} = -\nabla\mathbf{u}^T \cdot \mathbf{q}$$

Temperature gradient

$$\dot{\nabla T} = -\nabla\mathbf{u}^T \cdot \nabla T + \kappa\Delta\nabla T$$

Particles with a shape

Simple models of <u>inertial</u> particles with a shape

Inertial sphere: translation and rotation

$$m_p \frac{d\mathbf{v}}{dt} = \mathbf{F} = 6\pi\mu r_p(\mathbf{u} - \mathbf{v}) \quad \Rightarrow \quad \tau_p = \frac{m_p}{6\pi\mu r_p} = \frac{2}{9}\frac{\rho_p}{\rho_f}\frac{r_p^2}{\nu}$$

$$\frac{d(\mathbb{I}\,\boldsymbol{\omega}_p)}{dt} = \mathbf{T} = 8\pi\mu r_p^3(\boldsymbol{\omega} - \boldsymbol{\omega}_p) \quad \Rightarrow \quad \tau_{p,rot} = \frac{\frac{2}{5}m_p^2}{8\pi\mu r_p^3} = \frac{1}{15}\frac{\rho_p}{\rho_f}\frac{r_p^2}{\nu}$$

$$\mathbb{I}_{ij} = \frac{2}{5} m_p r_p^2\, \delta_{ij}$$

Rotation relaxes faster than translation

⇓

Decoupling of rotation from translation

Simple model of non-spherical inertial particle

$$m_p \frac{d\mathbf{v}}{dt} = \mathcal{K}(\mathbf{u} - \mathbf{v}) + m_p\mathbf{g} \qquad \mathcal{K} = c_\perp \mathcal{I} + (c_{||} - c_\perp)\mathbf{p}\mathbf{p}^T$$

$$\dot{\boldsymbol{p}}(t) = \boldsymbol{\Omega}\cdot\boldsymbol{p} + \frac{\alpha^2 - 1}{\alpha^2 + 1}(\mathcal{I} - \boldsymbol{p}\boldsymbol{p})\cdot\mathcal{S}\boldsymbol{p}$$

Orientation $\rightarrow$ / $\not\leftarrow$ drag

RAPID COMMUNICATION

Inertial spheroids in homogeneous, isotropic turbulence

Amal Roy[1,2,*], Anupam Gupta[3,†], and Samriddhi Sankar Ray[2,‡]

Show more

Phys. Rev. E **98**, 021101(R) – **Published 3 August, 2018**

DOI: https://doi.org/10.1103/PhysRevE.98.021101

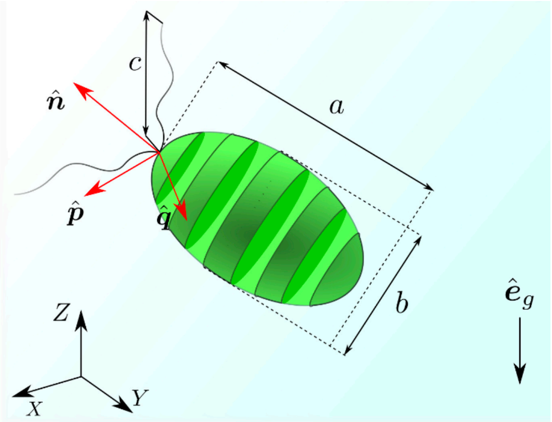
Particles with a shape

Fully Overdumped models

$$\dot{\mathbf{x}}_s(t) = \mathbf{u}(\mathbf{x}_s, t) + \mathbf{v}_s$$

$$\boldsymbol{v}_s\left(\boldsymbol{p}\right) = v_s^{min}\hat{\boldsymbol{e}}_g + \left(v_s^{max} - v_s^{min}\right)\left(\hat{\boldsymbol{e}}_g \cdot \boldsymbol{p}\right)\boldsymbol{p}$$

Settling aspherical particles



$$v_s \mathbf{p}(t)$$

Micro-swimmers

$$v_s \; \Theta(\dot{\theta}_s) \; \mathbf{p}(t)$$

Scalar-taxis and foraging

$$\mathbf{J}(\mathbf{p}, \dot{\gamma}_s, t)$$

Planktonic "jumps"

Particles with a shape

Translation-rotation coupled point-particle models

$$m_p \ddot{\mathbf{x}} = \mathbf{f} + m_p \mathbf{g} \qquad \dot{\mathbf{p}} = \boldsymbol{\omega} \wedge \mathbf{p} \qquad \frac{d}{dt}(\mathbb{I}\boldsymbol{\omega}) = \mathbf{T} \qquad \mathbb{I}_{ij} = \frac{m_p \; r_{p\perp}^2}{5}\left[(1+\alpha^2)\delta_{ij} + (1-\alpha^2)p_i p_j\right]$$

Force & Torque

Resistance tensor 6x6 matrix

$$\begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{T} \end{bmatrix} = m\gamma \begin{bmatrix} \mathcal{K} & 0 & 0 \\ 0 & \mathbb{M}^{(r1)} & \mathbb{M}^{(r2)} \end{bmatrix} \begin{bmatrix} \boldsymbol{u} - \boldsymbol{v} \\ \boldsymbol{\Omega} - \boldsymbol{\omega} \\ \mathbb{S} \end{bmatrix}$$

Resistance translation tensor

Resistance rotation tensors (2nd and 3rd rank)

$$\mathcal{K} = c_\perp \mathcal{I} + (c_{||} - c_\perp)\mathbf{p}\mathbf{p}^T$$

Statistical Model for the Orientation of Nonspherical Particles Settling in Turbulence

K. Gustavsson[1], J. Jucha[2,3], A. Naso[4], E. Lévêque[4], A. Pumir[2], and B. Mehlig[1]

Show more

Phys. Rev. Lett. **119**, 254501 – **Published 19 December, 2017**

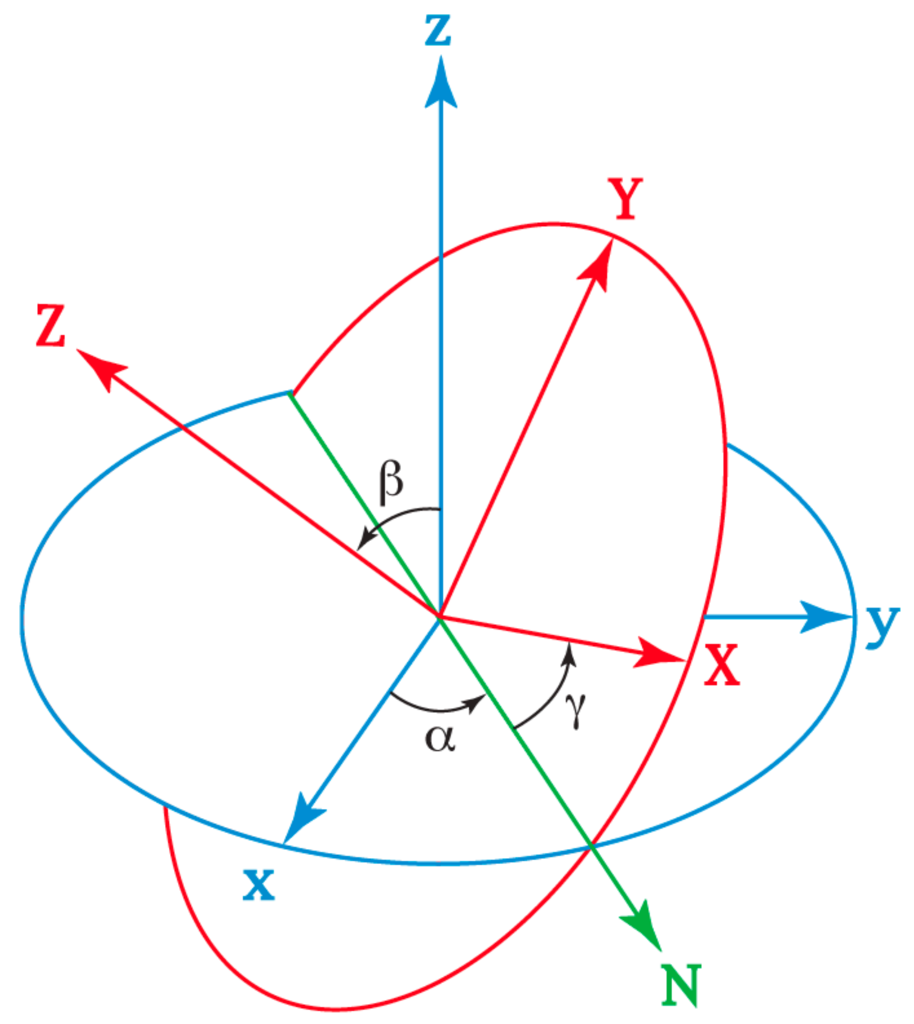
DOI: https://doi.org/10.1103/PhysRevLett.119.254501

Finite-sized particles

Back to basics: Rigid body motion

$$m_p \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \mathbf{F} \qquad \mathbf{F} = \oint_{S_p} \boldsymbol{\sigma} \cdot \mathbf{n} \, dS$$

$$\frac{\mathrm{d}\boldsymbol{\mathcal{I}\Omega}}{\mathrm{d}t} = \mathbf{T} \qquad \mathbf{T} = \oint_{S_p} (\mathbf{x} - \mathbf{r}) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) \, dS$$



Particle couplings

Dusty-gas model (Eulerian-Eulerian description)

On the stability of laminar flow of a dusty gas

By P. G. SAFFMAN
Department of Mathematics, King's College, London

(Received 19 December 1961)

$$\partial_t n + \nabla \cdot (n \ \mathbf{v}) = 0$$

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = \frac{\mathbf{u} - \mathbf{v}}{\tau_p}$$

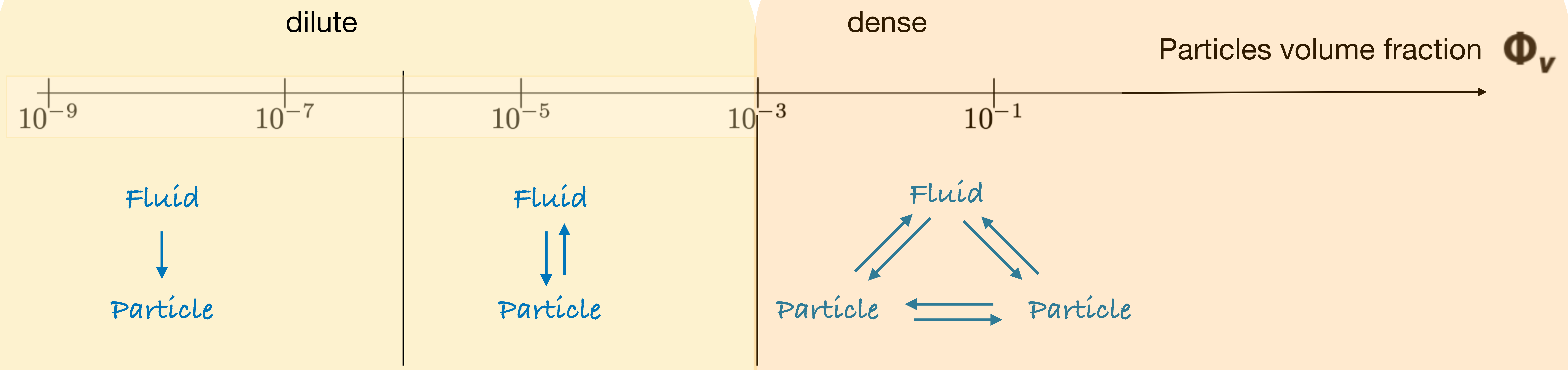
Two-way momentum coupling

$$\nabla \cdot \mathbf{u} = 0$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} - n \frac{\mathbf{u} - \mathbf{v}}{\tau_p}$$

Particle couplings

$$\Phi_v = V_p \int_V n \, dV = \frac{N_p V_p}{V}$$



one-way

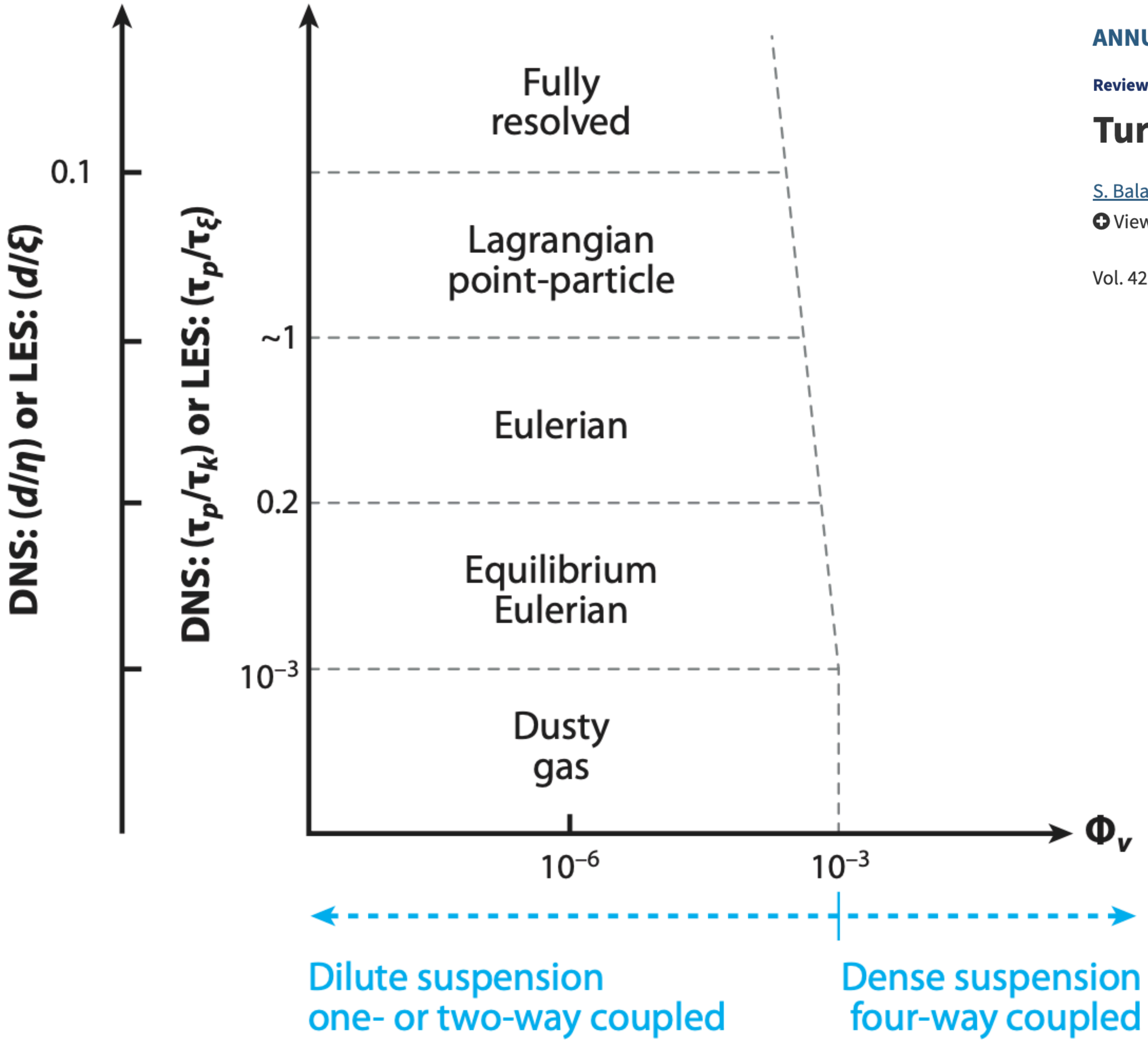
two-way

total momentum (and mass) conservation

4-way

Lubrication forces

Particle couplings



ANNUAL REVIEW OF FLUID MECHANICS Volume 42, 2010

Review Article

Turbulent Dispersed Multiphase Flow

S. Balachandar[1] and John K. Eaton[2]

View Affiliations

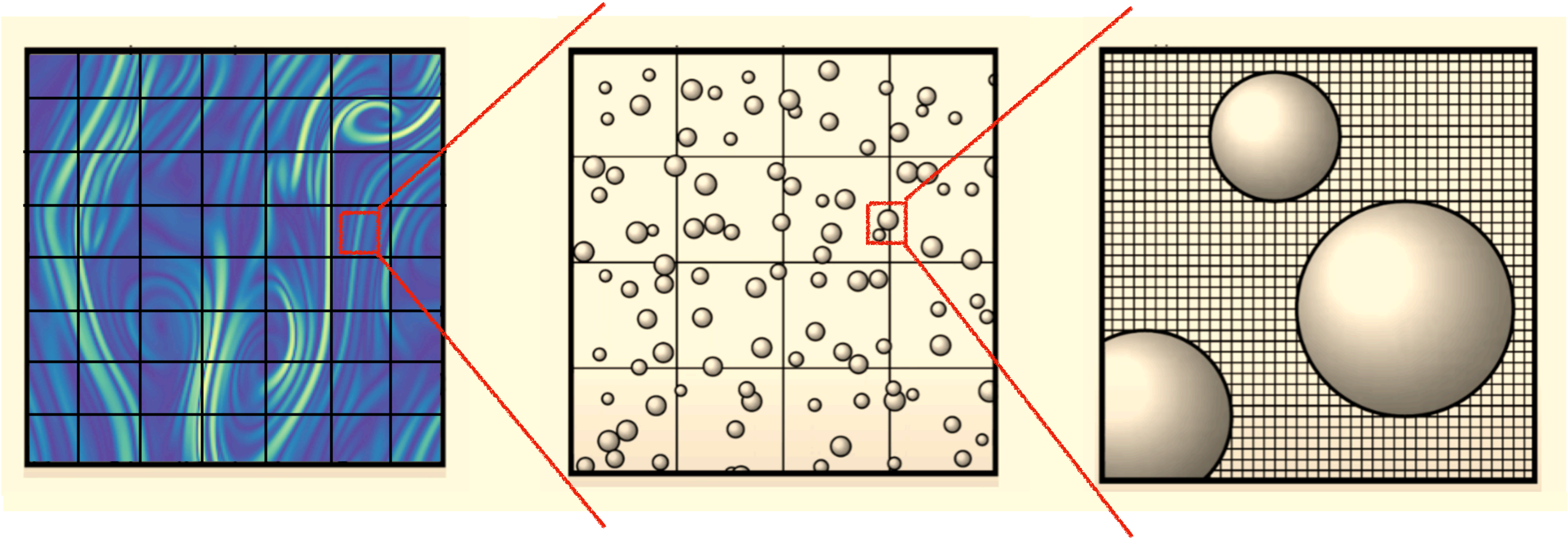
Vol. 42:111-133 (Volume publication date January 2010) | https://doi.org/10.1146/annurev.fluid.010908.165243

Part 2

Methods

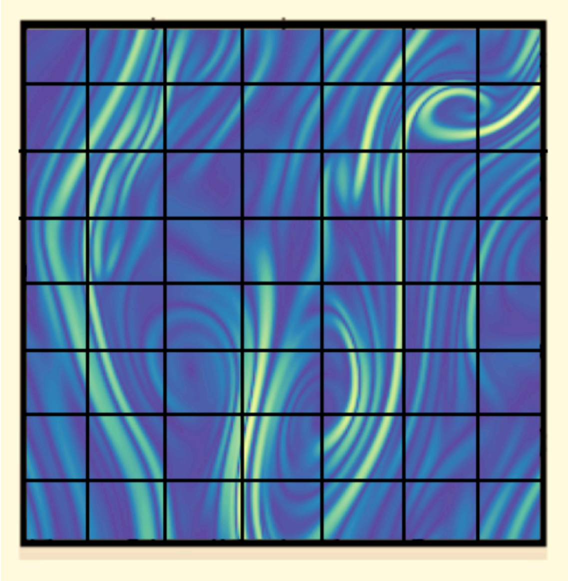
Which method?

A matter of scale



$\ell_{obs} \gg r_p$ $\ell_{obs} \gtrsim r_p$ $\ell_{obs} < r_p$

Eulerian-Eulerian



When? The continuum hypothesis holds

Advantages:

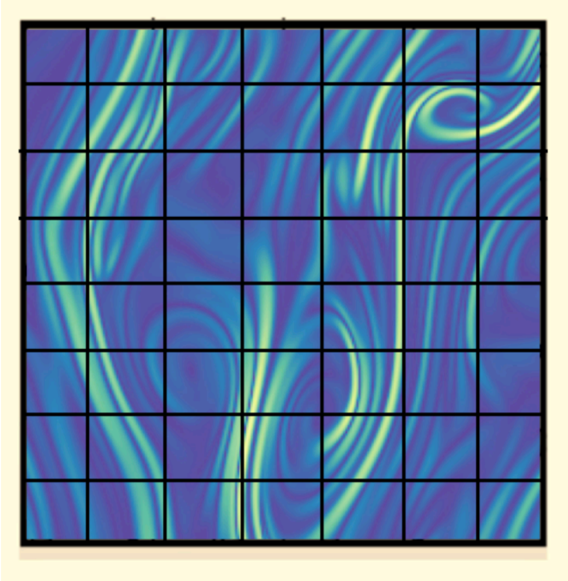
1) **Theoretical** PDE analysis, analytical understanding e.g. instabilities

   My view: In general, simpler (more abstract) models allow a deeper understanding of a complex physical system

2) **Numerical** Use same discretisation method for the carrier flow and particles

Choose your favourite method: Spectral, FD, FV, LBM

Eulerian-Eulerian



Difficulties: development of shocks due to the compressibility of particle velocity field.

Solutions:

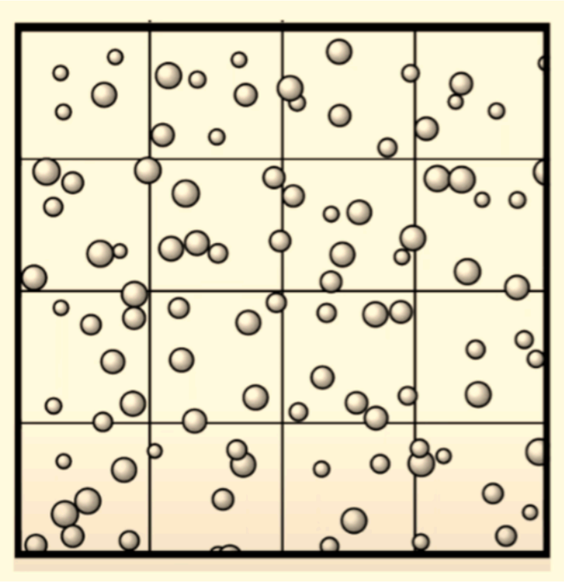
1) Regularisation through artificial dissipations (in mass and momentum conservation)

2) Use semi-Lagrangian methods for the advection term

3) Shock capturing schemes

4) different spatial/temporal resolutions for particles and fluid

Eulerian-Lagrangian



When? the observation scale is very large but the continuum hyp. does not hold

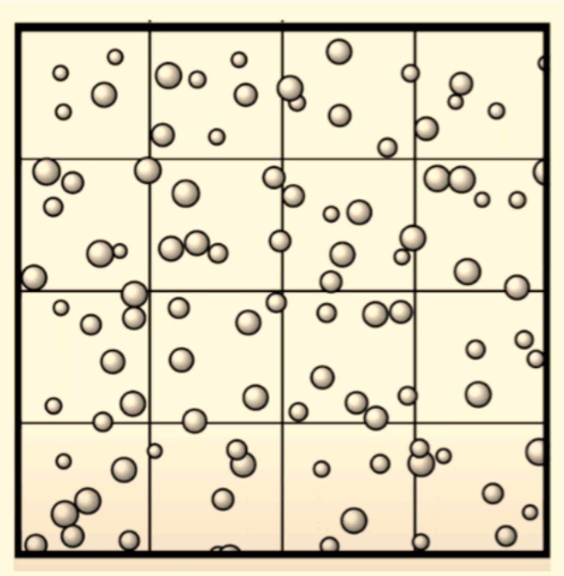
Eulerian fluid description as easy as before

Particle dynamics based on ODE (or ODIE)

One-way coupling—> interpolation

Two-way coupling —> interpolation and extrapolation

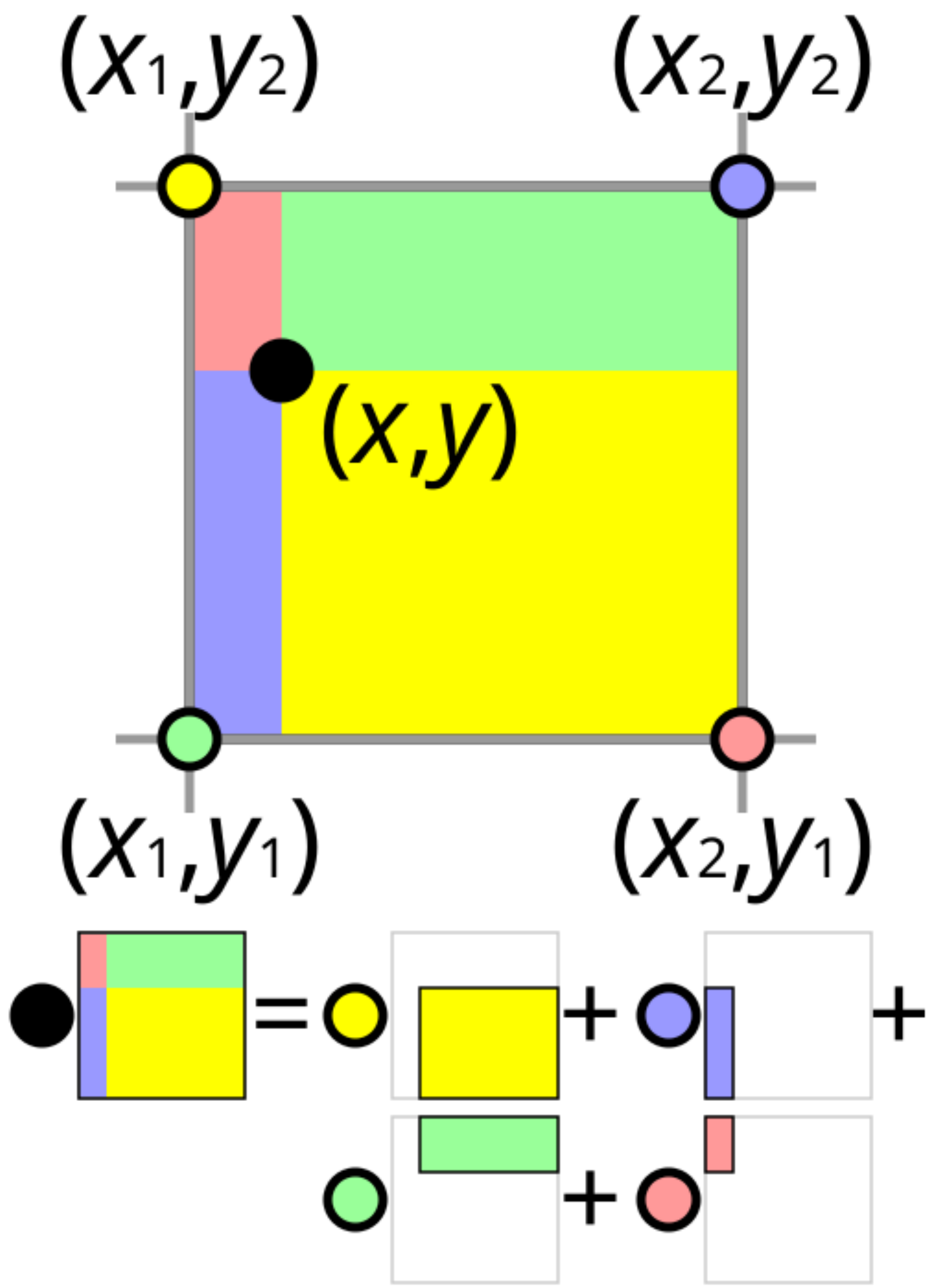
Eulerian-Lagrangian



Interpolation/extrapolation

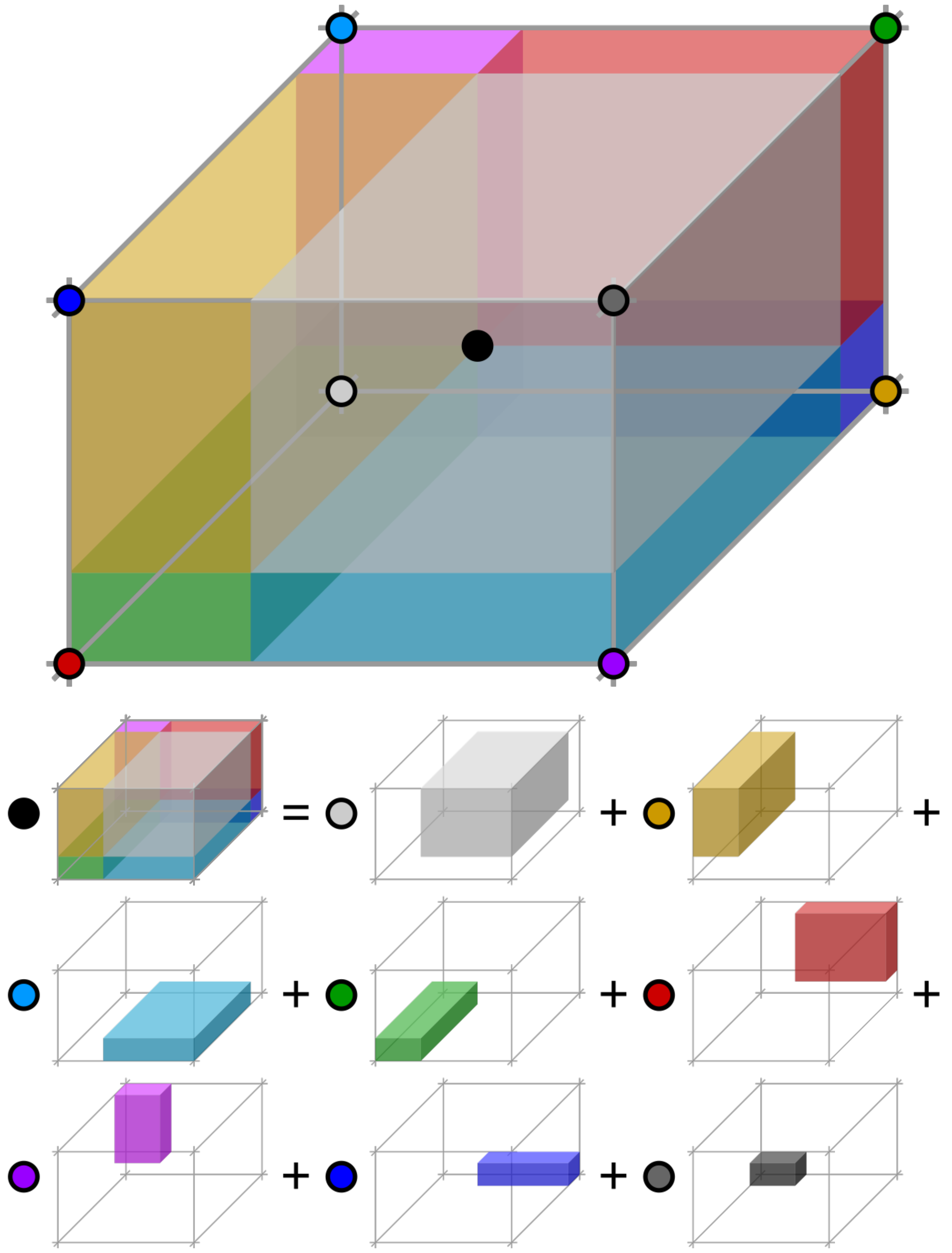
2D -> bilinear

Informations from 4 points



3D -> trilinear

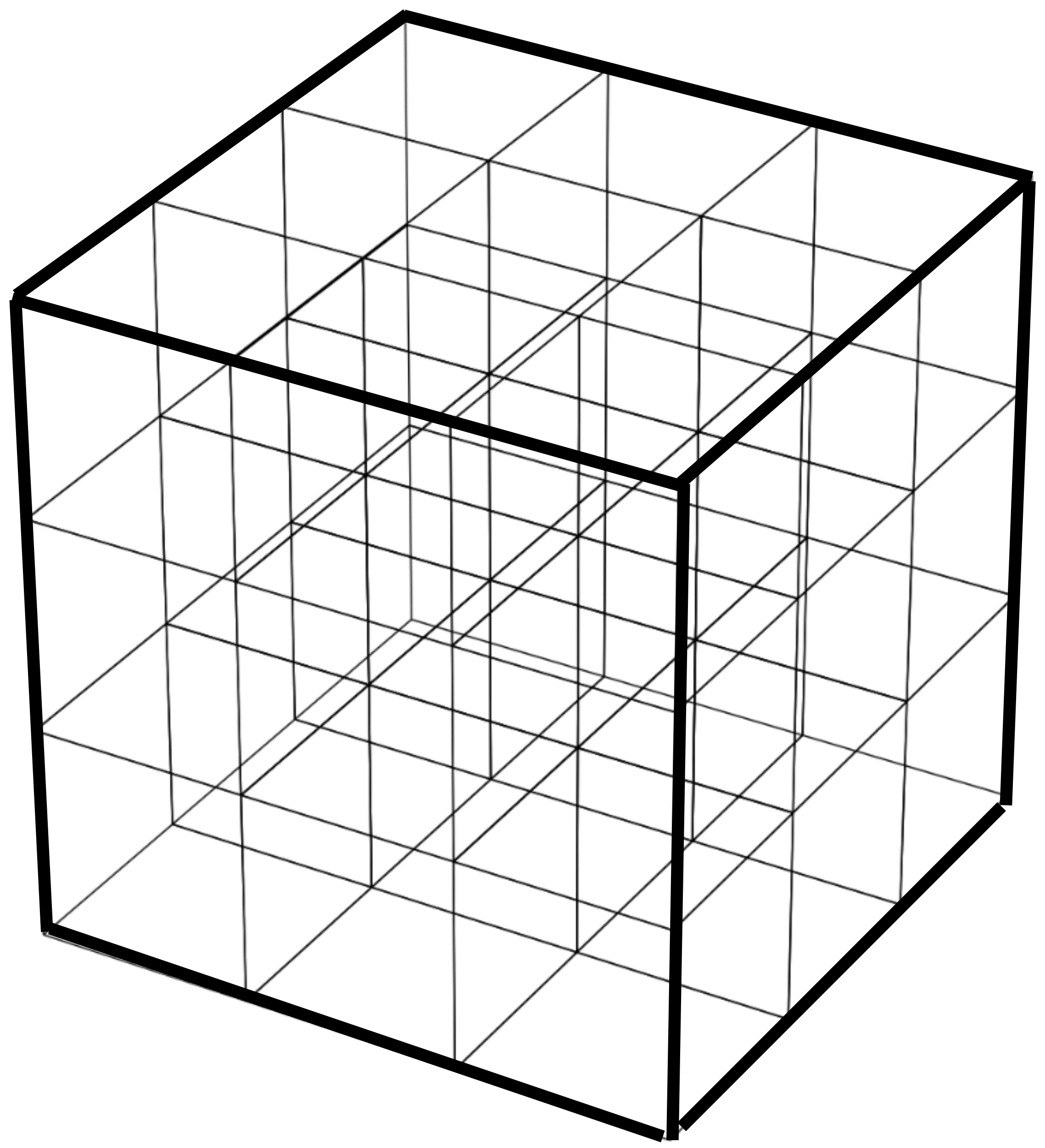
Informations from 8 points



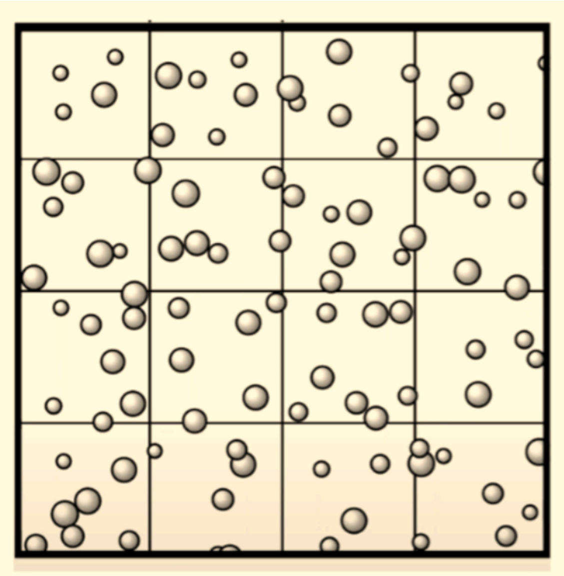
3D -> tricubic

Informations from 27 cubes 64 points

$$f(x,y,z) = \sum_{i=0}^{3}\sum_{j=0}^{3}\sum_{k=0}^{3} a_{ijk} x^i y^j z^k.$$



Eulerian-Lagrangian



How to compute the hydrodynamic forces on the particle?

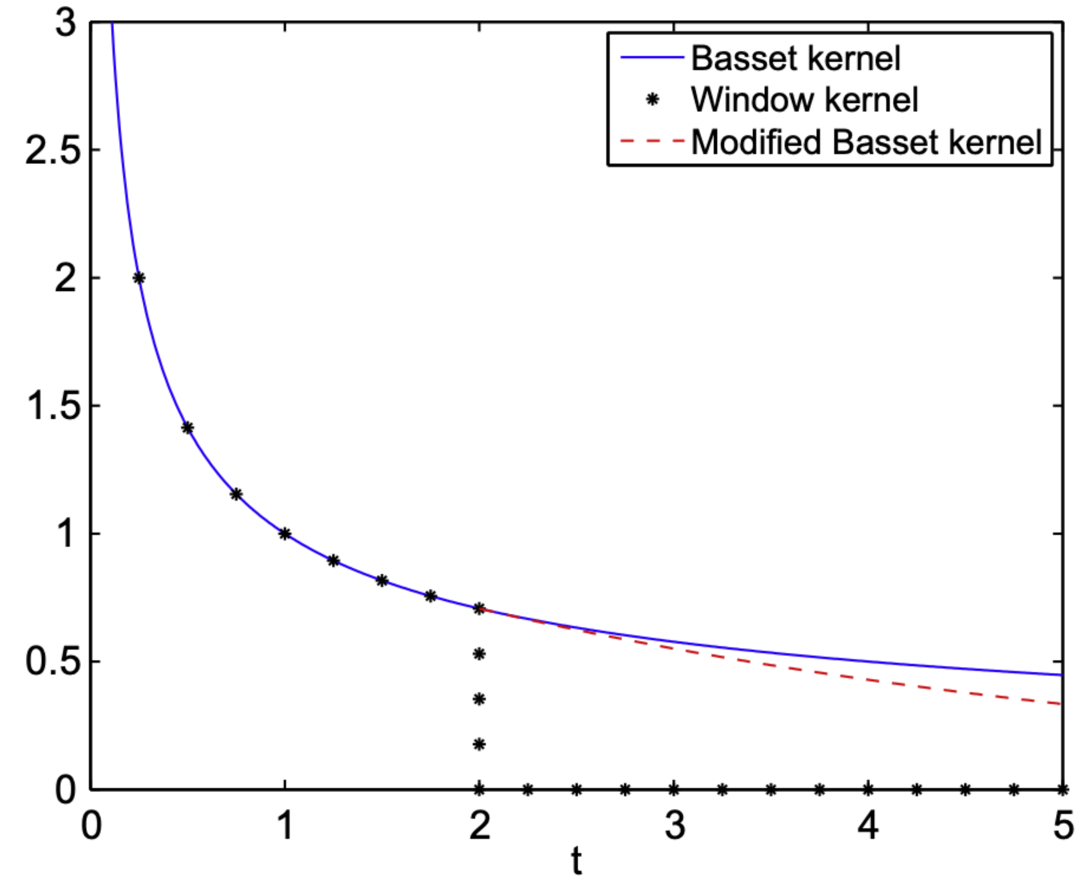
Fluid material derivative

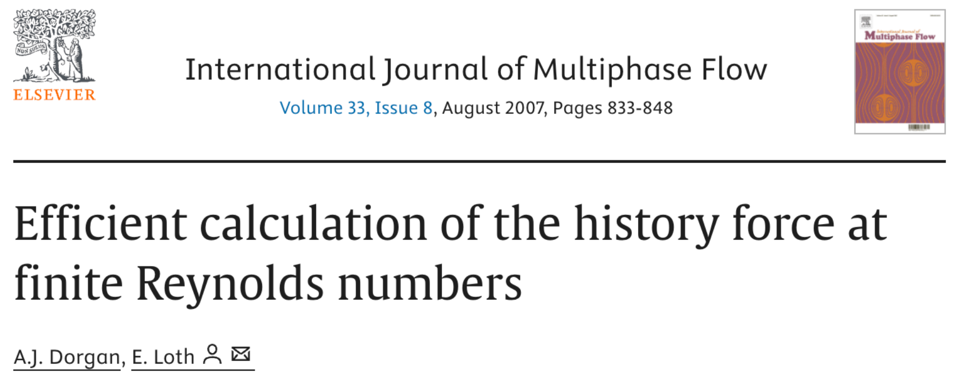
$$D_t\mathbf{u} \;= d_t\mathbf{u} + (\mathbf{u}-\mathbf{v})\cdot\nabla\mathbf{u} \;= \frac{\mathbf{u}_t - \mathbf{u}_{t-\delta t}}{\delta t} + (\mathbf{u}-\mathbf{v})\cdot\nabla\mathbf{u}$$

Or *r.h.s.* of NS $\quad -\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{f}$

History force

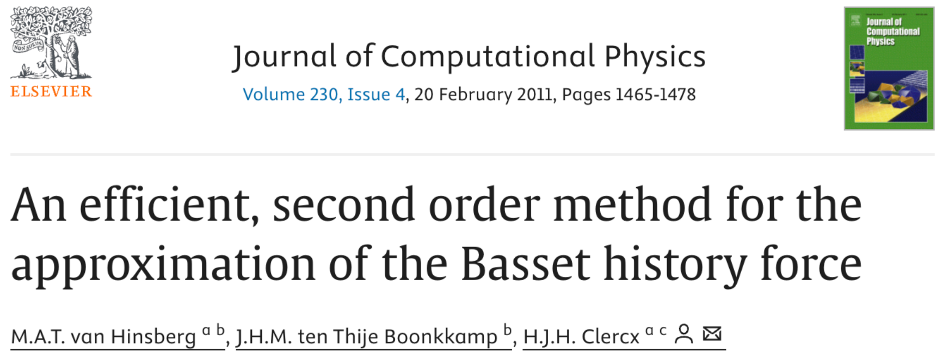
$$\frac{3\beta}{r_p}\int_{t-t_h}^{t}\left(\frac{\nu}{\pi(t-\tau)}\right)^{\frac{1}{2}}\frac{\mathrm{d}}{\mathrm{d}\tau}(\mathbf{u}-\mathbf{v})\,\mathrm{d}\tau$$




International Journal of Multiphase Flow
Volume 33, Issue 8, August 2007, Pages 833-848

Efficient calculation of the history force at finite Reynolds numbers

A.J. Dorgan, E. Loth


Journal of Computational Physics
Volume 230, Issue 4, 20 February 2011, Pages 1465-1478

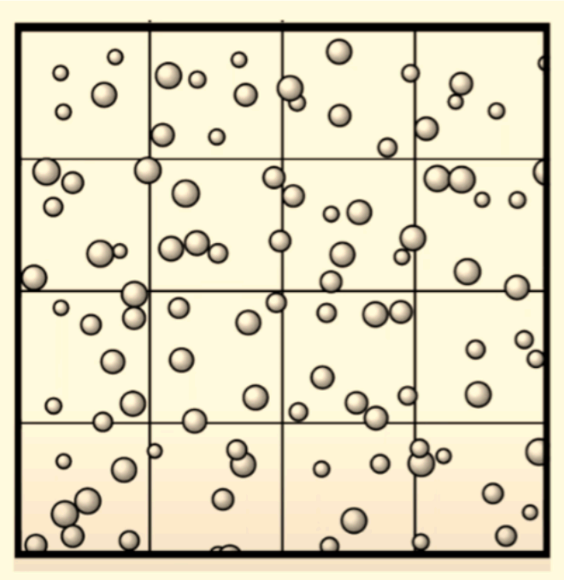
An efficient, second order method for the approximation of the Basset history force

M.A.T. van Hinsberg [a b], J.H.M. ten Thije Boonkkamp [b], H.J.H. Clercx [a c]

window method

empirically in turbulence $t_h \simeq 10\tau_\eta$

Eulerian Lagrangian



Temporal integration

Time-marching scheme

Taylor scheme

$$\mathbf{v}(t+\delta t) = \mathbf{v}(t) + \mathbf{a}(t)\delta t$$

$$\mathbf{x}(t+\delta t) = \mathbf{x}(t) + \mathbf{v}(t)\delta t + \frac{1}{2}\mathbf{a}(t)\delta t^2$$

AB2

$$\mathbf{v}(t+\delta t) = \mathbf{v}(t) + \left(\frac{3}{2}\mathbf{a}(t) + \frac{1}{2}\mathbf{a}(t-\delta_t)\right)\delta t$$

$$\mathbf{x}(t+\delta t) = \mathbf{x}(t) + \left(\frac{3}{2}\mathbf{v}(t) + \frac{1}{2}\mathbf{v}(t-\delta_t)\right)\delta t$$

Size of time-step

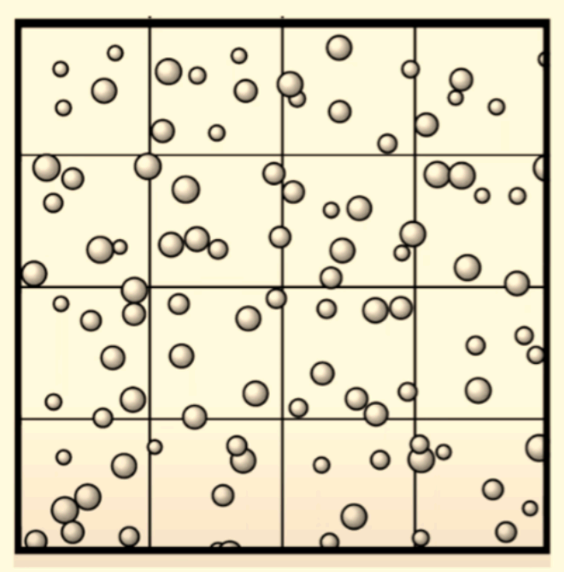
$$\delta t \ll \tau_p \qquad \tau_p = \frac{r_p^2}{3\nu\beta} \qquad \delta t \ll \min[\tau_p(Re_p)]$$

$$\delta t \ll \tau_f$$

$$\Rightarrow \qquad \delta t \leq \delta t_{Euler}$$

Eulerian Lagrangian

Particles with size and shape

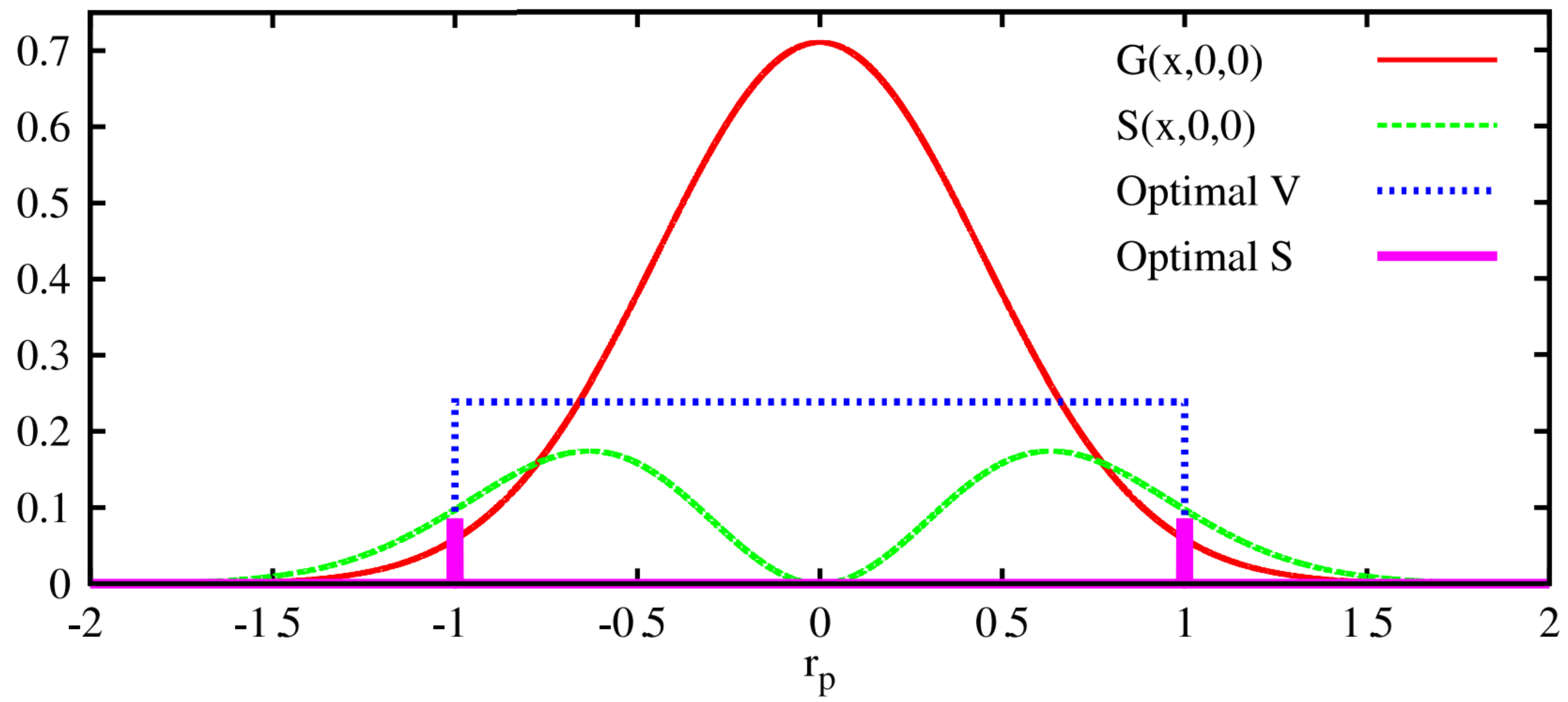


Faxén terms

$$\left[\frac{D\mathbf{u}}{Dt}\right]_V = (4/3\,\pi r_p^3)^{-1}\int_V \frac{D\mathbf{u}}{Dt}(\mathbf{x},t)\,\mathrm{d}^3x$$

$$[\mathbf{u}]_S = (4\pi r_p^2)^{-1}\int_S \mathbf{u}(\mathbf{x},t)\,\mathrm{d}^2x.$$

$$G(\mathbf{x}) = (1/(\sqrt{2\pi}\sigma))^3\exp(-\mathbf{x}^2/(2\sigma^2)),$$



Efficient implementation: Gaussian convolutions and FFTs

$$\left[\frac{D\mathbf{u}}{Dt}(\mathbf{x},t)\right]_V \simeq \int_{L^3} G(\mathbf{x}')\frac{D\mathbf{u}}{Dt}(\mathbf{x}-\mathbf{x}',t)\,\mathrm{d}^3x' = \mathcal{DFT}^{-1}\left[\tilde{G}(\mathbf{k})\frac{\widetilde{D\mathbf{u}}}{Dt}(\mathbf{k},t)\right]$$

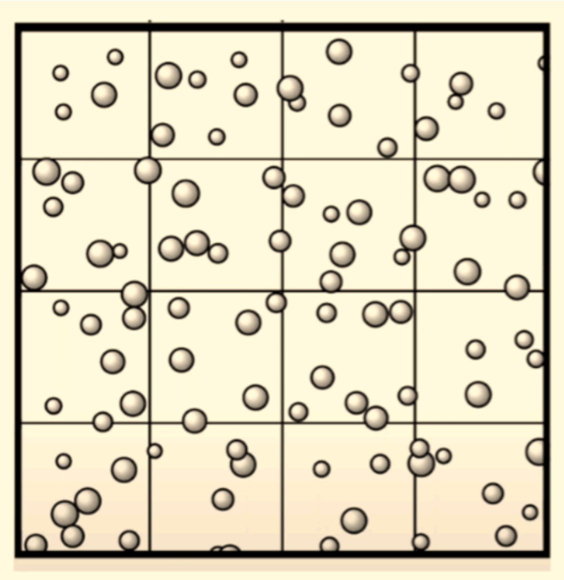
$$\tilde{G}(\mathbf{k}) = \exp(-\sigma^2\mathbf{k}^2/2) \simeq 1-\sigma^2\frac{\mathbf{k}^2}{2}$$

$$\text{if}\quad \sigma = \frac{r_p}{5} \quad \Rightarrow \quad [\mathbf{u}]_V \simeq \mathbf{u} + \frac{r_p^2}{10}\Delta\mathbf{u}$$

$$[\mathbf{u}(\mathbf{x},t)]_S = \frac{1}{3r_p^2}\frac{\mathrm{d}}{\mathrm{d}r_p}\left(r_p^3\,[\mathbf{u}(\mathbf{x},t)]_V\right) = \mathcal{DFT}^{-1}\left[\left(1-\sigma^2\mathbf{k}^2/3\right)\tilde{G}(\mathbf{k})\tilde{\mathbf{u}}(\mathbf{k},t)\right]$$

Acceleration statistics of finite-sized particles in turbulent flow: the role of Faxen forces,
E. Calzavarini, R. Volk, M. Bourgoin, E. Leveque, J.-F. Pinton and F. Toschi,
J.Fluid Mech., 630, 179-189 (2009)

Eulerian Lagrangian



Particles with shape

Need of different reference frames

1) Lab frame (or inertial) $\mathbf{x} = (x, y, z)$

2) Particle frame (or principal axis) $\mathbf{x}' = (x', y', z')$

3) Comoving frame $\mathbf{x}'' = (x'', y'', z'')$

Dynamics of prolate ellipsoidal particles in a turbulent channel flow

P. H. Mortensen; H. I. Andersson; J. J. J. Gillissen; B. J. Boersma

Check for updates

Physics of Fluids 20, 093302 (2008)
https://doi.org/10.1063/1.2975209

Motion of the center of mass

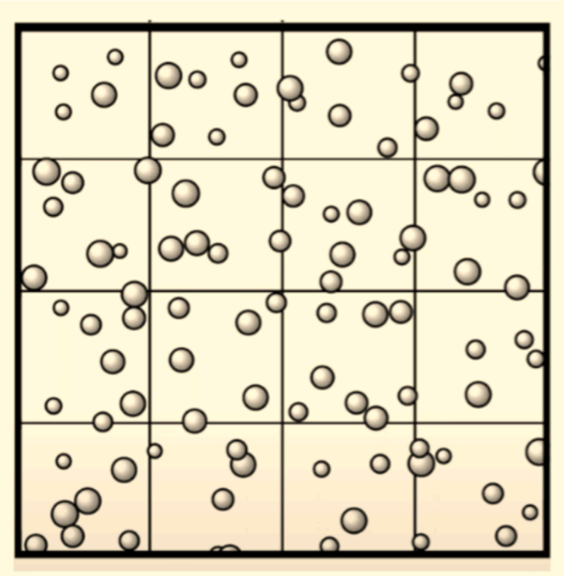
$\mathbf{x}' = \mathcal{A}\mathbf{x}''$ $\mathcal{A}(e_0, e_1, e_2, e_3)$ 3x3 Orthogonal matrix made of 4 Euler parameters a quaternion $\mathbf{q} = (e_0, e_1, e_2, e_3)$

$$\mathbf{K}' = \begin{pmatrix} k'_{xx} & 0 & 0 \\ 0 & k'_{yy} & 0 \\ 0 & 0 & k'_{zz} \end{pmatrix}$$

$$\mathbf{K} = \mathcal{A}^T \mathbf{K}' \mathcal{A}$$

$$m\frac{d\mathbf{v}}{dt} = \mathbf{F} = \mu \mathbf{A}^t \mathbf{K}' \mathbf{A}(\mathbf{u} - \mathbf{v})$$

Eulerian Lagrangian



Orientational dynamics

$$\frac{d}{dt}(\mathbb{I}\boldsymbol{\omega}_p) = \mathbf{T}$$

Lab frame

$$\mathbb{I}'\frac{d}{dt}(\boldsymbol{\omega}'_p) + \boldsymbol{\omega}'_p \wedge (\mathbb{I}'\boldsymbol{\omega}'_p) = \mathbf{T}'$$

Particle frame

Dynamics of prolate ellipsoidal particles in a turbulent channel flow

P. H. Mortensen; H. I. Andersson; J. J. J. Gillissen; B. J. Boersma

Physics of Fluids 20, 093302 (2008)
https://doi.org/10.1063/1.2975209

$\mathbb{I} = \mathcal{A}^T \mathbb{I}' \mathcal{A}$ $\mathbb{I}'$ is a diagonal matrix

$\mathbf{T}' = \mathcal{A}\mathbf{T}$ computed from Jeffery Torque model $\mathbf{T}'(\omega'_p, \nabla \mathbf{u}')$

Kinematic evolution

$$\frac{d\mathbf{q}}{dt} = \frac{1}{2}\mathcal{A}_q \mathbf{q}$$

$\mathcal{A}_q(\omega'_p)$ 4x4 matrix

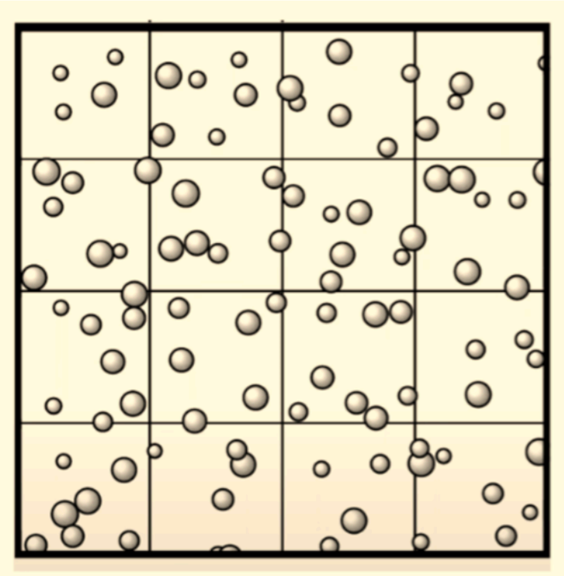
$||\mathbf{q}|| = 1$ condition to be checked at each time step

$$\begin{pmatrix} \dot{e}_0 \\ \dot{e}_1 \\ \dot{e}_2 \\ \dot{e}_3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} e_0 & -e_1 & -e_2 & -e_3 \\ e_1 & e_0 & -e_3 & e_2 \\ e_2 & e_3 & e_0 & -e_1 \\ e_3 & -e_2 & e_1 & e_0 \end{pmatrix}\begin{pmatrix} 0 \\ \omega'_x \\ \omega'_y \\ \omega'_z \end{pmatrix}$$

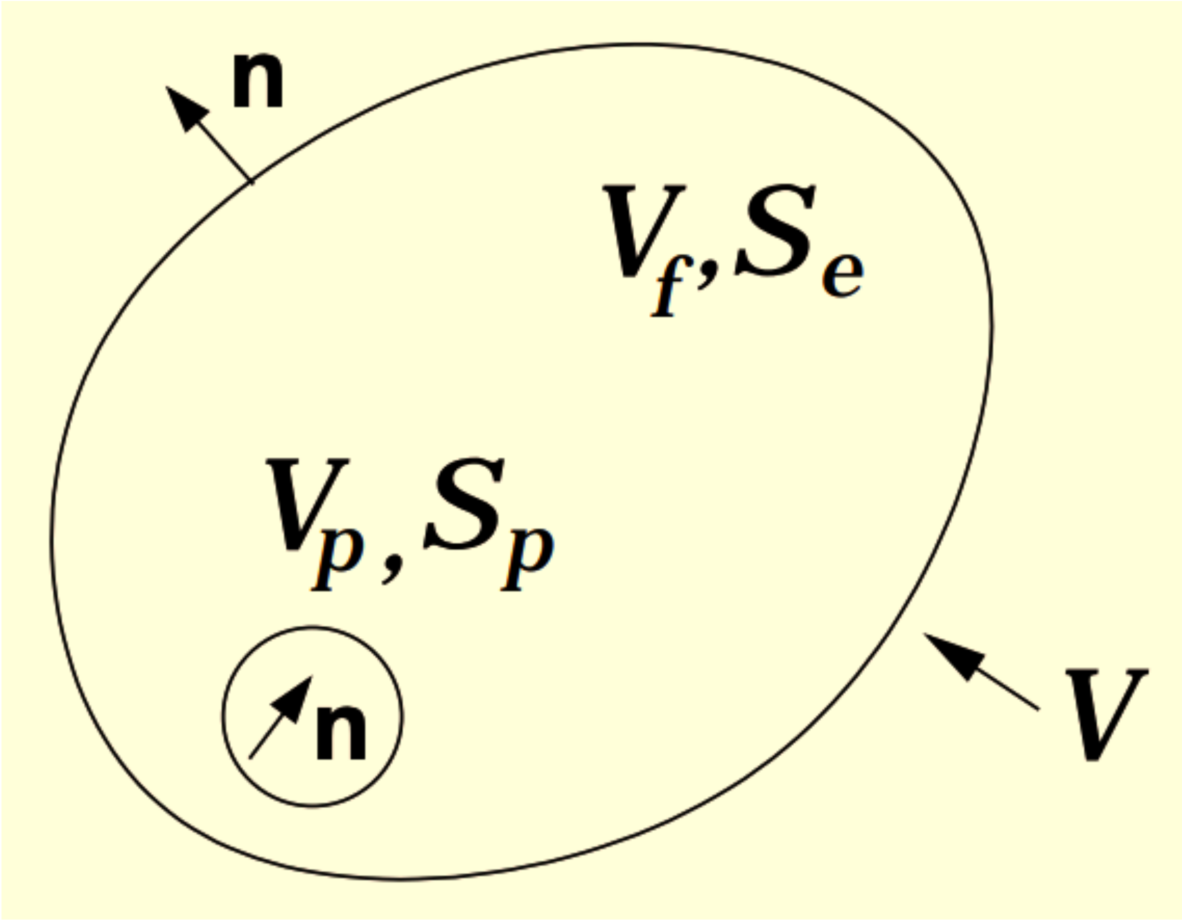
$$e_i = \frac{e_i}{\sqrt{e_0^2 + e_1^2 + e_2^2 + e_3^2}}$$

$$e_0^2 + e_1^2 + e_2^2 + e_3^2 = 1$$

Eulerian-Lagrangian



Two-way coupling



$$\mathcal{V} = \mathcal{V}_f + \mathcal{V}_p$$

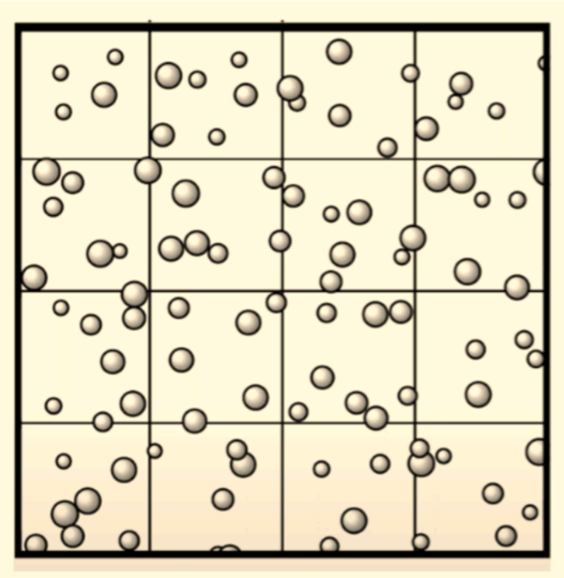
$$\int_{\mathcal{V}_f} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{S_e} \boldsymbol{\sigma} \cdot \mathbf{n} dS + \int_{S_p} \boldsymbol{\sigma} \cdot \mathbf{n} dS + \int_{\mathcal{V}_f} \rho_f \mathbf{g} d\mathcal{V}$$

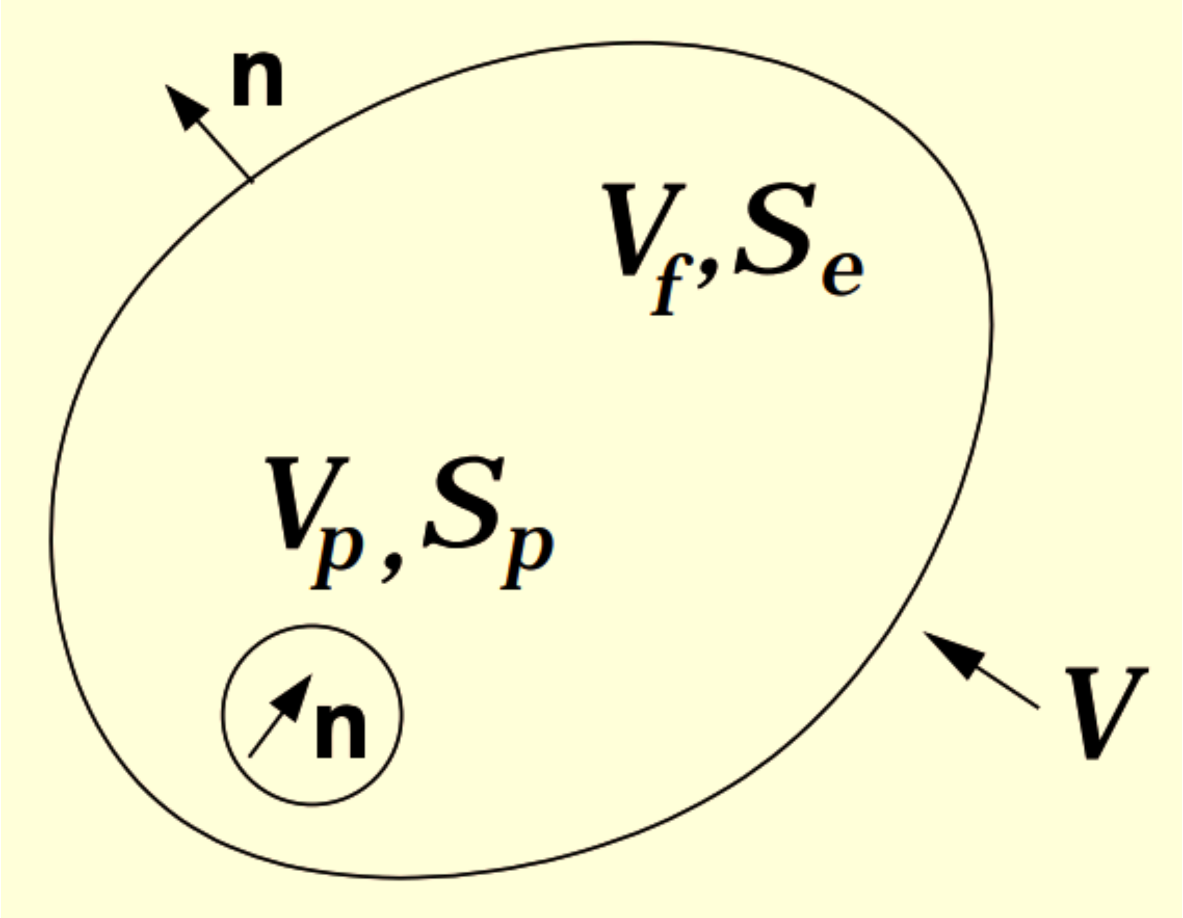
Momentum conservation eq.
For the fluid

$$\rho_p \mathcal{V}_p \frac{d\mathbf{v}}{dt} = -\int_{S_p} \boldsymbol{\sigma} \cdot \mathbf{n} dS + \rho_p \mathcal{V}_p \mathbf{g}$$

Eq. Of motion for the particle

Eulerian-Lagrangian





Two-way coupling

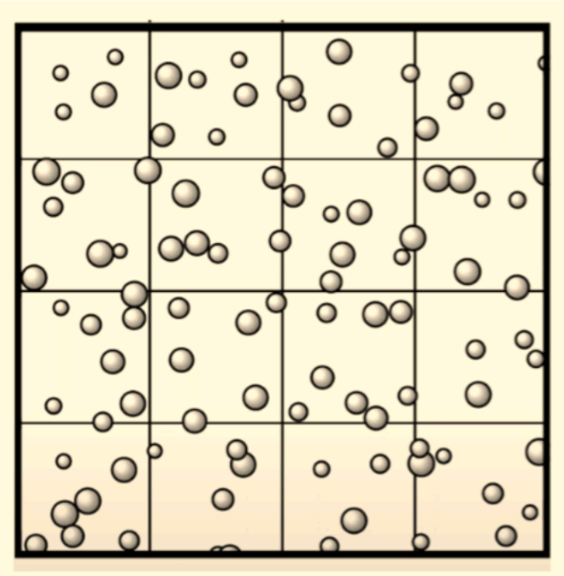
1.add the two equations

$$\int_{\mathcal{V}_f} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} + \rho_p \mathcal{V}_p \frac{d\mathbf{v}}{dt} = \int_{S_e} \boldsymbol{\sigma} \cdot \mathbf{n} dS + \int_{\mathcal{V}_f} \rho_f \mathbf{g} d\mathcal{V} + \rho_p \mathcal{V}_p \mathbf{g}$$

2.add the term $\int_{\mathcal{V}_p} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V}$ on both sides and use $\mathcal{V} = \mathcal{V}_f + \mathcal{V}_p$

$$\int_{\mathcal{V}} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{S_e} \boldsymbol{\sigma} \cdot \mathbf{n} \, dS + \int_{\mathcal{V}_f} \rho_f \mathbf{g} d\mathcal{V} + \rho_p \mathcal{V}_p \mathbf{g} + \int_{\mathcal{V}_p} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} - \rho_p \mathcal{V}_p \frac{d\mathbf{v}}{dt}$$

Eulerian Lagrangian



3. Use Gauss theorem

$$\int_{\mathcal{V}} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{\mathcal{V}} \nabla \cdot \boldsymbol{\sigma} + \rho_f \mathbf{g} \, d\mathcal{V} + \int_{\mathcal{V}_p} \rho_f (\frac{D\mathbf{u}}{Dt} - \mathbf{g}) d\mathcal{V} + \rho_p (\mathcal{V}_p \mathbf{g} - \mathcal{V}_p \frac{d\mathbf{v}}{dt})$$

$$\int_{\mathcal{V}} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{\mathcal{V}} \nabla \cdot \boldsymbol{\sigma} + \rho_f \mathbf{g} \, d\mathcal{V} + \int_{\mathcal{V}_p} \rho_f (\frac{D\mathbf{u}}{Dt} - \mathbf{g}) + \rho_p (\mathbf{g} - \frac{d\mathbf{v}}{dt}) d\mathcal{V}$$

Heavyside theta function

$$\int_{\mathcal{V}} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{\mathcal{V}} \nabla \cdot \boldsymbol{\sigma} + \rho_f \mathbf{g} \, d\mathcal{V} + \int_{\mathcal{V}} \left[\rho_f (\frac{D\mathbf{u}}{Dt} - \mathbf{g}) + \rho_p (\mathbf{g} - \frac{d\mathbf{v}}{dt}) \right] \Theta(\mathbf{x} - \mathbf{x}_p) d\mathcal{V}$$

4. assuming that the flow gradients are constant over the particle (or assuming point-like particles)

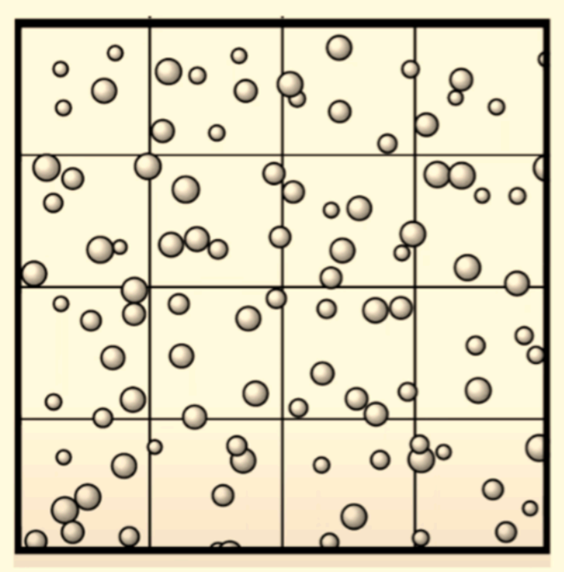
$$\int_{\mathcal{V}} \rho_f \frac{D\mathbf{u}}{Dt} d\mathcal{V} = \int_{\mathcal{V}} \nabla \cdot \boldsymbol{\sigma} + \rho_f \mathbf{g} \, d\mathcal{V} + \int_{\mathcal{V}} \left[\rho_f (\frac{D\mathbf{u}}{Dt} - \mathbf{g}) + \rho_p (\mathbf{g} - \frac{d\mathbf{v}}{dt}) \right] \mathcal{V}_p \delta(\mathbf{x} - \mathbf{x}_p) d\mathcal{V}$$

Dirac delta function

5. Consider that the volume V is arbitrary —> eq. In differential (local) form

Squires & Eaton (1990); Elghobashi & Truesdell (1993); Boivin et al. (1998), Mazzitelli (2003)

Eulerian Lagrangian



Single particle feedback on the flow

$$\frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{g} + \mathbf{a}_{pf} \qquad \mathbf{a}_{pf} = \left[\frac{D\mathbf{u}}{Dt} - \mathbf{g} + \frac{\rho_p}{\rho_f}(\mathbf{g} - \frac{d\mathbf{v}}{dt})\right] \frac{\mathcal{V}_p}{\mathcal{V}} \delta(\mathbf{x} - \mathbf{x}_p) \qquad \boldsymbol{\sigma} = -p\mathcal{I} + \mu_f(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$$

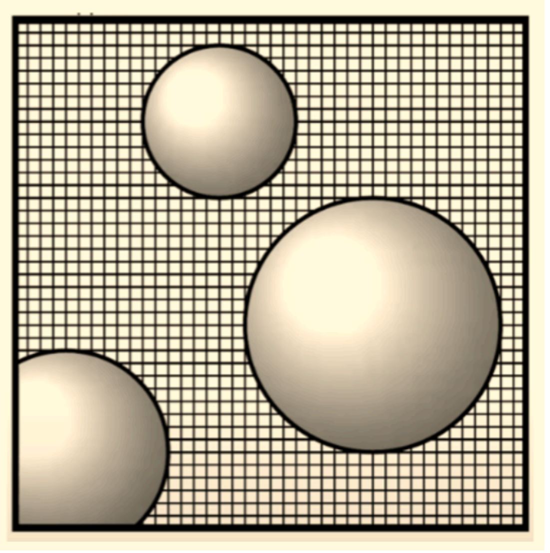
Many particles

$$\mathbf{a}_{pf} = \Sigma_{i=1}^{N} \left[\frac{D\mathbf{u}}{Dt} - \mathbf{g} + \frac{\rho_p}{\rho_f}(\mathbf{g} - \frac{d\mathbf{v}}{dt})\right] \frac{\mathcal{V}_p}{\mathcal{V}} \delta(\mathbf{x} - \mathbf{x}_p)$$

Eulerian description

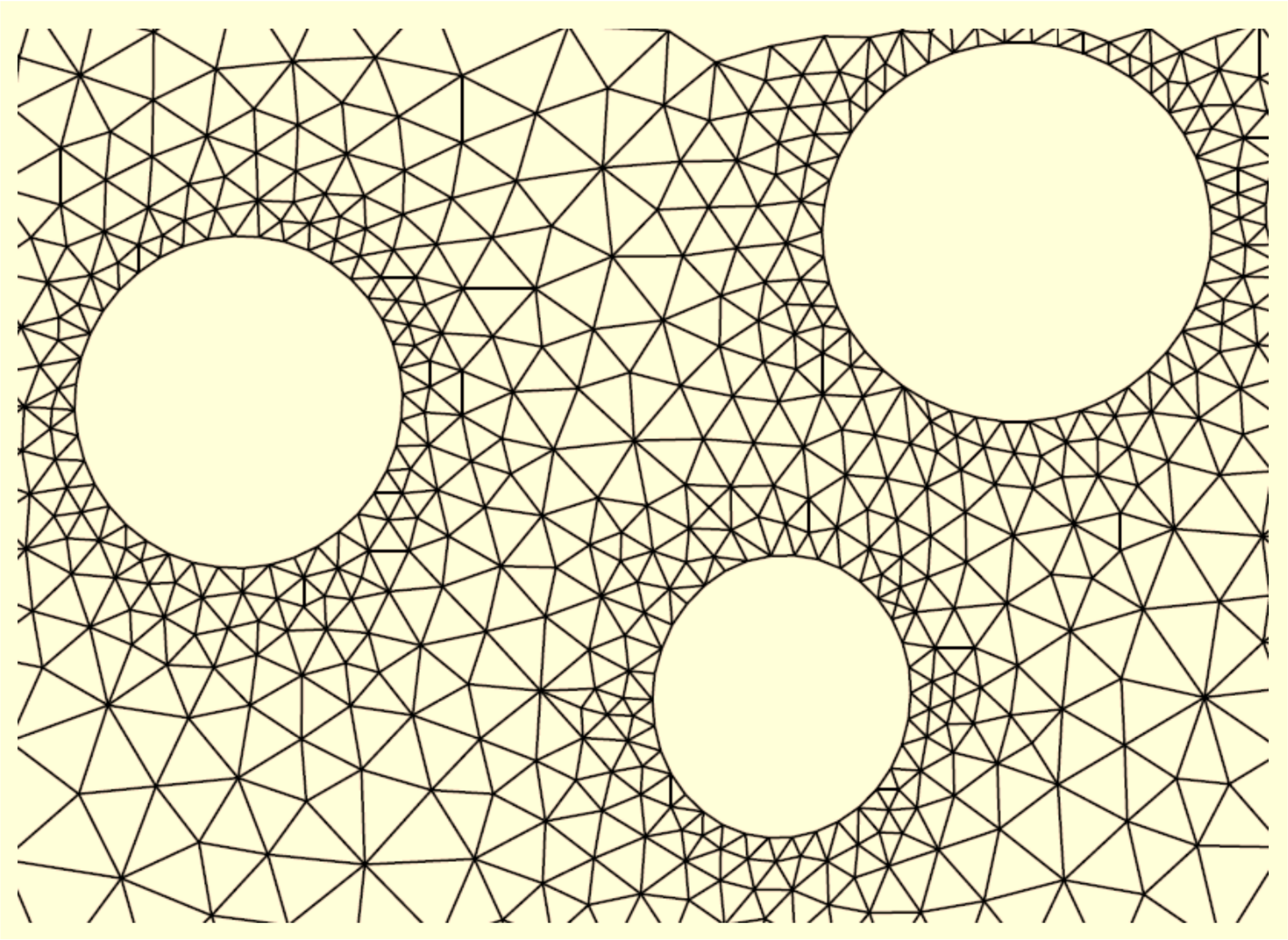
$$\mathbf{a}_{pf} = \left[\frac{D\mathbf{u}}{Dt} - \mathbf{g} + \frac{\rho_p}{\rho_f}(\mathbf{g} - \frac{d\mathbf{v}}{dt})\right] \mathcal{V}_p \; n(\mathbf{x}, \mathbf{t})$$ number density

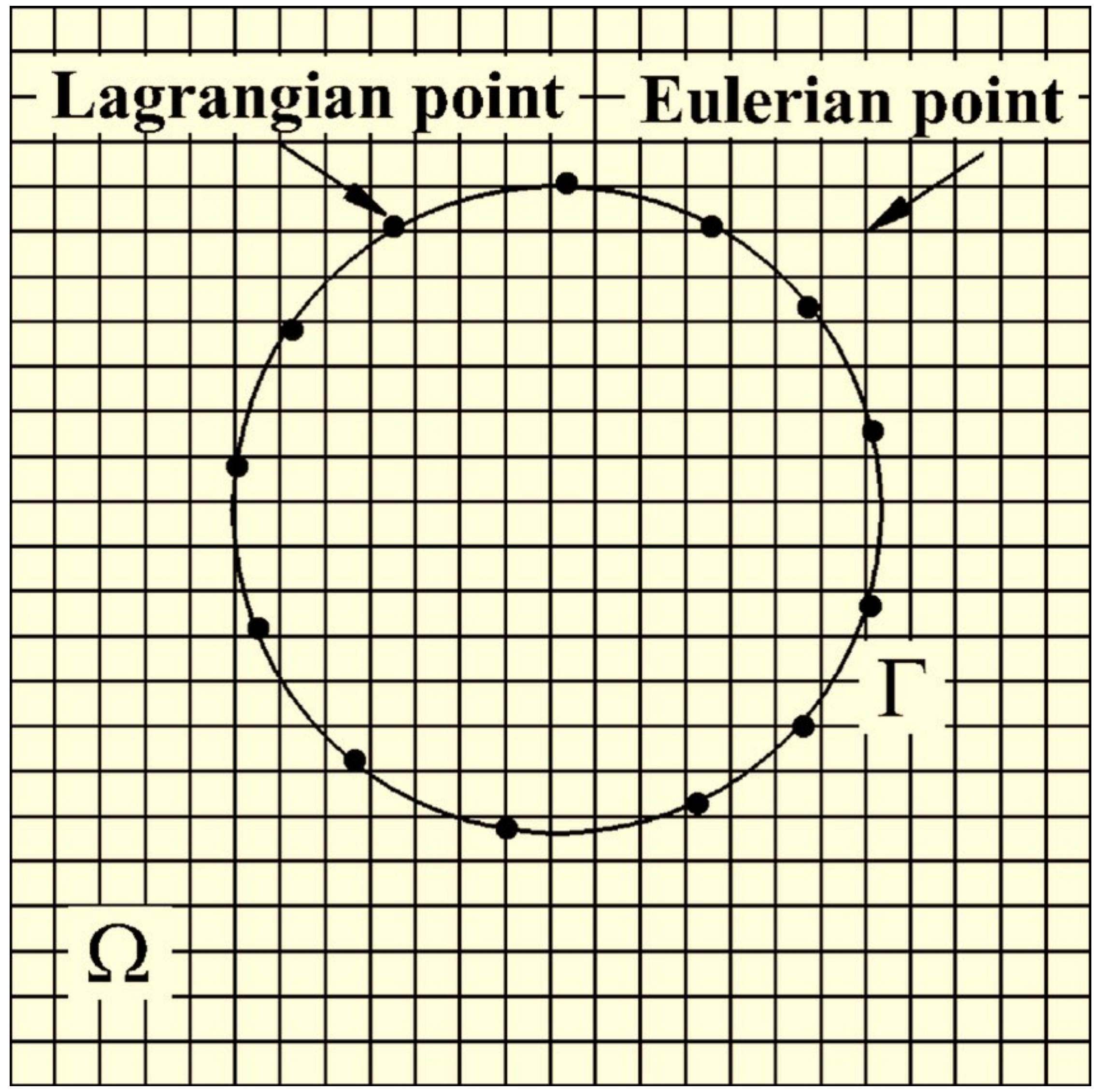
$$\mathbf{a}_{pf} = \left[\frac{D\mathbf{u}}{Dt} - \mathbf{g} + \frac{\rho_p}{\rho_f}(\mathbf{g} - \frac{d\mathbf{v}}{dt})\right] \Phi_p(\mathbf{x}, \mathbf{t})$$ volume density

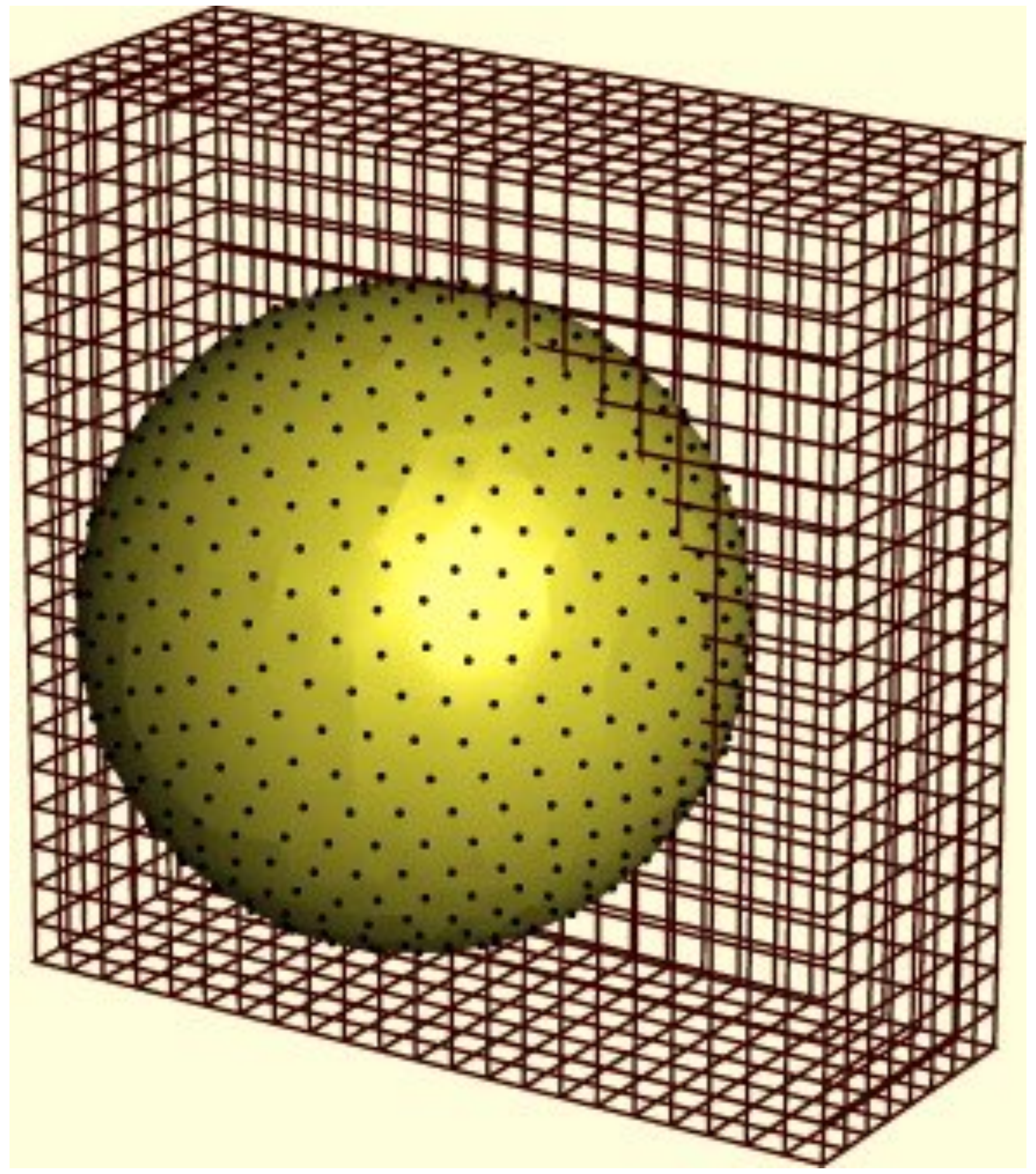


Particle-resolved

The real DNS

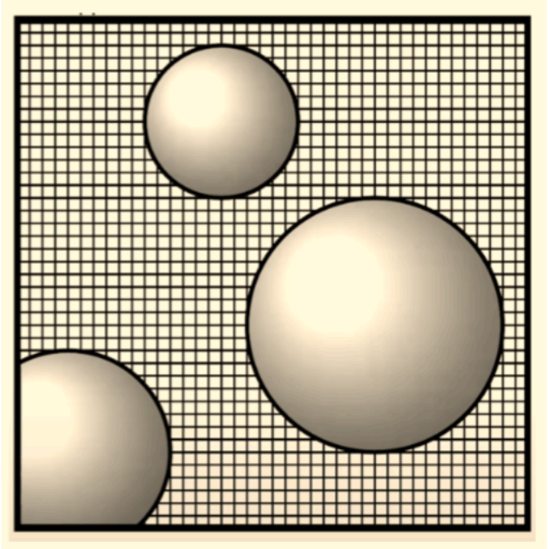






Body fitted

Fictitious domain



Particle-resolved

Penalisation method

$$\nabla \cdot \mathbf{u} = 0$$
$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} - \frac{\chi_s}{\eta}(\mathbf{u} - \mathbf{u}_s)$$

Penalization force

$$\mathbf{F} = \frac{\chi_s}{\eta}(\mathbf{u} - \mathbf{u}_s)$$

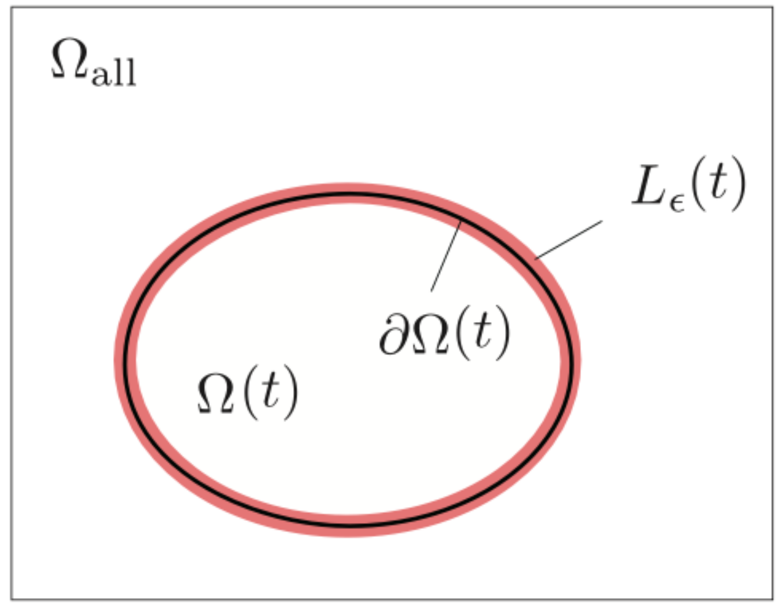
$$\chi_s(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \mathbf{x} \in \Omega_s(t) \\ 0 & \text{otherwise} \end{cases}$$

$\eta \ll 1$ penalization factor

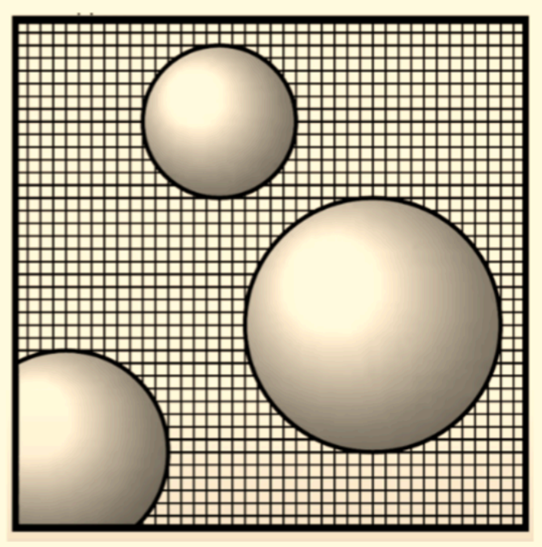
stress integration method to compute force and torque on the particle

$$\boldsymbol{\mathcal{F}}_f = \int_{\partial \Omega_s} \sigma \cdot \mathbf{n} dS \qquad \boldsymbol{\mathcal{T}}_f = \int_{\partial \Omega_s} \mathbf{r} \times \sigma \cdot \mathbf{n} dS$$

See: Erwan Liberge, Claudine Béghein. A comparison of force computations for modeling fluid - structure interaction problems with the lattice Boltzmann volume penalisation method. Discrete and Continuous Dynamical Systems - Series S, 2024, 17, pp.2420 - 2435.



Particle-resolved



Immersed Boundary Method

IB (body) force

$$\nabla \cdot \boldsymbol{u} = 0,$$

$$\rho_{\mathrm{f}}\left[\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right] = -\nabla p + \mu\nabla^2\boldsymbol{u} + \boldsymbol{g}$$

$$M\frac{d\boldsymbol{U}_{\mathrm{c}}}{dt} = \boldsymbol{F},$$

$$\boldsymbol{I}_{\mathrm{B}}\frac{d^{\mathrm{B}}\boldsymbol{\Omega}_{\mathrm{c}}}{dt} + {}^{\mathrm{B}}\boldsymbol{\Omega}_{\mathrm{c}} \times (\boldsymbol{I}_{\mathrm{B}}{}^{\mathrm{B}}\boldsymbol{\Omega}_{\mathrm{c}}) = \boldsymbol{S}^{\mathrm{T}}\boldsymbol{T}.$$

$$\boldsymbol{F}(t) = \boldsymbol{F}_{\mathrm{tot}}(t) + \boldsymbol{F}_{\mathrm{in}}(t).$$

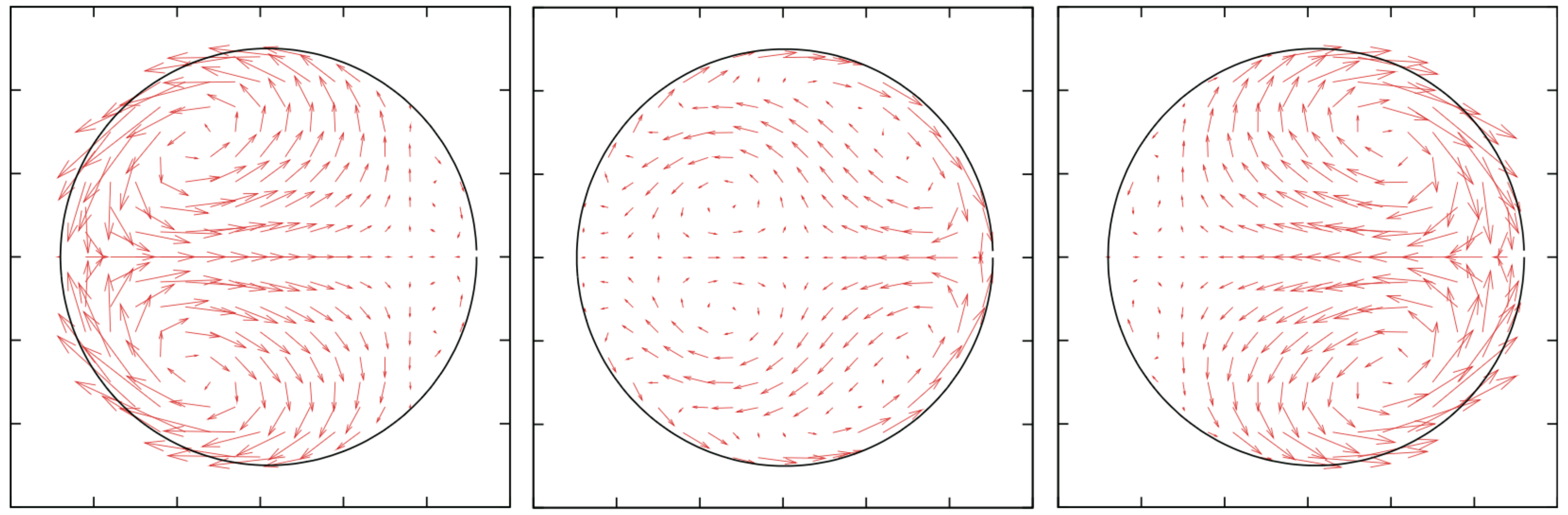
$$\boldsymbol{F}_{\mathrm{tot}}(t) = -\int_{\boldsymbol{x}\in L_\epsilon(t)} \boldsymbol{g}(\boldsymbol{x},t)\,d\boldsymbol{x}.$$

$$\boldsymbol{F}_{\mathrm{in}}(t) = \rho_{\mathrm{f}}\frac{d}{dt}\int_{\boldsymbol{x}\in\Omega(t)} \boldsymbol{u}(\boldsymbol{x},t)\,d\boldsymbol{x}.$$

$$\boldsymbol{T}(t) = \boldsymbol{T}_{\mathrm{tot}}(t) + \boldsymbol{T}_{\mathrm{in}}(t),$$

$$\boldsymbol{T}_{\mathrm{tot}}(t) = -\int_{\boldsymbol{x}\in L_\epsilon(t)} [\boldsymbol{x} - \boldsymbol{X}_{\mathrm{c}}(t)] \times \boldsymbol{g}(\boldsymbol{x},t)\,d\boldsymbol{x},$$

$$\boldsymbol{T}_{\mathrm{in}}(t) = \rho_{\mathrm{f}}\frac{d}{dt}\int_{\boldsymbol{x}\in\Omega(t)} [\boldsymbol{x} - \boldsymbol{X}_{\mathrm{c}}(t)] \times \boldsymbol{u}(\boldsymbol{x},t)\,d\boldsymbol{x}$$



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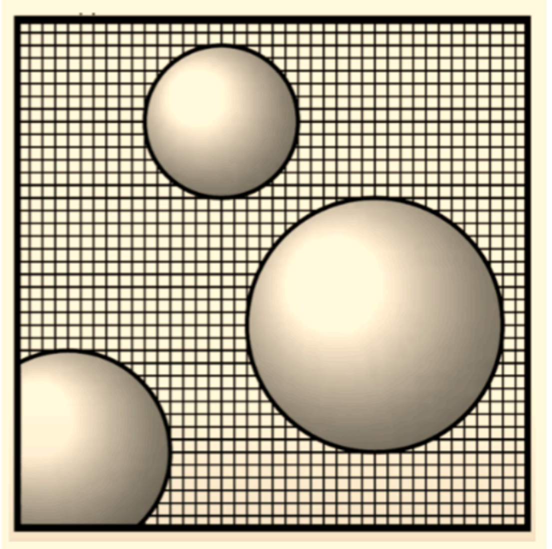
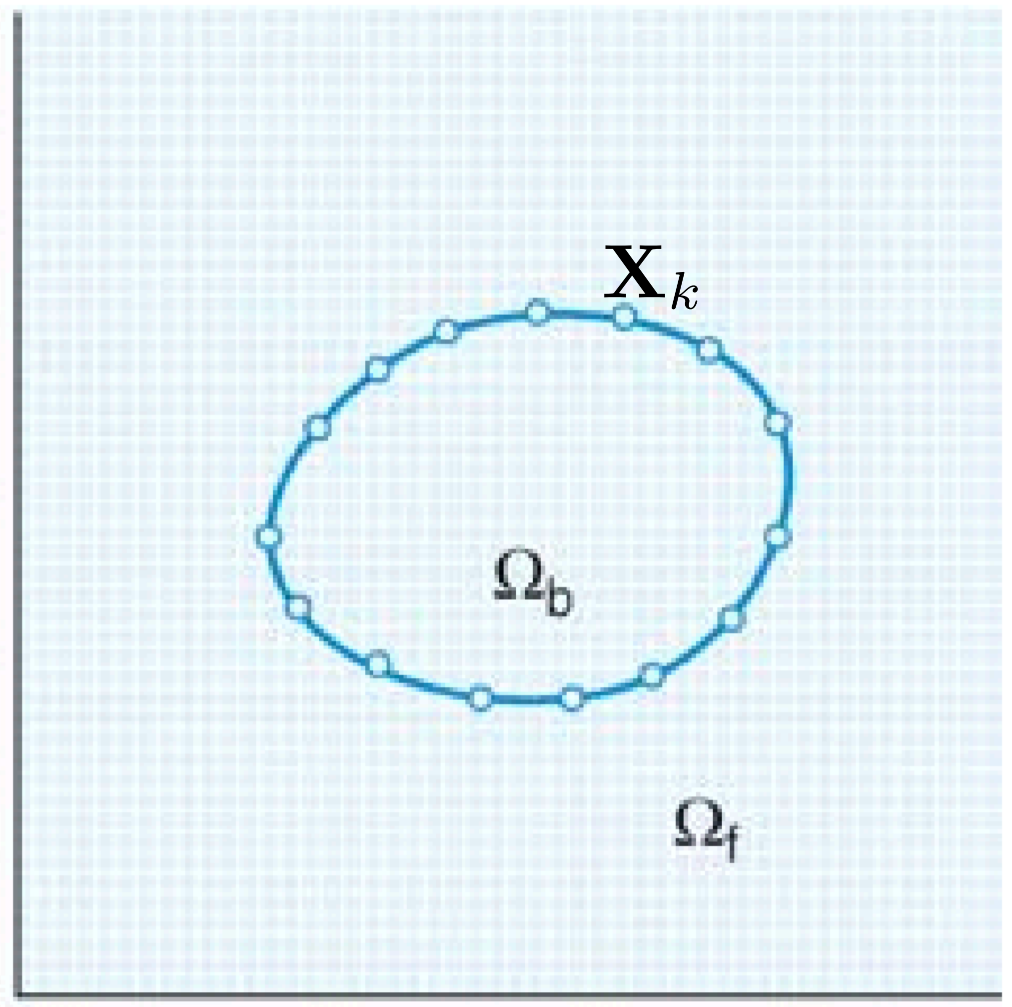
Effect of internal mass in the simulation of a moving body by the immersed boundary method

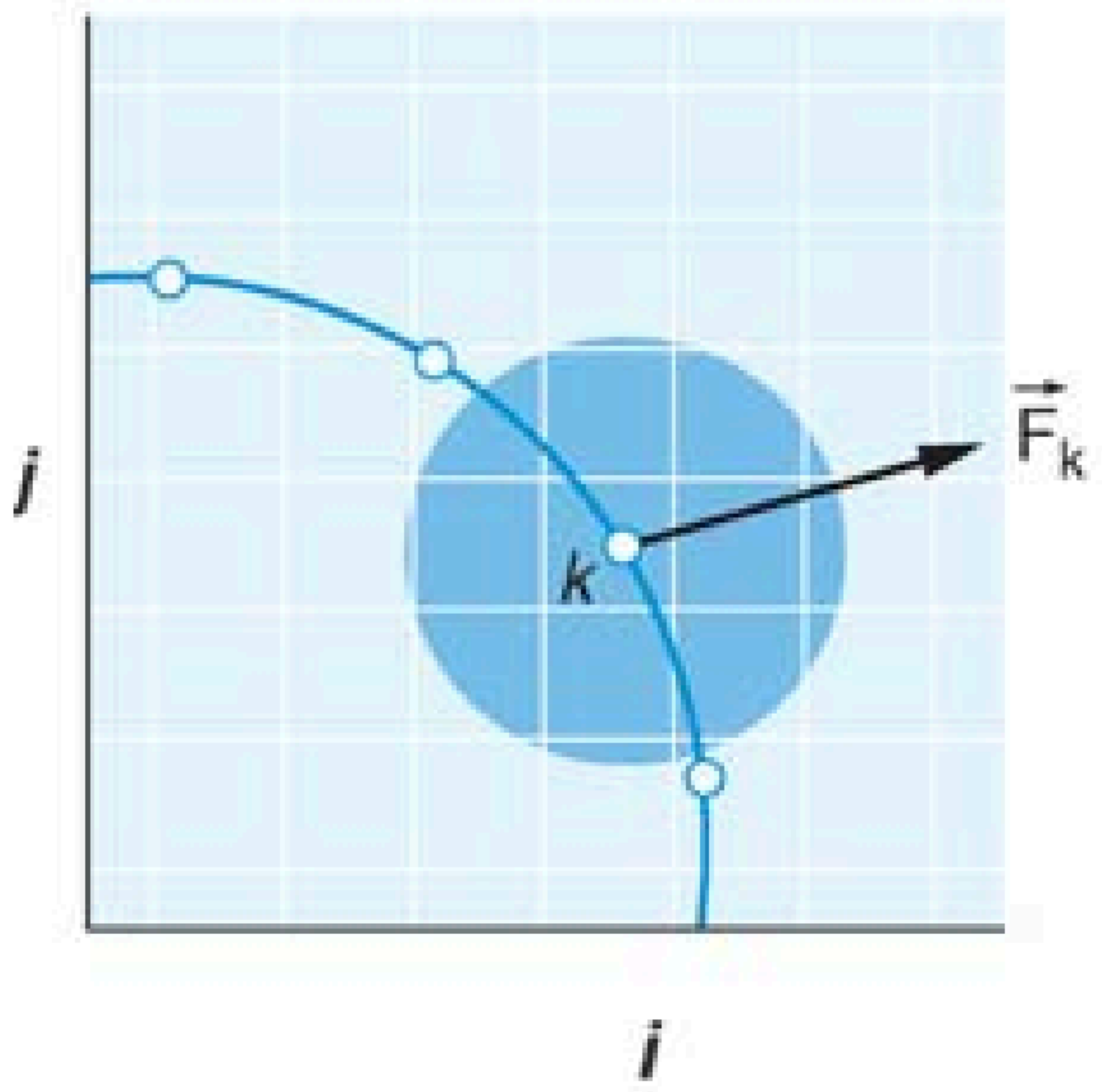
Kosuke Suzuki [a], Takaji Inamuro [a,b,*]

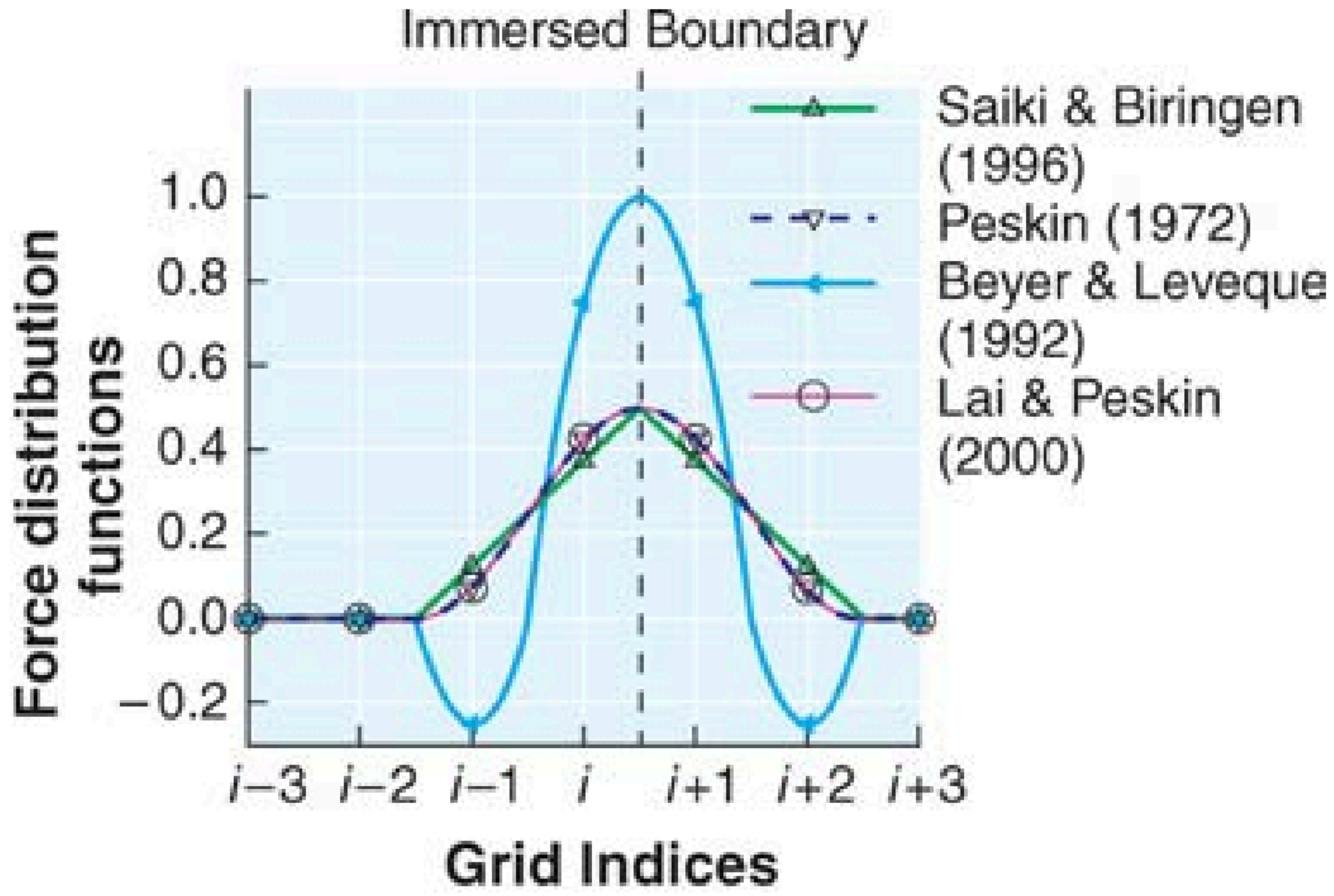
Particle-resolved

Immersed Boundary Method







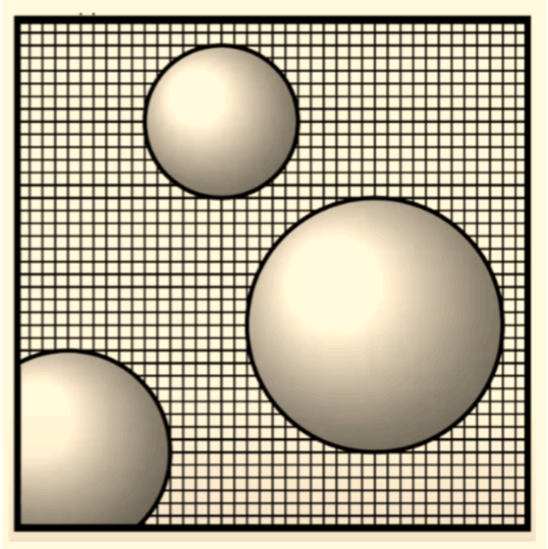


$\boldsymbol{X}_k(t+\Delta t)$ and $\boldsymbol{U}_k(t+\Delta t)(k=1,\ldots,N)$ are Lagrangian particle interface marker points

known $\boldsymbol{u}(\boldsymbol{x},t)$ and $p(\boldsymbol{x},t)$ $\longrightarrow$ $\boldsymbol{u}_i^*(\boldsymbol{x},t+\Delta t)$ evolved velocity without the body force

Particle-resolved

Immersed Boundary Method



How to compute and apply the IB force? Multi Direct Forcing method

$$\boldsymbol{u}^*(\boldsymbol{X}_k, t+\Delta t) = \sum_{\boldsymbol{x}} \boldsymbol{u}^*(\boldsymbol{x}, t+\Delta t) W(\boldsymbol{x}-\boldsymbol{X}_k)(\Delta x)^d$$

$$\boldsymbol{g}_0(\boldsymbol{X}_k, t+\Delta t) = \frac{\boldsymbol{U}_k - \boldsymbol{u}^*(\boldsymbol{X}_k, t+\Delta t)}{\Delta t}$$

Step 1 $$\boldsymbol{g}_\ell(\boldsymbol{x}, t+\Delta t) = \sum_{k=1}^{N} \boldsymbol{g}_\ell(\boldsymbol{X}_k, t+\Delta t) W(\boldsymbol{x}-\boldsymbol{X}_k)\Delta V,$$

Step 2 $$\boldsymbol{u}_\ell(\boldsymbol{x}, t+\Delta t) = \boldsymbol{u}^*(\boldsymbol{x}, t+\Delta t) + \Delta t\, \boldsymbol{g}_\ell(\boldsymbol{x}, t+\Delta t)$$

Step 3 $$\boldsymbol{u}_\ell(\boldsymbol{X}_k, t+\Delta t) = \sum_{\boldsymbol{x}} \boldsymbol{u}_\ell(\boldsymbol{x}, t+\Delta t) W(\boldsymbol{x}-\boldsymbol{X}_k)(\Delta x)^d$$

Step 4 $$\boldsymbol{g}_{\ell+1}(\boldsymbol{X}_k, t+\Delta t) = \boldsymbol{g}_\ell(\boldsymbol{X}_k, t+\Delta t) + \frac{\boldsymbol{U}_k - \boldsymbol{u}_\ell(\boldsymbol{X}_k, t+\Delta t)}{\Delta t}$$

Peskin 1972 weighting function

$$W(x,y,z) = \frac{1}{\Delta x} w\left(\frac{x}{\Delta x}\right) \cdot \frac{1}{\Delta x} w\left(\frac{y}{\Delta x}\right) \cdot \frac{1}{\Delta x} w\left(\frac{z}{\Delta x}\right),$$

$$w(r) = \begin{cases} \frac{1}{8}\left(3 - 2|r| + \sqrt{1 + 4|r| - 4r^2}\right), & |r| \leqslant 1 \\ \frac{1}{8}\left(5 - 2|r| - \sqrt{-7 + 12|r| - 4r^2}\right), & 1 \leqslant |r| \leqslant 2 \\ 0, & \text{otherwise.} \end{cases}$$

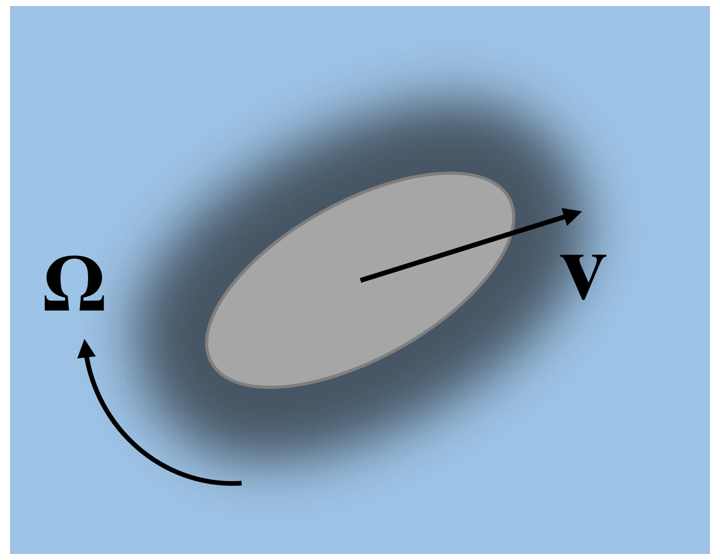
After ~5 iterations b.c. are satisfied at the Lagrangian points

Auxiliary particle models

$$\mathbf{F} = \oint_{S_p} \boldsymbol{\sigma} \cdot \mathbf{n} \; dS$$

$$\mathbf{T} = \oint_{S_p} (\mathbf{x} - \mathbf{r}) \times (\boldsymbol{\sigma} \cdot \mathbf{n}) \; dS$$

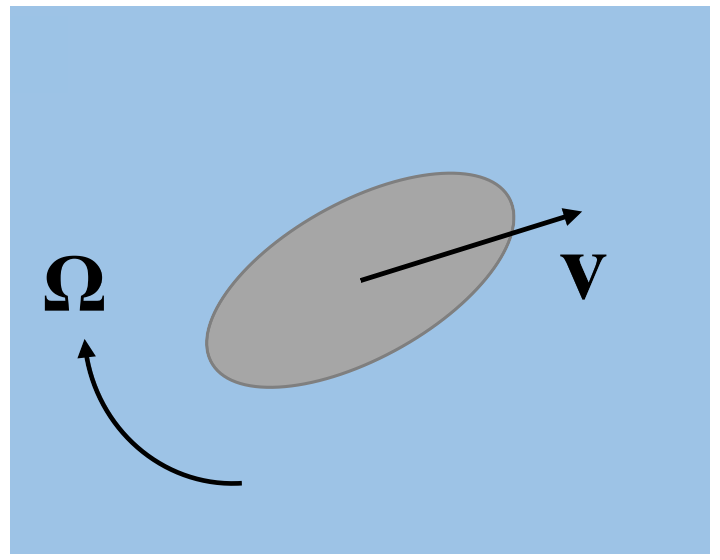
Real Particles (RP)



$$\mathbf{F}_{VP} = \int_{V_p} \rho \frac{D\mathbf{u}}{Dt} d^3x$$

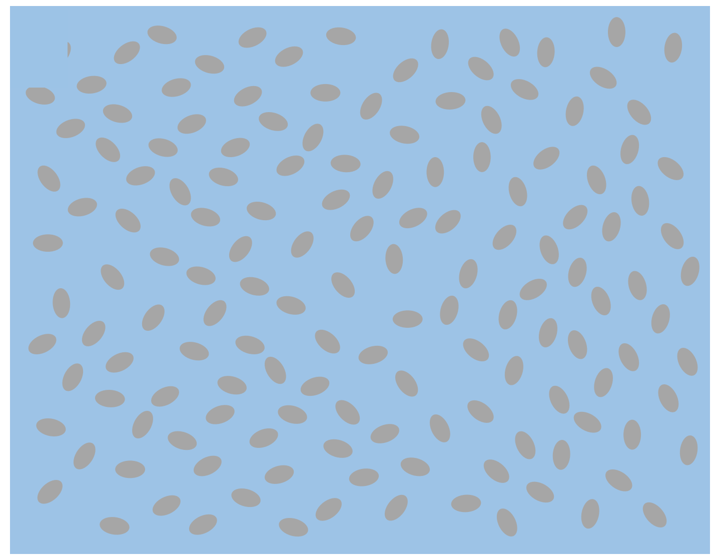
$$\mathbf{T}_{VP} = \int_{V_p} (\mathbf{x} - \mathbf{r}) \times \rho \frac{D\mathbf{u}}{Dt} d^3x$$

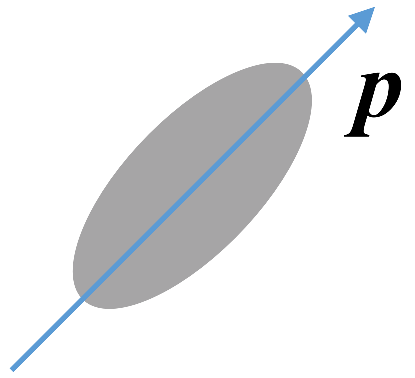
Virtual Particles (VP)



Zero inertia particles

Jeffery fluid tracers (JFT)



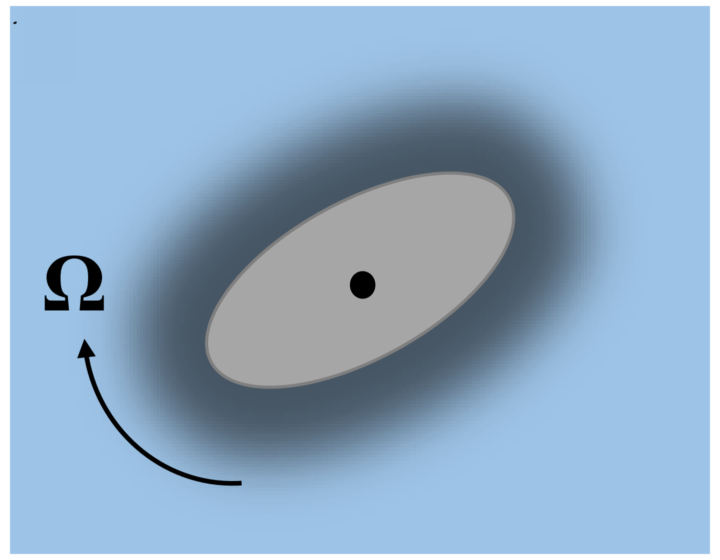


$$\dot{\mathbf{r}} = \mathbf{u}(\mathbf{r}(t), t),$$

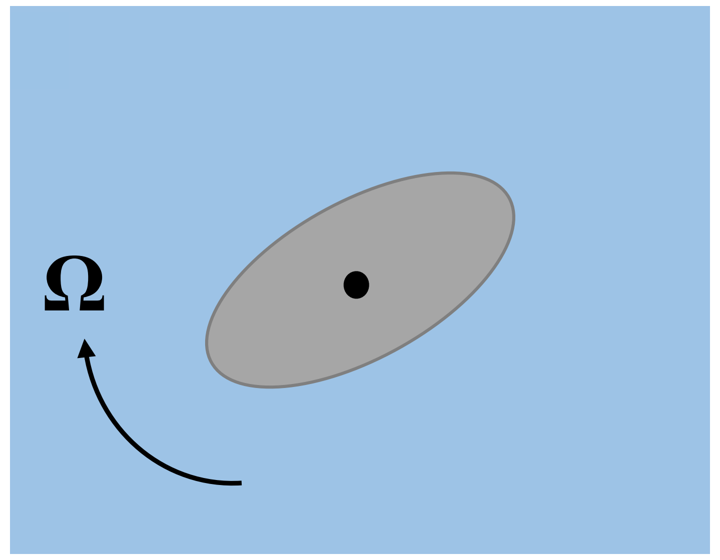
$$\dot{\mathbf{p}} = \boldsymbol{\Omega} \times \mathbf{p}$$ Jeffery (1922)

$$\boldsymbol{\Omega} = \frac{1}{2}\boldsymbol{\omega}(\mathbf{r}(t), t) + \Lambda \; \mathbf{p} \times \mathcal{S}(\mathbf{r}(t), t)\mathbf{p}$$

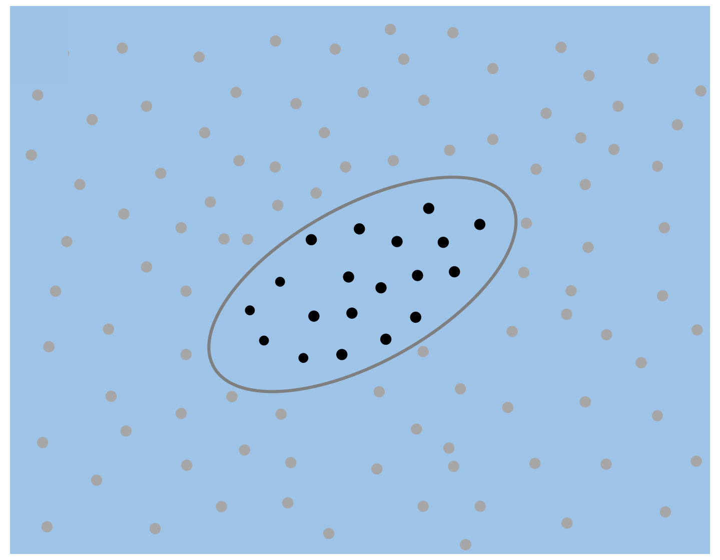
$$\Lambda = \frac{\alpha^2 - 1}{\alpha^2 + 1}$$



Real Particles Fixed Location (RPFL)



Virtual Particles Fixed Location (VPFL)



Volume Averages (VA)

$$\mathbf{a}_{VA} = \frac{1}{V_p} \int_{V_p} \frac{D\mathbf{u}}{Dt} d^3x$$

$$\boldsymbol{\Omega}_{VA} = \frac{1}{V_p} \int_{V_p} \nabla \times \mathbf{u} \; d^3x$$

Numerical Experiments	Model Equations
Real Particles (RP)	NSE + NEE + IBM
Volume Averages (VA)	NSE
Virtual Particles (VP)	NSE + NEE
Real Particles with Fixed Locations (RPFL)	NSE + EE + IBM
Virtual Particles with Fixed Locations (VPFL)	NSE + EE
Jeffery Fluid Tracers (JFT)	NSE + tracer eq.+ Jeffery eq.

Dynamics of finite-size spheroids in turbulent flow: the roles of flow structures and particle boundary layers, L. Jiang, C. Wang, S. Liu, C. Sun, E. Calzavarini, **J. Fluid Mech** (2022)

Hands on session

Simulations to the people!

Goal: Everyone can do CFD

- Solve the Navier-Stokes equation in 2D, fully understanding the code
- Simulate inertial particle dispersion
- Visualize and analyze particle clustering

We will use Python (v3) and jupyter notebook

See https://github.com/ecalzavarini/copartcoflow

NS in Fourier space

$$\hat{\mathbf{v}}(\mathbf{k}) = \mathcal{F}(\mathbf{v}(\mathbf{k}))$$

$\hat{\mathbf{v}}(\mathbf{k}) = \mathcal{FFT}(\mathbf{v}(\mathbf{k}))$ $O(N \log_2 N)$ operations

$$\mathbf{v}(\mathbf{x}) \to \hat{\mathbf{v}}(\mathbf{k})$$
$$\nabla^2 \to -k^2$$
$$\nabla \to i\mathbf{k}$$

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{f}$$
$$\nabla \cdot \mathbf{v} = 0$$

$$\partial_t \hat{\mathbf{v}} + \hat{\mathbf{v}} * i\mathbf{k}\hat{\mathbf{v}} = -i\mathbf{k}\hat{p} - \nu \mathbf{k}^2 \hat{\mathbf{v}} + \hat{\mathbf{f}}$$
$$i\mathbf{k} \cdot \hat{\mathbf{v}} = 0$$

$$(f * g)(t) := \int_{-\infty}^{\infty} f(\tau) g(t - \tau)\, d\tau$$

$$(f * g)[n] = \sum_{m=-\infty}^{\infty} f[m] g[n - m]$$

$O(N^2)$ operations

Pseudo-spectral method

Treatment of non-linear and forcing terms

$$\hat{\mathbf{v}} * i\mathbf{k}\hat{\mathbf{v}} = \mathcal{FFT}(\mathbf{v} \cdot \mathcal{FFT}^{-1}(i\mathbf{k}\hat{\mathbf{v}}))$$ + dealiasing $k_i < \frac{2}{3}k_{max}$

$$r.h.s. \equiv -\hat{\mathbf{v}} * i\mathbf{k}\hat{\mathbf{v}} + \hat{\mathbf{f}}$$

$$\partial_t \hat{\mathbf{v}} = r.h.s. \quad \Rightarrow \quad \hat{\mathbf{v}}^{(n+1)} = \hat{\mathbf{v}}^{(n)} + \Delta t \; r.h.s.^{(n)}$$

Explicit Euler

Pressure gradient

$$\mathbf{r.h.s.} = \nabla \times \mathbf{A} + \nabla P$$

$$\nabla \cdot (\mathbf{r.h.s.}) = \nabla^2 P \quad \Rightarrow \quad i\mathbf{k} \cdot \widehat{\mathbf{r.h.s.}} = -\mathbf{k}^2 \hat{P}$$

Pressure correction step

$$\hat{\mathbf{v}}^{(n+1)} \leftarrow \hat{\mathbf{v}}^{(n+1)} - \Delta t \; i\mathbf{k}\hat{P}$$

Treatment of viscous dissipation

$$\frac{\partial \mathbf{v}}{\partial t} = \nu \nabla^2 \mathbf{v} \quad \Rightarrow \quad \frac{\hat{\mathbf{v}}^{(n+1)} - \hat{\mathbf{v}}^{(n)}}{\Delta t} = -\nu k^2 \hat{\mathbf{v}}^{(n+1)}$$

Implicit Euler

Thanks

www.ecalzavarini.info