Some problems and simulation methods motivated by the modeling of particle–laden flows

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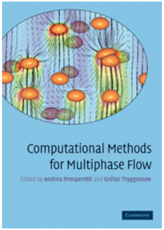
Computational Methods for Multiphase Flows, '07

- Many aspects of the modelling issues are unclear or questionable.
- Changing a "detail" might drastically modify the structure of the PDEs system



The formulation of a satisfactory set of averaged-equations models emerges as the single highest priority in the modeling of complex multiphase flows. [...] It seems justified to take a pragmatic view of the situation, using the available models and methods with open eyes and full awareness of their potential limitations. An exploration of the sensitivity of the results to the constitutive relations, parameter values, and numerics [...] becomes a vital necessity in this field

A. Prosperetti, G. Tryggvason.

A hydrodynamic system for mixture flows

Unknowns

Particle volume fraction ϕ, particle bulk velocity V, carrier fluid velocity u, pressure p

Incompressibility assumption

Mass densities of each phase $\bar{\rho}_p, \bar{\rho}_f$ are constant

Equations (1D)

Mass conservation and momentum balance

$$\partial_t(\bar{\rho}_p \phi) + \partial_x(\bar{\rho}_p \phi V) = 0,$$

$$\partial_t(\bar{\rho}_f (1-\phi)) + \partial_x(\bar{\rho}_f (1-\phi) u) = 0,$$

$$\partial_t(\bar{\rho}_p \phi V) + \partial_x(\bar{\rho}_p \phi V^2) + \bar{\rho}_p c^2 \pi(\phi) + \phi \partial_x p = \bar{\rho}_p \big(\phi D(u - V) + \phi g\big),$$

$$\begin{aligned}\partial_t(\bar{\rho}_f (1-\phi) u) + \partial_x(\bar{\rho}_f (1-\phi) u^2) + (1-\phi)\partial_x p \\ = \bar{\rho}_p \phi D(V-u) + \bar{\rho}_f (1-\phi) g + \partial_x((1-\phi)\mu \partial_x u).\end{aligned}$$

Where does it come from ? Fluid-kinetic models

Particles

- $\frac{4}{3}\pi a^3 f(t,x,\xi)\,\mathrm{d}\xi\,\mathrm{d}x$=volume fraction in $B(x,\,\mathrm{d}x)$ of particles with velocity in $B(\xi,\,\mathrm{d}\xi)$
- $\phi(t,x) = \frac{4}{3}\pi a^3 \int f\,\mathrm{d}\xi$=volume fraction.
- Vlasov-type eq: $\partial_t f + \xi\cdot\nabla_x f + \nabla_\xi\cdot(Af) = Q(f)$
- A accounts for **interactions with the fluid**, external forces (like gravity...), Q accounts for particles interactions

Fluid

Description my means of continuum mechanics: unknowns ρ_f, u. Euler or NS system with a coupling term describing the force exerted by the dispersed phase on the carrier phase.

Leading effect: Drag forces

Proportional to $u-\xi$. But the coefficient can be quite complicated. Stokes law: $D = \frac{9\mu}{2\rho_d a^2}$

Fluid-kinetic models for mixtures: **Thick** Sprays

Modeling assumptions

- Strong coupling: volume occupied by the particles is not neglected
- Pressure efforts taken into account
- **Close packing** term: $\pi(\phi) \to +\infty$ as $\phi = \frac{4}{3}\pi a^3 \int f \, \mathrm{d}\xi \to \phi_\star \in (0,1)$. Ex.: $\pi(\phi) = \frac{c^2\phi^\beta}{\phi_\star - \phi}$
- $Q(f) = 0$,
$$A = A(t,x,\xi) = D(u-\xi) + g - \frac{1}{\bar\rho_p}\nabla P - \frac{c^2}{\phi}\nabla_x \pi(\phi)$$
- incompressibility $\rho_f(t,x) = \bar\rho_f\big(1-\phi(t,x)\big)$

A non linear system of PDEs

Kinetic eq. (dispersed phase)

$$\partial_t f + \xi \cdot \nabla_x f + \nabla_\xi \cdot \left(\left[D(u - \xi) - \frac{1}{\bar{\rho}_p} \nabla_x P - \frac{c^2}{\phi} \nabla_x \pi(\phi) + g \right] f \right) = 0.$$

Hydrodynamic system (carrier phase)

$$\begin{aligned} &\partial_t n + \nabla_x \cdot (nu) = 0, \\ &\partial_t (nu) + \nabla_x \cdot (nu \otimes u) + \frac{1}{\bar{\rho}_f} \nabla_x P - \text{Visc. Terms} \\ &\qquad = ng + \frac{\bar{\rho}_p}{\bar{\rho}_f} \frac{4}{3} \pi a^3 \int f \left(D(\xi - u) + \frac{1}{\bar{\rho}_p} \nabla_x P \right) \mathrm{d}\xi, \end{aligned}$$

Constraint

$$n = 1 - \phi = 1 - \frac{4}{3} \pi a^3 \int f \, \mathrm{d}\xi.$$

Moment system

Set

$$\phi(t,x) = \frac{4}{3}\pi a^3 \int f(t,x,\xi)\,\mathrm{d}\xi, \qquad \phi V(t,x) = \frac{4}{3}\pi a^3 \int \xi f(t,x,\xi)\,\mathrm{d}\xi$$

and $\rho = \bar{\rho}_p \phi + \bar{\rho}_f(1-\phi)$, $\rho\bar{u} = \bar{\rho}_p \phi V + \bar{\rho}_f(1-\phi)u$. We have

$$\partial_t \phi + \nabla_x \cdot (\phi V) = 0 = \partial_t n + \nabla_x \cdot (nu)$$

with $\phi + n = 1$, so that the **mean volume velocity** is div-free

$$\nabla_x \cdot (\phi V + nu) = 0.$$

Besides, we get

$$\partial_t(\rho\bar{u}) + \nabla_x \cdot \big(\rho_f nu \otimes u + P + \bar{\rho}_p \mathbb{P} + \bar{\rho}_f c^2 \pi(\phi)\big) = \rho g + \text{Visc. Terms}$$

with $\mathbb{P} = \displaystyle\int \xi \otimes \xi f \,\mathrm{d}\xi$.

Mono-kinetic system

Assuming that particles are **mono-kinetic**

$$f(t,x,\xi) = \phi(t,x)\delta(\xi = V(t,x))$$

yields a closed system

$$\partial_t \phi + \nabla_x \cdot (\phi V) = 0 = \partial_t n + \nabla_x \cdot (nu).$$

$$\partial_t(\phi V) + \nabla_x \cdot \big(\phi V \otimes V + c^2 \pi(\phi)\big) = D\phi(u - V) - \frac{\phi}{\bar\rho_p}\nabla_x P + \phi g,$$

$$\partial_t(nu) + \nabla_x \cdot (nu \otimes u) + \frac{1}{\bar\rho_f}\nabla_x P$$

$$= ng + \frac{\bar\rho_p}{\bar\rho_f} D\phi(V - u) + \frac{\phi}{\bar\rho_f}\nabla_x P + \text{Visc. Terms},$$

and the constraint $\nabla_{\mathbf{x}} \cdot (\phi \mathbf{V} + \mathbf{nu}) = \mathbf{0}$

Rmk.: the system for $\phi, \phi V$ has a hyperbolic structure, owing to the close packing pressure. See Saurel, Cayré-Hérard, Sainsaulieu... for similar pbs.

Dissipation properties ($\Phi''(z) = c^2\pi(z)/z$)

Microscopic model

$$\partial_t \left(\frac{4}{3}\pi a^3 \bar\rho_p \int \frac{\xi^2}{2} f \,\mathrm{d}\xi + \frac{1}{2}\bar\rho_f n u^2 + \mathscr{G}\left(\bar\rho_p \rho + \bar\rho_f n\right) + \bar\rho_p \Phi(\phi) \right)$$
$$+\nabla_x \cdot (smthg.) + \frac{4}{3}\pi a^3 \bar\rho_p \int D(\xi - u)^2 f \,\mathrm{d}\xi + n\mu |\nabla_x u|^2 = 0.$$

Hydrodynamic model

$$\partial_t \left(\bar\rho_p \phi \frac{V^2}{2} + \bar\rho_f n \frac{u^2}{2} + \bar\rho_p \Phi(\phi) + \mathscr{G}(\bar\rho_p \phi + \bar\rho_f n) \right)$$
$$+\nabla_x \cdot (smthg.) + \bar\rho_p D\phi (V-u)^2 + n\mu |\nabla_x u|^2 = 0.$$

Rmk.: For compressible models, hyperbolicity of the system is far from clear.

Numerical difficulties

$$\partial_t \phi + \partial_x(\phi V) = 0,$$

$$\partial_t(\phi V) + \partial_x(\phi V^2) + c^2\pi(\phi) + \frac{\phi}{\bar{\rho}_p}\partial_x p = \phi D(u - V) + \phi g,$$

$$\partial_t n + \partial_x(nu) = 0,$$

$$\partial_t(nu) + \partial_x(nu^2) + \frac{n}{\bar{\rho}_f}\partial_x p = \frac{\bar{\rho}_p}{\bar{\rho}_f}\phi D(V - u) + ng + \frac{1}{\bar{\rho}_p}\partial_x(n\mu\partial_x u).$$

- Incompressibility $n = (1 - \phi)$ yields $\partial_x(\phi V + (1 - \phi)u) = 0$. It motivates to work with **staggered grids**.
- Close–packing effect $\lim_{\phi \to \phi_\star} \pi(\phi) = +\infty$ It induces specific stability conditions.

Numerical method: Projection & kinetic schemes

Two difficulties

- To satisfy $0 \leq \phi < \phi_\star$,
- To satisfy the constraint $n + \phi = 1$, $\nabla_x \cdot (\phi V + nu) = 0$.

Prediction-correction approach

- Predict $\phi, u, J = \phi V$ by getting rid of the constraint: $\phi^{k+1}, u^\star, J^\star$
- Correct by setting $n^{k+1} u^{k+1} = n^{k+1} u^\star - n^{k+1} \dfrac{\Delta t}{\bar{\rho}_f} \nabla_x \Pi^\star$, $J^{k+1} = J^\star - \phi^{k+1} \dfrac{\Delta t}{\bar{\rho}_p} \nabla_x \Pi^\star$. It yields a **Poisson-like eq.**

$$-\nabla_x \cdot \left(\left(\frac{\phi^{k+1}}{\bar{\rho}_p} + \frac{n^{k+1}}{\bar{\rho}_f} \right) \nabla_x \Pi^\star \right) = -\frac{1}{\Delta t} \nabla_x \cdot (J^\star + n^{k+1} u^\star).$$

Numerical method: Projection & kinetic schemes, Ctn'd

"Naive" idea

Just discretize the Poisson eq.
cf. : Ciarelli, Di Russo, Natalini, Ribot, models for biofilms formation; Cayré-Hérard
But, we have

$$\phi^{k+1} = \phi^k - \frac{\Delta t}{\Delta x}(\mathscr{F}^k_{j+1/2} - \mathscr{F}^k_{j-1/2}), \quad n_j^{k+1} = n_j^k - \frac{\Delta t}{\Delta x}(\mathscr{G}^k_{j+1/2} - \mathscr{G}^k_{j-1/2})$$

and it is not clear that the approximation is consistent with

$$\mathscr{F}^k_{j+1/2} - \mathscr{F}^k_{j-1/2} + \mathscr{G}^k_{j+1/2} - \mathscr{G}^k_{j-1/2} = 0.$$

Use staggered grids

- Volume fractions and pressures at $(j+1/2)\Delta x$ and velocities at $j\Delta x$: exact mass conservation, avoid odd/even decoupling
- It yields a **non linear** system for the correction Π (which degenerates to the standard 3 points scheme when $\phi = Cst.$).

A new scheme for barotropic Euler equations

Euler equations

- Mass conservation $\partial_t \, \phi + \partial_x(\phi V) = 0$,
- Momentum conservation $\partial_t(\phi V) + \partial_x(\phi V^2 + \pi(\phi)) = 0$
- Pressure: $\phi \mapsto \pi(\phi)$ is non decreasing, and strictly convex. The sound speed $\phi \mapsto c(\phi) = \sqrt{\pi'(\phi)}$ is non decreasing. Ex.: $\pi(\phi) = \phi^\gamma$, with $\gamma \geq 1$... but we can consider a more complex pressure law, like e. g. $\pi(\phi) = \frac{\phi^\beta}{\phi_\star - \phi}$.

Hyperbolicity and wave speeds

Set $\mathscr{U} = (\phi, \mathscr{J} = \phi V)$ and rewrite $\partial_t \mathscr{U} + A(\mathscr{U})\partial_x \mathscr{U} = 0$ with

$$F(\mathscr{U}) = \begin{pmatrix} \mathscr{J} \\ \dfrac{\mathscr{J}^2}{\phi} + \pi(\phi) \end{pmatrix}, \; A(\mathscr{U}) = \nabla_{\mathscr{U}} F(\mathscr{U}) = \begin{pmatrix} 0 & 1 \\ \pi'(\phi) - \dfrac{\mathscr{J}^2}{\phi^2} & 2\dfrac{\mathscr{J}}{\phi} \end{pmatrix}.$$

The eigenvalues of $A(\mathscr{U})$ are $\lambda_\pm(\mathscr{U}) = V \pm c(\phi)$.

Features of the scheme

- **Finite Volume** framework
  $\mathscr{U}_j^{k+1} = \mathscr{U}_j^k - \frac{\Delta t}{\Delta x}(F_{j+1/2}^k - F_{j-1/2}^j)$ where $F_{j+1/2}^k$ depends on $\mathscr{U}_j^k, \mathscr{U}_{j+1}^k$.
- Consistency $\mathbb{F}(\mathscr{U}, \mathscr{U}) = F(\mathscr{U})$.
- Design of the numerical fluxes with a flavor of Kinetic Schemes: integral over an auxiliary variable ξ of some "equilibrium function" $M(\mathscr{U})$ & UpWinding principles.
- Staggered grids: densities and velocities are not stored n the same gridpoints.
- Explicit formula: no "abstract formula" for M, no need of integration procedure... for **any** pressure law.
- Stability analysis: we can find Δt^k small enough so that $\phi^{k+1} > 0$ and $E^{k+1} \leq E^k$, discrete version of

$$\frac{\mathrm{d}}{\mathrm{d}t} \int \left(\phi \frac{V^2}{2} + \Phi(\phi)\right) \mathrm{d}x \leq 0$$

where $\phi \Phi'(\phi) - \Phi(\phi) = \pi(\phi)$. Ent

A kinetic scheme on staggered grids for barotropic gas dynamics

$$\begin{cases} \partial_t \phi + \partial_x(\phi V) = 0, \\ \partial_t(\phi V) + \partial_x(\phi V^2 + \pi(\phi)) = 0. \end{cases}$$

The pressure $\phi \mapsto \pi(\phi)$ is strictly increasing and strictly convex;
the sound speed $\phi \mapsto c(\phi) = \sqrt{\pi'(\phi)}$ is strictly increasing.
[Not true for "real" gases like the Bizarrium.]
The system is hyperbolic, the characteristic speeds are $V \pm c(\phi)$.

Kinetic scheme

Define a "generalized Maxwellian" $M = (M_0, M_1)(\phi, V)$ with

$$\int M \,\mathrm{d}\xi = \begin{pmatrix} \phi \\ \phi V \end{pmatrix} = U, \quad \int \xi M \,\mathrm{d}\xi = \begin{pmatrix} \phi V \\ \phi V^2 + \pi(\phi) \end{pmatrix} = F(U).$$

Set $F^{\pm}(U) = \displaystyle\int_{\xi \gtrless 0} \xi M(\phi, V)(\xi) \,\mathrm{d}\xi.$

Consistency : $F(U) = F^+(U) + F^-(U)$.

Construction of the kinetic scheme: Basic principles

The system of conservation laws is seen as the **hydrodynamic limit**

$$\partial_t f + \xi \partial_x f = \frac{1}{\tau}(M - f), \qquad \tau \ll 1.$$

Time splitting

- Transport $\partial_t f + \xi \partial_x f = 0$:

  UpWind $$\frac{\Delta x}{\Delta t}(f_j^{k+1/2} - f_j^k) + \xi_+(f_j^k - f_{j-1}^k) + \xi_-(f_{j+1}^k - f_j^k) = 0.$$

- Stiff ODE $\partial_t f = \frac{1}{\tau}(M - f)$

  Note that $M^{k+1} = M^{k+1/2}$ so that
  $f^{k+1} = e^{-\Delta t/\tau} f^{k+1/2} + (1 - e^{-\Delta t/\tau}) M^{k+1/2}$.

Inria

Construction of the kinetic scheme: Basic principles

Time splitting

- Transport $\partial_t f + \xi \partial_x f = 0$:

$$\mathrm{UpWind}\ \frac{\Delta x}{\Delta t}(f_j^{k+1/2} - f_j^k) + \xi_+(f_j^k - f_{j-1}^k) + \xi_-(f_{j+1}^k - f_j^k) = 0.$$

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Kinetic Fluxes: Let $\tau \to 0$ and $\xi-$average

$$\frac{\Delta x}{\Delta t} \int f_j^{k+1}\, \mathrm{d}\xi = \frac{\Delta x}{\Delta t} \int M_j^{k+1}\, \mathrm{d}\xi = \begin{pmatrix} \phi^{k+1} \\ (\phi V)^{k+1} \end{pmatrix}$$

$$= \begin{pmatrix} \phi_j^k \\ (\phi V)_j^k \end{pmatrix} - \int \Big(\xi_+ (M_j^k - M_{j-1}^k) + \xi_- (M_{j+1}^k - M_j^k) \Big)\, \mathrm{d}\xi$$

A kinetic scheme on staggered grids

Principle : Fluxes are constructed from **moments of M** & **Upwinding**

Maxwellian (Kaniel's fashion)

$$M_0(\phi, V)(\xi) = \frac{\phi}{2c(\phi)} \mathbf{1}_{|\xi - V| \le c(\phi)},$$
$$M_1(\phi, V)(\xi) = V M_0(\phi, V)(\xi) + \tilde{M}(\phi, V)(\xi)$$

with $\tilde{M}(\phi, V)(\xi) = \xi L(\phi, V) \mathbf{1}_{|\xi| \le |V| + c(\phi)}$ (encoding the pressure)

Staggered grids: Mass flux

Densities known at $x_{j+1/2}$, velocities at the interface x_j.
Upwinding is natural ▸ StMaF

$$\frac{h_{j+1/2}}{\Delta t}(\phi^{k+1}_{j+1/2} - \phi^k_{j+1/2}) + \mathscr{F}^k_{j+1} - \mathscr{F}^k_j = 0,$$
$$\mathscr{F}^k_j = \int_{\xi>0} \xi M_0(\phi_{j-1/2}, V^k_j)\,\mathrm{d}\xi + \int_{\xi<0} \xi M_0(\phi_{j+1/2}, V^k_j)\,\mathrm{d}\xi$$

The flux $\mathscr{F}^k_j$ involves the velocity V^k_j **only**.

Staggered grids: Momentum

- Set $\phi_j^k = \dfrac{h_{j+1/2}\phi_{j+1/2}^k + h_{j-1/2}\phi_{j-1/2}^k}{2h_j} = \dfrac{1}{h_j}\displaystyle\int \phi_h^k(y)\,\mathrm{d}y$.
- FV scheme
$\dfrac{h_j}{\Delta t}(\phi_j^{k+1}V_j^{k+1} - \phi_j^k V_j^{k+1}) + \tilde{\mathscr{F}}_{j+1/2}^k - \tilde{\mathscr{F}}_{j-1/2}^k = 0.$
- **Pressure flux**: Since

$$\int_{\xi>0} \xi \tilde{M}(\rho, V)\,\mathrm{d}\xi + \int_{\xi<0} \xi \tilde{M}(\rho', V')\,\mathrm{d}\xi = \frac{1}{2}(\pi(\rho) + \pi(\rho'))$$

  the pressure gradient is **centered** $\pi(\phi_{j+1/2}^k) - \pi(\phi_{j-1/2}^k)$.
- **Convection flux**: $\phi V \times V$ =Mass flux $\times$ V involves
$\displaystyle\int_{\xi\gtrless 0} \xi M_0(\phi, V)(\xi) \times V\,\mathrm{d}\xi$. Idea: Upwind of V and average
on $x_{j+1/2}$ of the mass fluxes known at x_j, x_{j+1}: ▸ StMtF

$$V_j \frac{\mathscr{F}^+(\phi_{j-1/2}, V_j) + \mathscr{F}^+(\phi_{j+1/2}, V_{j+1/2})}{2} + V_{j+1}\frac{\mathscr{F}^-(\phi_{j+1/2}, V_j) + \mathscr{F}^-(\phi_{j+3/2}, V_{j+1})}{2}$$

Numerical Analysis

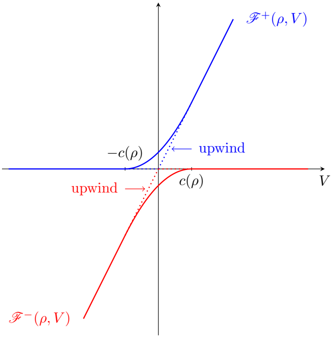
We have an **explicit** formula for the numerical mass flux

$$\mathscr{F}^+(\rho, V) = \left| \begin{array}{l} 0 \\ \dfrac{\rho}{4c(\rho)}(V + c(\rho))^2 = \dfrac{\rho}{4c(\rho)}\lambda_+(\rho, V)^2 \\ \rho V = \dfrac{\rho}{4c(\rho)}(\lambda_+(\rho, V)^2 - \lambda_-(\rho, V)^2) \end{array} \right.$$

$$\mathscr{F}^-(\rho, V) = \left| \begin{array}{l} \rho V = \dfrac{\rho}{4c(\rho)}(\lambda_+(\rho, V)^2 - \lambda_-(\rho, V)^2) \\ -\dfrac{\rho}{4c(\rho)}(V - c(\rho))^2 = -\dfrac{\rho}{4c(\rho)}\lambda_-(\rho, V)^2 \\ 0 \end{array} \right.$$

according to the three cases $V + c(\rho) \leqslant 0$,
$V - c(\rho) < 0 < V + c(\rho)$ and $0 < V - c(\rho)$, respectively.

Properties of the flux



Accordingly $0 \leqslant \pm\mathscr{F}^{\pm}(\rho, V) \leqslant \rho\big[\lambda_{\pm}(\rho, V)\big]^{\pm}$

Stability: discrete maximum principle

If $\Delta t([\lambda_+]^+ + [\lambda_-]^-) \leq \Delta x$, then the discrete density remains ≥ 0.

Numerical Analysis

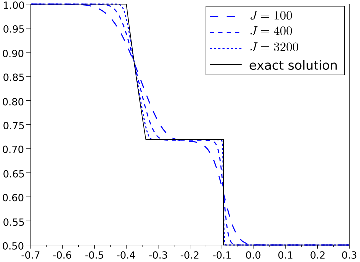
Under suitable CFL condition:

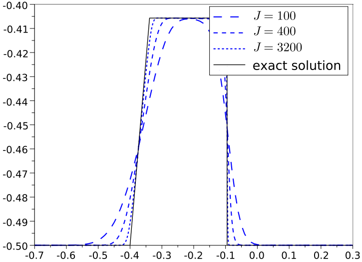
- Positivity of the density is preserved $\phi_{j+1/2}^{k+1} \geq 0$,
- The physical entropy is decaying: with $\pi(\rho) = \rho\Phi'(\rho) - \Phi(\rho)$,

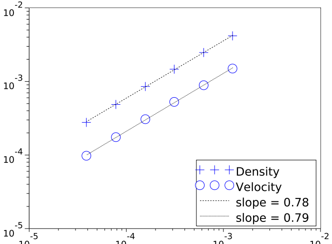
$$h_j \sum_j \phi_j^{k+1} |V_j^{k+1}|^2 + h_{j+1/2} \sum_j \Phi(\phi_{j+1/2}^{k+1}) \leq h_j \sum_j \phi_j^k |V_j^k|^2 + h_{j+1/2} \sum_j \Phi(\phi_{j+1/2}^k).$$

  In fact we have both **local** and **global** versions of the entropy dissipation. It holds for **general (convex) pressure laws**. Proof: mixing of Bouchut's and Herbin-Latché techniques. Unusual: "work with 2 eq. rather than a system".
- Consistency analysis works too and a convergence statement of "Lax-Wendroff type" can be established.
- Performs well in vacuum regions.

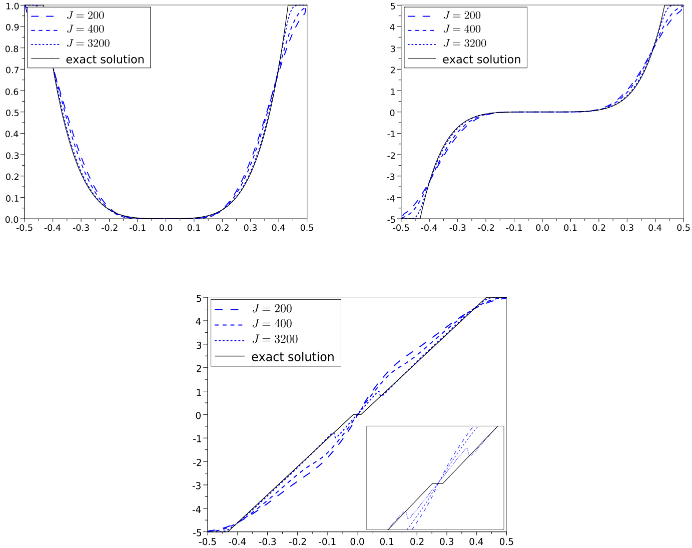
Numerical results (Density, Velocity, L^1-Error)







A simulation with vacuum (Density, Velocity, Momentum)



Remarks on numerical diffusion

Set $$\begin{cases} \mathscr{F}^{|\cdot|}(\phi, V) = \int |\xi| M_0(\phi, V)(\xi)\,\mathrm{d}\xi > 0, \\ d^{|\cdot|}(\phi, \phi', V) = \dfrac{\mathscr{F}^{|\cdot|}(\phi, V) - \mathscr{F}^{|\cdot|}(\phi', V)}{\phi - \phi'} > 0. \end{cases}$$

The mass flux recasts as

$$\begin{aligned} \mathscr{F}_j &= \mathscr{F}^{+}(\phi_{j-1/2}, V_j) + \mathscr{F}^{-}(\phi_{j+1/2}, V_j) \\ &= \frac{\phi_{j+1/2} + \phi_{j-1/2}}{2} V_j - \frac{1}{2}\left(\mathscr{F}^{|\cdot|}(\phi_{j+1/2}, V_j) - \mathscr{F}^{|\cdot|}(\phi_{j-1/2}, V_j)\right) \end{aligned}$$

$$\mathscr{F}_{j+1} - \mathscr{F}_j = \left(\frac{\phi_{j+3/2} + \phi_{j+1/2}}{2} V_{j+1} - \frac{\phi_{j+1/2} + \phi_{j-1/2}}{2} V_j\right) - \Delta_j^{\mathrm{mass}}$$

with Δ_j^{mass} a discrete diffusion term, with coefficients involving $d^{|\cdot|} > 0$. Id. for the momentum flux.

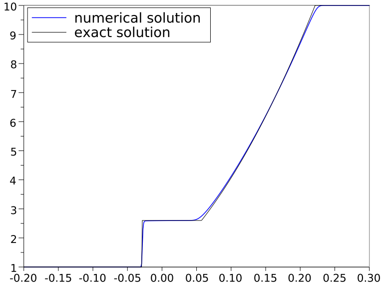
The "Purely UpWind" version of the scheme: why to be kinetic matters!

Replace M_0 by $\phi\delta(\xi = V)$.

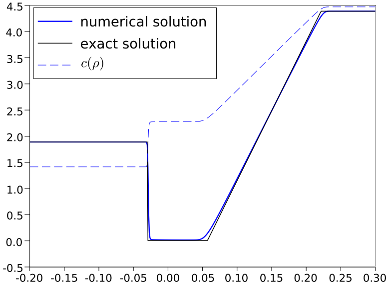
The mass flux becomes

$$\mathscr{F}_j^{\mathrm{UpW}} = \phi_{j-1/2}\big[V_j\big]^+ - \phi_{j+1/2}\big[V_j\big]^-.$$

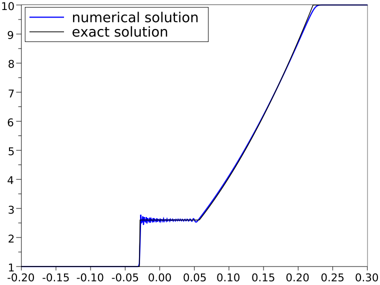
- Note that CFL for the maximum principle would now involve only the **material velocity** V instead of the wave speed $V \pm c(\phi)$.
- Numerical diffusion might vanish (when the material velocity vanishes) since $\mathscr{F}_j^{|\cdot|,\mathrm{UpW}} = \rho|V|$ and $d^{|\cdot|,\mathrm{UpW}} = |V|$.
- Scheme by Herbin-Latché-Nguyen: "Purely UpWind" and momentum fluxes defined by using positive/negative parts of the average of the mass fluxes, instead of the average of the positive and the average of the negative mass fluxes. Oscillations might appear which need to add artificial viscosity in the HLN scheme.



numerical solution
exact solution



numerical solution
exact solution
$c(\rho)$



numerical solution
exact solution

Coming back to the coupled problem

1-Update of the volume fraction ϕ et n

$$\frac{\phi - \phi^k}{\Delta t} + \mathrm{div}_h^{(1)}(\phi^k, V^k) = 0, \qquad n = 1 - \phi.$$

2-Prediction of the velocities $\widetilde{V}$ et $\widetilde{u}$

$$\frac{\phi\widetilde{V} - \phi^k V^k}{\Delta t} + \mathrm{div}_h^{(2)}(\phi^k, V^k) = D\phi(\widetilde{u} - \widetilde{V}) - \frac{\phi}{\bar{\rho}_p}\nabla_h p^k + \phi g,$$

$$\frac{n\widetilde{u} - n^k u^k}{\Delta t} + \mathrm{div}_h^{(2)}(n^k, u^k) - \frac{\mu}{\bar{\rho}_f}\Delta_h \widetilde{u} = \frac{\bar{\rho}_p}{\bar{\rho}_f} D\phi(\widetilde{V} - \widetilde{u}) - \frac{1-n}{\bar{\rho}_f}\nabla_h p^k + ng.$$

3-Computation of the pressure p it becomes a **nonlinear** step!

$$\mathrm{div}_h^{(1)}\left(\phi, \widetilde{V} - \frac{\Delta t}{\bar{\rho}_p}\nabla_h\left(p - p^k\right)\right) + \mathrm{div}_h^{(1)}\left(n, \widetilde{u} - \frac{\Delta t}{\bar{\rho}_f}\nabla_h\left(p - p^k\right)\right) = 0.$$

4-Correction of the velocities u_p, u_f

$$V = \widetilde{u}_p - \frac{\Delta t}{\bar{\rho}_p}\nabla_h(p - p^k), \qquad u = \widetilde{u} - \frac{\Delta t}{\bar{\rho}_f}\nabla_h(p - p^k).$$

Properties of the scheme

- At each time step, mass conservation holds

$$\frac{n - n^k}{\Delta t} + \mathrm{div}_h^{(1)}(n^k, u^k) = 0.$$

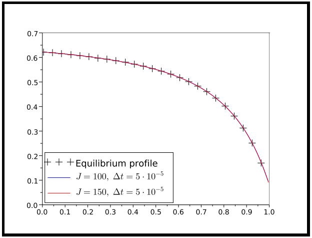
Accordingly, discrete **energy inequality** holds for the full system (with CFL) !

- Price to be paid: we are led to a non linear problem for obtaining the pressure.

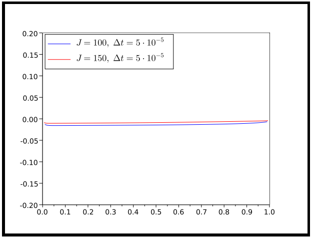
Existence of a solution can be proved by a topological degree argument. In practice, a few Newton iterations give the solution.

Sedimentation flow

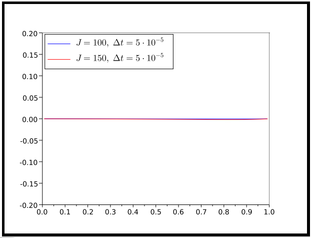
Volume Fraction ϕ



Particles Velocity V



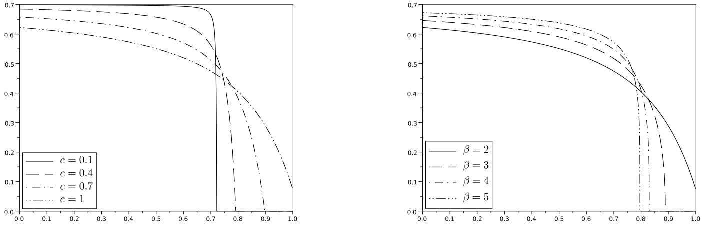
Fluid Velocity u



Parameters

- $\pi(\phi) = \dfrac{\phi^2}{\phi_\star - \phi}, \quad \phi_\star = 0.7$
- $\varrho_f = 1, \quad \varrho_p = 10^3, \quad g = -10$
- $\mu = 10^{-4}, \quad D = 0$

Equilibrium profiles ($\alpha_\star = .7$, make c or β vary)



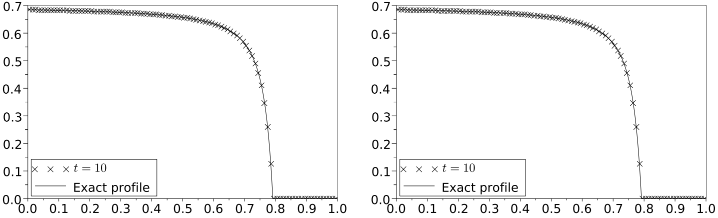


Figure: $c = 0.4$ and $\beta = 2$ (left) vs. $c = 0.2$ and $\beta = 4$ (right).

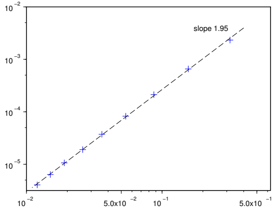
Analysis of the close-packing threshold

A stability condition guaranteeing that the numerical solution remains $\leq \alpha_\star$ can be identified:

$$\frac{\delta t}{h_{j+1/2}}(\lambda_+ + \lambda_-) \leq 1 - \frac{\alpha^k_{j+1/2}}{\alpha_\star}$$

Very demanding!! It might explain the lack of robustness reported for many simulations of the problem.

[This model, however, couldn't completely prevent the particle volume fraction to exceed the close packing limit and some numerical instabilities were experienced in the present unstructured code.]



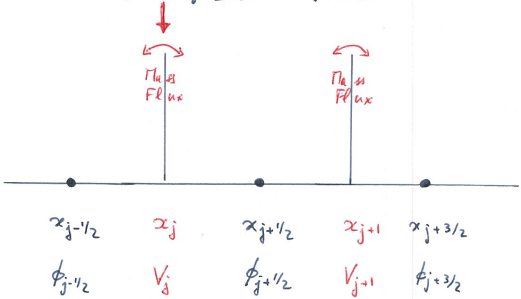
Maximal "acceptable" time step Δt as a function of $1 - \alpha_{Max}/\alpha_\star$.

Related Works

- Numerical analysis of the Kinetic Scheme on Staggered Grids (with F. Berthelin and S. Minjeaud): stability and Lax-Wendroff theorem.
- Simulation of fluid-kinetic models via **semi-Lagrangian methods** (with A. Champmartin, J.P. Braeunig, C. Fochesato)
- Schemes for asymptotic regimes (with P. Lafitte, J.-A. Carrillo, with S. Jin, J.-G. Liu, B. Yan)
- A **"new" model for mixtures**, generalizing KS: derivation from a microscopic description (kinetic theory of multiphase flows, e. g. Savage), dissipation properties, stability of solutions (with A. Vasseur) ▸ KS
- Numerical scheme, based on **DDFV techniques**, for the generalized KS model (with S. Krell)

Staggered grid: Mass fluxes

$$\mathcal{F}_j = \mathcal{F}^+(\phi_{j-1/2}, V_j) + \mathcal{F}^-(\phi_{j+1/2}, V_j)$$

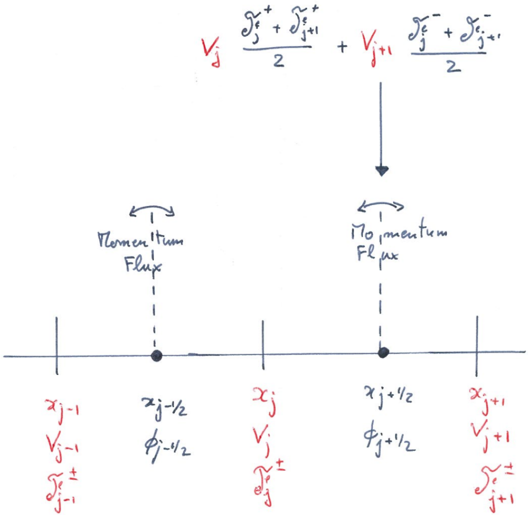


$$\frac{h_{j+1/2}}{\Delta t}\left(\phi^{k+1}_{j+1/2} - \phi^{k}_{j+1/2}\right) + \mathcal{F}_{j+1} - \mathcal{F}_j = 0$$

$$\mathcal{F}^{\pm}(\phi, V) = \int_{\pm\xi>0} \xi\, M_0(\phi, V)\, d\xi$$

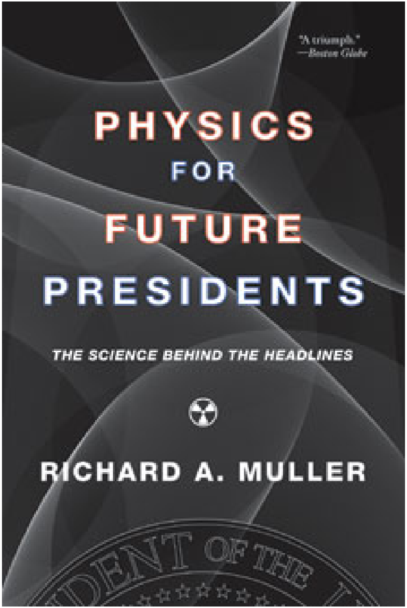
S1

Staggered grid: Momentum fluxes



▸ S2

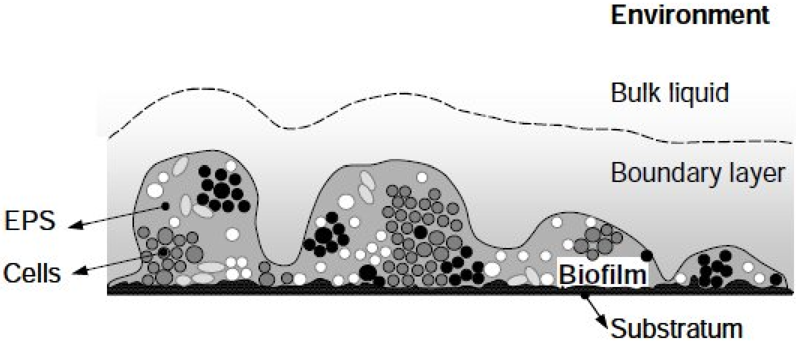
To know more on fluidized beds ▸ Bk0



Biological degradation ▸ Bk0

What is a biofilm ?

a complex mixture of **microorganisms** embedded in an **Extracellular matrix of Polymeric Substances (EPS)**



Entropy dissipation FS

Free energy balance

$$\partial_t \Phi(\phi) + \partial_x \big(\Phi(\phi) V\big) = \big(\Phi(\phi) - \phi \Phi'(\phi)\big) \partial_x V = -\pi(\phi)\ \partial_x V.$$

Kinetic energy balance

$$\partial_t \Big(\phi \frac{V^2}{2}\Big) + \partial_x \Big(\phi \frac{V^2}{2} V\Big) = \big(\partial_t(\phi V) + \partial_x(\phi V^2)\big) V = -\partial_x \pi(\phi)\ V.$$

Conclusion

Adding the two relations yields the **local** relation

$$\partial_t \Big(\phi \frac{V^2}{2} + \Phi(\phi)\Big) + \partial_x \Big(\Big(\phi \frac{V^2}{2} + \Phi(\phi) + \pi(\phi)\Big) V\Big) = 0$$

that can be integrated over the domain.

A new mixture model (generalizing KS) ▸ WP

$$\partial_t n + \nabla_x \cdot (nu) = 0,$$

$$\partial_t (nu) + \nabla_x \cdot (nu \otimes u) + \nabla_x p - \nabla_x \cdot (\mu \mathbb{D}(u)) = -(\kappa n + \bar{\phi}\phi)\nabla_x \mathscr{E} - \nabla_x \phi,$$

$$n = 1 - \bar{\phi}\phi, \qquad \nabla_x \cdot \left(u - \frac{\bar{\phi}\phi}{\mu\nu} \nabla_x (\ln(\phi) + \bar{\phi} p + \bar{\phi}\mathscr{E}) \right) = 0,$$

$$\partial_t \phi = -\nabla_x \cdot (\phi u) + \frac{1}{\bar{\phi}} \nabla_x \cdot u = -\nabla_x \cdot \left(\phi \left(u - \frac{1}{\mu\nu} \nabla_x (\bar{\phi} p + \bar{\phi}\mathscr{E}) \right) \right) + \nabla_x \cdot \left(\frac{1}{\mu\nu} \nabla_x \phi \right).$$

- Derivation from a kinetic model (hydrodynamic regime)
- “hybrid” behavior
- Entropy dissipation (in any dimension)
- An additional entropy dissipation in 1D: no formation of vacuum, compactness and stability of weak solutions.

Inria