SOME ISSUES AND REMARKS ON LAGRANGIAN STOCHASTIC MODELS FOR SINGLE-PHASE TURBULENCE AND FIBRE SUSPENSIONS

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Plan

1. General guidelines: Modelling approach and actual models
   - Choice of a modelling approach for single-phase reactive flows
   - Choice of a modelling approach for polydispersed two-phase flows
2. The framework of present Lagrangian two-phase flow models
   - The (one-particle) PDF formalism: from SDEs to Mean fields
   - An reminder on the physical contents
3. Consistency issues in the fluid limit case
   - Correspondence with Reynolds-stress modelling
     - The spurious issue of spurious drifts
     - Various forms of the Langevin equations
   - Consistency issues in the hybrid "Euler/Lagrange" formulation

Do all roads lead to Rome?

- In turbulence, the issue of "modelling" is to reduce the number of degree of freedom and to come up with a "relevant" *contracted statistical description* (for single-phase and two-phase flow turbulence)
- From microscopic to macroscopic descriptions

(i) Microscopic level: DNS for the carrier fluid and "exact" fiber tracking

$$\Downarrow$$

(ii) PDF closures (Lagrangian stochastic models)

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(iii) Macroscopic or continuum modelling: two-fluid approaches

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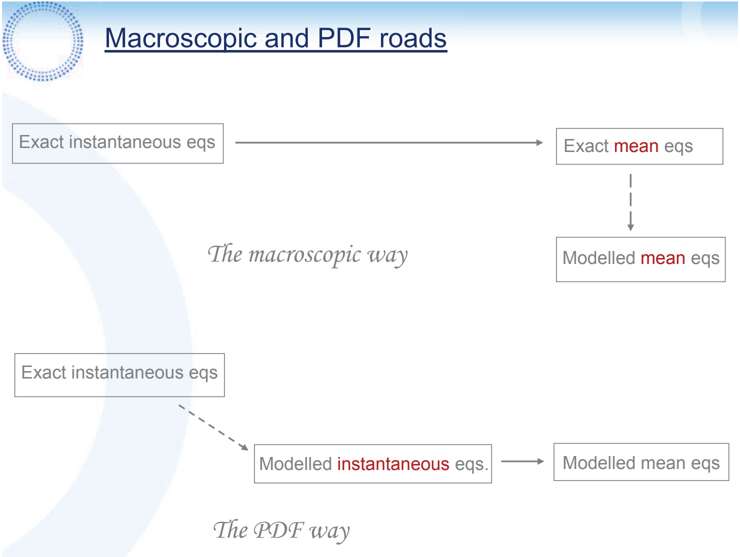
(iv) Macroscopic or continuum modelling: single-fluid approaches with modified rheological properties

Along the PDF road



Distinguishing the frame from the painting

- It is important to distinguish between the **modelling framework** and **actual modelling proposals**
- The choice of a modelling framework is an essential step, resulting from the **physical analysis** of *the situations to be addressed* (what flows are we trying to simulate?) and from **the choice** of *a set of precise statistical quantities* (what specific details are we trying to capture?)
- The "game" is then to tailor the "best model" within a chosen framework
- For example, is it relevant to criticise $k - \epsilon$ models because they cannot predict the fluid kinetic energy turbulence spectrum?
- Or is it relevant to criticise present (one-particle) Langevin models for two-phase flows because they contain no-length information?
- A double hierarchy and a double choice in the PDF world
  one or N-fiber PDF?/What variables for each fiber (fiber state-vector)?

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The issue of the closure of the chemical source term (1)

- In turbulent reactive flows, one may look for reduced information on some one-point moments on scalars $\phi = (T, c_1, c_2, \dots, c_\alpha)$
- For instance, the mean scalar equation has the form

$$\frac{\partial \langle \phi_l \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle \phi_l \rangle}{\partial x_k} = -\frac{\partial \langle u_k\, \phi_l^{'} \rangle}{\partial x_k} + \langle S_l(\phi) \rangle$$

- The moments equations involve typical terms such as the mean chemical source term $\langle S_l(\phi) \rangle$ and the scalar turbulent flux $\langle u_k\, \phi_l^{'} \rangle$
- These terms cannot be easily closed when *only moments* are known

$$\langle S(\phi) \rangle \stackrel{?}{=} \mathcal{F}(\langle \phi \rangle, \dots, \langle (\phi)^m \rangle)$$

- However, these terms are **closed** if the *one-point pdf* is known

$$\langle S(\phi) \rangle (t, \mathbf{x}) = \int S(\psi)\, p(t, \mathbf{x}; \psi)\, d\psi$$

$$\langle U_k \phi \rangle = \int V_k\, \psi\, p(t, \mathbf{x};\, V_k, \psi)\, dV_k\, d\psi$$

The issue of the closure of the chemical source term (2)

- if we wish to be able to treat the chemical source term, $\langle S_l(\phi)\rangle$, and turbulent fluxes (convective effects), $\langle u_k\, \phi_l^{'}\rangle$, *without approximation*, then, at least, the one-point pdf $p(t,\mathbf{x};\mathbf{V},\psi)$ must be known
- But do we need more detailed information such as the two-point pdf, $p(t,\mathbf{x}_1,\mathbf{x}_2;\mathbf{V}_1,\psi_1,\mathbf{V}_2,\psi_2)$?
- For turbulent reactive flows, **if we choose to describe only** one-point moments, then one-point pdfs are necessary but.. nothing more
- In that case, one-point pdfs closures appear as the best "tailor choice" with respect to **this given objective**
- Once this framework is chosen, it is important to know what is inside

$$\langle c^m\rangle(t,\mathbf{x}) = \int \varphi^m \underbrace{p(t,\mathbf{x};\varphi)}_{known}\, d\varphi \quad \forall m$$

- and what is outside, such as the concentration spatial correlation

$$\langle c(t,\mathbf{x}_1)c(t,\mathbf{x}_2)\rangle = \int \varphi_1\,\varphi_2\, \underbrace{p(t,\mathbf{x}_1,\mathbf{x}_2;\varphi_1,\varphi_2)}_{unknown}\, d\varphi_1\, d\varphi_2$$

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Dispersed two-phase Flow Modelling: point particles

- "exact equations" : Navier-Stokes eqs. and forces on a particle

$$\begin{cases} \dfrac{d\mathbf{x}_p}{dt} = \mathbf{U}_p \\ \dfrac{d\mathbf{U}_p}{dt} = \dfrac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p} + \dfrac{\rho_p - \rho_f}{\rho_p}\mathbf{g} + \dfrac{\rho_f}{\rho_p}\left(\dfrac{d\mathbf{U}_s}{dt}\right) + \dfrac{1}{2}\dfrac{\rho_f}{\rho_p}\left(\dfrac{d\mathbf{U}_s}{dt} - \dfrac{d\mathbf{U}_p}{dt}\right) \end{cases}$$

$$\tau_p = \frac{\rho_p}{\rho_f}\frac{4d}{3C_D|\mathbf{U}_s - \mathbf{U}_p|} \quad C_D = \frac{24}{Re}[1 + 0.15Re^{0.687}] \quad Re = \frac{d\,|\mathbf{U}_s - \mathbf{U}_p|}{\nu}$$

- case of 'heavy' particles $\rho_p \gg \rho_f$

$$\begin{cases} \dfrac{d\mathbf{x}_p}{dt} = \mathbf{U}_p \\ \dfrac{d\mathbf{U}_p}{dt} = \dfrac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p} + \mathbf{g} \end{cases}$$

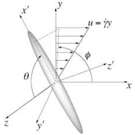
- key word: turbulence $\Rightarrow$ statistical approach

But how "exactly" should we describe each fiber?

- The rigid-fiber approach

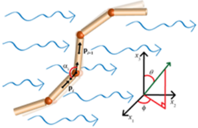
$$\frac{d\mathbf{U}_p}{dt} \sim \mathbf{K}\left(\mathbf{U}_s - \mathbf{U}_p\right)$$

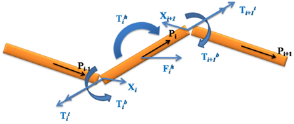
$$\frac{d\boldsymbol{\omega}_p}{dt} \sim \mathcal{F}(\boldsymbol{\omega}_p, S^f_{ij}, \Omega^f_{ij})$$



$\Rightarrow$ need of a local (one-point) fluid information on U_i and $\partial U_i/\partial x_j$

- The chain-rod approach for flexible fibers: N-connected rods

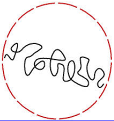




$\Rightarrow$ need of a spatial (multi-point) fluid information on U_i and $\partial U_i/\partial x_j$

- A new and intermediate description with a reduced state-vector?

define a few variables: $l, \theta, \ldots$



Modelling constraints

- limitations of the macroscopic road
  1. detailed information is needed
  2. it is too difficult to close directly at the macroscopic level through constitutive relations between macroscopic variables.
- need of different physical descriptions
  1. the important physical phenomena are treated without approximation,
  2. enough information is available to handle correctly issues of complex physics (combustion, polydispersed particles),
  3. the resulting numerical model is tractable for non-homogeneous flows,
  4. the model can be coupled to other approaches, either more fundamental or applied descriptions.

Let's go stochastic

- (one) central issue: turbulent dispersion

$$\frac{d\mathbf{U}_p}{dt} = \frac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p} + \mathbf{g}$$

  $\mathbf{U}_s(t) = \mathbf{U}[t, \mathbf{x}_p(t)]$ is the *instantaneous* fluid velocity 'seen' by the particle along its trajectory as it moves across the flow.

- limited available information on $\mathbf{U}_s$ (ex : first two moments provided by the turbulence model)

  $\Rightarrow$ stochastic modelling

- compromise is sought between physical accuracy, information content and tractability to (or possible generalisation to) general flows

  $\Rightarrow$ one-particle pdf

- key issue: proper choice of the variables retained in the state vector and those that are eliminated from the PDF description

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PDF approach to dispersed two-phase flow

- The fluid 'seen' is included in the state vector $\mathbf{Z} = (\mathbf{x}_p, \mathbf{U}_p, \mathbf{U}_s)$ which is modelled by a general diffusion process

$$\begin{cases} d\mathbf{x}_p = \mathbf{U}_p\, dt \\ d\mathbf{U}_p = \mathbf{A}_p(t,\mathbf{Z}), dt \qquad (= \dfrac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p}\, dt + \mathbf{g}\, dt) \\ d\mathbf{U}_s = \mathbf{A}_s\,(t,\mathbf{Z},\langle\mathcal{F}[\,\mathbf{Z}\,]\rangle)\; dt + \mathbf{B}_s\,(t,\mathbf{Z},\langle\mathcal{G}[\,\mathbf{Z}\,]\rangle)\; d\mathbf{W} \end{cases}$$

- particle tracking approach $\equiv$ PDF approach
  Monte Carlo simulation of the pdf $p_L(t;\mathbf{y}_p,\mathbf{V}_p,\mathbf{V}_s)$
- hierarchy of descriptions (marginal pdfs)

$$p_L(t;\mathbf{y}_p,\mathbf{V}_p) = \int p_L(t;\mathbf{y}_p,\mathbf{V}_p,\mathbf{V}_s)d\mathbf{V}_s$$

$$p_L(t;\mathbf{y}_p) = \int\int p_L(t;\mathbf{y}_p,\mathbf{V}_p,\mathbf{V}_s)d\mathbf{V}_s\, d\mathbf{V}_p$$

- The PDF formalism for the fluid case is retrieved by taking $\tau_p \to 0$

The PDF formalism (1)

- Lagrangian model for a large number N of stochastic particles

$$\begin{cases} d\mathbf{x}_p = \mathbf{U}_p \, dt, \\ d\mathbf{U}_p = \mathbf{A}_p(t, \mathbf{Z}), dt \\ d\mathbf{U}_s = \mathbf{A}_s\left(t, \mathbf{Z}, \langle \mathcal{F}[\,\mathbf{Z}\,] \rangle\right) \, dt + \mathbf{B}_s\left(t, \mathbf{Z}, \langle \mathcal{G}[\,\mathbf{Z}\,] \rangle\right) \, d\mathbf{W} \end{cases}$$

- Discrete Lagrangian and Eulerian Mass Density Functions (MDFs)

$$\begin{aligned} F_p^L(t; \mathbf{y}, \mathbf{V}_p, \mathbf{V}_s) &= M_p \, p_L(t; \mathbf{y}, \mathbf{V}_p, \mathbf{V}_s) \\ F_p^E(t, \mathbf{x}; \mathbf{V}_p, \mathbf{V}_s) &= F_p^L(t; \mathbf{y} = \mathbf{x}, \mathbf{V}_p, \mathbf{V}_s) \\ &= \int F_p^L(t; \mathbf{y}, \mathbf{V}_p, \mathbf{V}_s) \delta(\mathbf{y} - \mathbf{x}) \, d\mathbf{y} \end{aligned}$$

- The general definition of an average quantity is

$$\alpha_p(t, \mathbf{x}) \, \rho_p \langle H_p \rangle(t, \mathbf{x}) = \int H(\mathbf{V}_p, \psi_p) F_p^E(t, \mathbf{x}; \mathbf{V}_p, \mathbf{V}_s) \, d\mathbf{V}_p \, \mathbf{V}_s.$$

The PDF formalism (2)

- Discrete Lagrangian and Eulerian MDFs

$$F^L_{p,N}(t; \mathbf{y}, \mathbf{V}_p, \mathbf{V}_s) = \sum_{i=1}^{N} m_p^{(i)} \delta(\mathbf{y} - \mathbf{x}_p^{(i)}) \otimes \delta(\mathbf{V}_p - \mathbf{U}_p^{(i)}) \otimes \delta(\mathbf{V}_s - \mathbf{U}_s^{(i)})$$

$$F^E_{p,N}(t, \mathbf{x}; \mathbf{V}_p, \mathbf{V}_s) = F^L_{p,N}(t; \mathbf{y} = \mathbf{x}, \mathbf{V}_p, \mathbf{V}_s)$$

- In the discrete formulation, in a given cell with N_x^p particles

$$\langle H_p \rangle \simeq H_{p,N} = \frac{\sum_{i=1}^{N_x^p} m_p^i H(\mathbf{U}_p^i(t), \mathbf{U}_s^i(t))}{\sum_{i=1}^{N_x^p} m_p^i}.$$

- The Eulerian MDF satisfies the same Fokker-Planck as p_L

$$\frac{\partial F_p^E}{\partial t} + V_{p,i} \frac{\partial F_p^E}{\partial x_i} = -\frac{\partial}{\partial V_{p,i}}(A_{p,i}\, F_p^E\,) - \frac{\partial}{\partial V_{s,i}}(A_{s,i}\, F_p^E\,) + \frac{1}{2} \frac{\partial^2}{\partial V_{s,i} \partial V_{s,j}} \left((B_s B_s^T)_{ij}\, F_p^E \right).$$

Resulting mean field equations

- Mean continuity and mean momentum equations

$$\frac{\partial}{\partial t}(\alpha_p \rho_p) + \frac{\partial}{\partial x_i}(\alpha_p\, \rho_p \langle U_{p,i}\rangle) = 0.$$

$$\alpha_p\, \rho_p \frac{d}{dt}\langle U_{p,i}\rangle = -\frac{\partial}{\partial x_j}(\alpha_p\, \rho_p \langle u_{p,i} u_{p,j}\rangle) + \alpha_p\, \rho_p \langle A_{p,i}\rangle.$$

- The (rather intricate) second-order equations

$$\begin{aligned}\alpha_p \rho_p \frac{d}{dt}\langle u_{p,i} u_{p,j}\rangle = &- \frac{\partial}{\partial x_k}(\alpha_p\, \rho_p \langle u_{p,i} u_{p,j} u_{p,k}\rangle) - \alpha_p \rho_p \langle u_{p,i} u_{p,k}\rangle \frac{\partial \langle U_{p,j}\rangle}{\partial x_k} \\ &- \alpha_p \rho_p \langle u_{p,j} u_{p,k}\rangle \frac{\partial \langle U_{p,i}\rangle}{\partial x_k} + \alpha_p\, \rho_p \langle A_{p,i}\, v_{p,j} + A_{p,j}\, v_{p,i}\rangle, \\ \alpha_p \rho_p \frac{d}{dt}\langle u_{s,i} u_{p,j}\rangle = &- \frac{\partial}{\partial x_k}(\alpha_p\, \rho_p \langle u_{s,i} u_{p,j} u_{p,k}\rangle) - \alpha_p \rho_p \langle u_{s,i} u_{p,k}\rangle \frac{\partial \langle U_{p,j}\rangle}{\partial x_k} \\ &- \alpha_p \rho_p \langle u_{p,j} u_{p,k}\rangle \frac{\partial \langle U_{s,i}\rangle}{\partial x_k} + \alpha_p\, \rho_p \langle A_{s,i}\, v_{p,j}\rangle + \alpha_p\, \rho_p \langle A_{p,j}\, v_{s,i}\rangle,\end{aligned}$$

Plan

Lagrangian stochastic modelling (fluid case): key physical notions

- $\mathbf{Z} = (\mathbf{x}, \mathbf{U})$ is treated as a diffusion process
- At $Re \gg 1$, the acceleration $\mathbf{a}$ is seen as a **fast-variable** and eliminated
- Kolmogorov theory yields a coarse-grained description $\tau_\eta \ll dt \ll T$
- decomposition of a fluid particle acceleration

$$\mathbf{a} = -\frac{1}{\rho}\frac{\partial\langle P\rangle}{\partial\mathbf{x}} + \underline{\mathbf{G}}\,(\mathbf{U} - \langle\mathbf{U}\rangle) + \gamma.$$

- Kolmogorov theory at $Re \gg 1$: $\langle(\gamma)^2\rangle \sim \langle\mathbf{a}^2\rangle \Rightarrow \langle(\gamma)^2\rangle \simeq \dfrac{\langle\epsilon\rangle}{\tau_\eta}$
- fast-variable elimination: $\langle(\gamma)^2\rangle \times \tau_\eta \xrightarrow{Re\to\infty} D \simeq \langle\epsilon\rangle$
- **slaving principle**: γ is a function of the local value of the **slow mode** $\mathbf{x}$

$$\gamma\, dt \approx \sqrt{C_0\,\langle\epsilon\rangle(\mathbf{x})}\, d\mathbf{W}$$

- This slaving principle has direct relevance to the mean-field equations

Lagrangian stochastic modelling (fluid case): the resulting form

- one-point description (at present)

$$\begin{cases} dx_i^+ = U_i^+ \, dt \\ dU_i^+ = \left(-\dfrac{1}{\rho} \dfrac{\partial P}{\partial x_i} + \nu \Delta U_i \right)^+ dt \\ d\phi_l^+ = (\Gamma \Delta \phi_l)^+ \, dt + S_l(\phi^+) \, dt \end{cases}$$

$$\Downarrow$$

$$\begin{cases} dx_i = U_i \, dt \\ dU_i = -\dfrac{1}{\rho} \dfrac{\partial \langle P \rangle}{\partial x_i} \, dt + D_i \, dt + \sqrt{C_0 \langle \epsilon \rangle} dW_i \\ d\phi_l = A_{\phi_l} \, dt + S_l(\phi) \, dt \end{cases}$$

$$D_i = G_{ij} \left(U_j - \langle U_j \rangle \right) = -\left(\frac{1}{2} + \frac{3}{4} C_0 \right) \frac{\langle \epsilon \rangle}{k} (U_i - \langle U_i \rangle) + G_{ij}^a \left(U_j - \langle U_j \rangle \right)$$

$$A_{\phi_l} = -\frac{\phi_l - \langle \phi_l \rangle}{\tau_\phi} \qquad \tau_\phi = \frac{2k}{C_\phi \langle \epsilon \rangle}$$

Mean velocity Equations

- mass conservation and mean momentum equation (high-Reynolds case)

$$\begin{cases} \dfrac{\partial \langle U_i \rangle}{\partial x_i} = 0 \\ \dfrac{\partial \langle U_i \rangle}{\partial t} + \langle U_j \rangle \dfrac{\partial \langle U_i \rangle}{\partial x_j} + \dfrac{\partial \langle u_i u_j \rangle}{\partial x_j} = -\dfrac{1}{\rho} \dfrac{\partial \langle P \rangle}{\partial x_i} \end{cases}$$

- second-order equation (high-Reynolds case)

$$\frac{\partial \langle u_i u_j \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle u_i u_j \rangle}{\partial x_k} + \frac{\partial \langle u_i u_j u_k \rangle}{\partial x_k} = -\langle u_i u_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} - \langle u_j u_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}$$
$$\langle u_i D_j \rangle + \langle u_j D_i \rangle + C_0 \langle \epsilon \rangle \delta_{ij}$$

$$\frac{\partial \langle u_i u_j \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle u_i u_j \rangle}{\partial x_k} = -\frac{\partial \langle u_i u_j u_k \rangle}{\partial x_k} - \langle u_i u_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} - \langle u_j u_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}$$
$$+ G^a_{ik} \langle u_j u_k \rangle + G^a_{jk} \langle u_i u_k \rangle - (1 + \frac{3}{2} C_0) \frac{\langle \epsilon \rangle}{k} \left(\langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij} \right) - \frac{2}{3} \langle \epsilon \rangle \delta_{ij}$$

Mean scalar Equations

- mean scalar equation

$$\frac{\partial \langle \phi_l \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle \phi_l \rangle}{\partial x_k} = -\frac{\partial \langle u_k \, \phi_l^{'} \rangle}{\partial x_k} + \langle S_l(\phi) \rangle$$

- second-order scalar transport equation

$$\frac{\partial \langle u_i \phi_l^{'} \rangle}{\partial t} + \langle u_k \rangle \frac{\partial \langle u_i \, \phi_l^{'} \rangle}{\partial x_k} + \frac{\partial \langle u_i u_k \phi_l^{'} \rangle}{\partial x_k} = -\langle u_i u_k \rangle \frac{\partial \langle \phi_l \rangle}{\partial x_k} - \langle u_k \phi_l^{'} \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}$$
$$+ \langle u_i S_l(\phi) \rangle - \left(G_{ik} - \frac{1}{2} C_\phi \frac{\langle \epsilon \rangle}{k} \delta_{ik} \right) \langle u_k \phi_l^{'} \rangle$$

- All convective and source terms are in **closed form**
- No *instantaneous* field but **mean fields** $\langle \mathbf{U} \rangle(t, \mathbf{x})$, $\langle u_i u_j \rangle(t, \mathbf{x})$, $\langle \phi \rangle(t, \mathbf{x})$..
- **Closures with white-noise terms** in the **particle stochastic equations** correspond to **local closures** (in space) in the **mean-field equations**

White-noise terms and local mean-field closures (1)

- The white-noise term in the particle stochastic equation

$$dU_i = -\frac{1}{\rho}\frac{\partial\langle P\rangle}{\partial x_i}\,dt + D_i\,dt + \underbrace{\sqrt{C_0\langle\epsilon(\mathbf{x})\rangle}dW_i}_{\textit{fast term}}$$

  which has a **zero correlation timescale** correspond to

$$\frac{\partial\langle u_i u_j\rangle}{\partial t} + \langle U_k\rangle\frac{\partial\langle u_i u_j\rangle}{\partial x_k} + \frac{\partial\langle u_i u_j u_k\rangle}{\partial x_k} = -\langle u_i u_k\rangle\frac{\partial\langle U_j\rangle}{\partial x_k} - \langle u_j u_k\rangle\frac{\partial\langle U_i\rangle}{\partial x_k}$$
$$\langle u_i D_j\rangle + \langle u_j D_i\rangle + \underbrace{C_0\langle\epsilon\rangle(\mathbf{x})}_{\textit{local term}}\,\delta_{ij}$$

- The **memory-less** term in the particle velocity equation induce a "*transport-less*" or **local term** in the corresponding equation (which appears always as the level of the work performed by these "forces")

White-noise terms and local mean-field closures (2)

- If the fast-acceleration terms is now regularised (with a "coloured noise")

$$dU_i = -\frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i}\,dt + D_i\,dt + \gamma_i\,dt$$

which is a defined process with a **non-zero integral timescale**, then

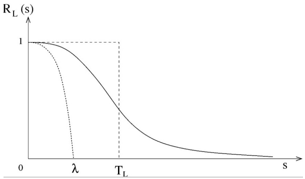
$$\frac{\partial \langle u_i u_j \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle u_i u_j \rangle}{\partial x_k} + \frac{\partial \langle u_i u_j u_k \rangle}{\partial x_k} = -\langle u_i u_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} - \langle u_j u_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}$$
$$\langle u_i D_j \rangle + \langle u_j D_i \rangle + \underbrace{\langle u_i \gamma_j \rangle + \langle u_j \gamma_i \rangle}_{non-local\ term}$$

- For example, if γ is also a Langevin model $d\gamma_i = -\frac{\gamma_i}{\tau}\,dt + K_i\,dW_i$ then $\langle u_i \gamma_i \rangle$ is the solution of a **transport equation**: non-locality ($\tau > 0$)

$$\begin{cases} \dfrac{\partial \langle u_i \gamma_i \rangle}{\partial t} + \langle U_k \rangle \dfrac{\partial \langle u_i \gamma_i \rangle}{\partial x_k} + \dfrac{\partial \langle u_k u_i \gamma_i \rangle}{\partial x_k} = \langle D_i \gamma_i \rangle - \dfrac{\langle u_i \gamma_i \rangle}{\tau} + \langle (\gamma_i)^2 \rangle \\ \dfrac{\partial \langle (\gamma_i)^2 \rangle}{\partial t} + \langle U_k \rangle \dfrac{\partial \langle (\gamma_i)^2 \rangle}{\partial x_k} + \dfrac{\partial \langle u_k (\gamma_i)^2 \rangle}{\partial x_k} = -2\dfrac{\langle (\gamma_i)^2 \rangle}{\tau} + \underbrace{K_i^2}_{local\ term} \end{cases}$$

Acceleration and the derivative of the velocity auto-correlation (1)

- Lagrangian velocity auto-correlation $R_L(t,s) = \dfrac{\langle U(t)U(t+s)\rangle}{\sqrt{\langle U^2(t)\rangle\langle U^2(t+s)\rangle}}$



In stationary homogeneous turbulence, the Lagrangian velocity auto-correlation, $R_L(s)$ depends only on the time lag, s, and is an even $\mathcal{C}^2$-function. Thus, at the origin, $R_L^{'}(s=0)=0$

- With a Langevin model for particle velocity written simply as

$$dU(t) = -\frac{U(t)}{T}\,dt + K\,dW_t$$

then the auto-correlation is an exponential function

$$R(s) = \exp\left(-\frac{s}{T}\right) \Longrightarrow R^{'}(s=0) = -\frac{1}{T} \neq 0$$

- The form of R_L is a **consequence** of a Langevin model but **not** its input

Acceleration and the derivative of the velocity auto-correlation (2)

- Is there a defect of Lagrangian models? Is it even a result or a surprise?
- The derivative of the velocity auto-correlation is governed by acceleration

$$R_L'(s=0) = \langle U(t) \left(\frac{dU(t)}{dt} \right) \rangle$$

- Yet, the *basic starting idea* behind the Langevin model was to *skip over details of the acceleration* and describe it as a *fast-variable process*
- The non-zero slope is **not** a result but **reflects** the **modelling choice**
- If acceleration is important, it should be treated as a non-infinite process

$$\begin{cases} dU(t) = -\dfrac{U(t)}{T}\, dt + \gamma\, dt \\ d\gamma = \dfrac{\gamma}{\tau}\, dt + K_a\, dW \end{cases} \Rightarrow \begin{cases} R_L(s) = \dfrac{1}{1-\tau/T} \left[e^{-s/T} - \dfrac{\tau}{T} e^{-s/\tau} \right] \\ \lim\limits_{\tau \to 0} R_L'(s=0) \neq \left(\lim\limits_{\tau \to 0} R_L \right)'(s=0) \end{cases}$$

- Auto-correlations **result from the choice** of a stochastic model
- Numerically, Stratonovich calculus can be used (cf. Lectures 4-5)

Kolmogorov hypothesis for the fluid seen

- Kolmogorov theory in the inertial range

$$\langle (d\mathbf{U}_f)^2 \rangle = C_0 \langle \epsilon \rangle dt$$

Langevin equation for fluid particle velocities

$$dU_{f,i} = -\frac{1}{\rho_f} \frac{\partial \langle P \rangle}{\partial x_i} dt - \frac{U_{f,i} - \langle U_{f,i} \rangle}{T_L} dt + \sqrt{C_0 \langle \epsilon \rangle} dW_i$$

- construction in two steps : step 1 (particle inertia) and step 2 (CTE)
- present models neglect step 1 $\rightarrow$ statistics of the fluid seen ($\mathbf{U}_s$) differ from the statistics of fluid particle velocities due to mean drifts
- Fluid seen $d\mathbf{U}_s = \delta \mathbf{u}[dt, \langle \mathbf{U}_r \rangle dt] \Rightarrow$ **space and time issue**
- Langevin models (diffusion process for the velocity of the fluid seen)

$$dU_{s,i} = A_{s,i} dt + B_{s,ij} dW_j$$

Langevin model for turbulent dispersion

- One general model

$$
\begin{aligned}
dU_{s,i} = & -\frac{1}{\rho_f}\frac{\partial \langle P\rangle}{\partial x_i}\,dt + \left(\langle U_{p,j}\rangle - \langle U_{f,j}\rangle\right)\frac{\partial \langle U_{f,i}\rangle}{\partial x_j}\,dt \\
& - \frac{\left(U_{s,i} - \langle U_{f,i}\rangle\right)}{T^*_{L,i}}\,dt + \sqrt{\langle \epsilon\rangle \left(C_0 b_i \tilde{k}/k + \frac{2}{3}(b_i\tilde{k}/k - 1)\right)}\,dW_i
\end{aligned}
$$

$$
\tilde{k} = \frac{3}{2}\frac{\sum_{i=1}^{3} b_i \langle u^2_{f,i}\rangle}{\sum_{i=1}^{3} b_i} \qquad b_i = \frac{T_L}{T^*_{L,i}} \quad 1/T_L = \left(\frac{1}{2} + \frac{3}{4}C_0\right)\frac{\langle\epsilon\rangle}{k}
$$

$$
T^*_{L,1} = \frac{T_L}{\sqrt{1 + \beta^2 \frac{|\langle \mathbf{U}_r\rangle|^2}{2k/3}}} \qquad T^*_{L,2} = T^*_{L,3} = \frac{T_L}{\sqrt{1 + 4\beta^2 \frac{|\langle \mathbf{U}_r\rangle|^2}{2k/3}}}
$$

- When $\tau_p \rightarrow 0$, the Langevin model for fluid particles is retrieved

$$
dU_{s,i} = -\frac{1}{\rho_f}\frac{\partial \langle P\rangle}{\partial x_i}\,dt - \frac{U_{s,i} - \langle U_{f,i}\rangle}{T_L}\,dt + \sqrt{C_0\langle\epsilon\rangle}\,dW_i
$$

Plan

A chosen list of specifications

- In two-phase flow modelling, stochastic (or pdf) models are used to predict averaged equations and constitutive relations
- It is important to check that the fluid limit is "well reproduced"
- An important issue to decide: what makes a given (fluid) particle stochastic model acceptable?
- Among other possible criteria, at least two appear compulsory:
  1. *the stochastic model should be free of spurious drifts and respect the mean-continuity equation*
  2. *All convective terms in the mean Navier-Stokes equation AND in the second-order must be exactly reproduced (as well as dissipative terms)*
- These two items means that, at least, the first two moment equations should be physically and well reproduced
- Other criteria include, for example, Gaussian pdfs in homogeneous cases and the ability to predict non-Gaussianity in inhomogeneous flows

The issue of spurious drifts

- The issue of "spurious drifts" refers to the possibility of having (fluid) particles which tend to accumulate in some areas
- Concentration build-ups amounts to a false accumulation of mass (in incompressible flows): *the mean continuity equation is not respected* !
- Uniform particle concentration (no spurious drift) and respect of the mean continuity equation is equivalent (cf. Pope)

$$\left(\frac{\partial}{\partial t} + \langle U \rangle_k \frac{\partial}{\partial x_k}\right) \ln p(t, \mathbf{x}) = -\frac{\partial \langle U_k \rangle}{\partial x_k}, \quad \langle U \rangle_k(t, \mathbf{x}) = \langle U_k \,|\, \mathbf{x}(t) = \mathbf{x} \rangle$$

- **Any stochastic model formulated with instantaneous velocity as**

$$\begin{cases} dx_{f,i} = U_{f,i}\, dt \\ dU_{f,i} = -\dfrac{1}{\rho}\dfrac{\partial \langle P \rangle}{\partial x_i}\, dt + StM(\mathbf{x}_f, \mathbf{U}_f) \end{cases}$$

where $\langle P \rangle$ is such that the mean-continuity equation is satisfied and with $\langle StM(\mathbf{x}_f, \mathbf{U}_f) \,|\, \mathbf{x}(t) = \mathbf{x} \rangle = 0$ is **free of spurious drifts**

Instantaneous or fluctuating velocities? (1)

- Any stochastic model can be expressed in terms of the instantaneous velocity, $\mathbf{U}(t)$, or of the fluctuating velocitiy $\mathbf{u}(t) = \mathbf{U}(t) - \langle \mathbf{U} \rangle (t, x_f(t))$
- This is not an issue of stochastic modelling but a change of variables
- Indeed, any stochastic model formulated in terms of $\mathbf{U}$ as

$$\begin{cases} dx_{f,i} = U_{f,i}\, dt \\ dU_{f,i} = \underbrace{-\frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i}\, dt}_{\textit{no spurious drift}} + \underbrace{StM(\mathbf{x}_f, \mathbf{U}_f)}_{\textit{model}} \end{cases}$$

- is equivalent to a stochastic model in terms of $\mathbf{u}$ formulated as

$$\begin{cases} dx_{f,i} = \left(\langle U \rangle_{f,i} + u_{f,i} \right)\, dt \\ du_{f,i} = \underbrace{\frac{\partial \langle u_i u_k \rangle}{\partial x_k}\, dt}_{(a)\ \textit{no spurious drift}} - \underbrace{u_k \frac{\partial \langle U_{f,i} \rangle}{\partial x_k}\, dt}_{(b)\ \textit{production term}} + \underbrace{StM(\mathbf{x}_f, \mathbf{u}_f)}_{\textit{model}} \end{cases}$$

Instantaneous or fluctuating velocities? (2)

- The first two terms on the rhs of the equation for **u** are **essential** and **compulsory**: they **must be respected** by any acceptable model
- The term (a) is necessary to ensure that no spurious drifts occur: *consistency with the mean Navier-Stokes equation*
- The term (b) is compulsory in order to treat correctly **convective terms** and, in particular to obtain the correct form of the second-order equations: *consistency with Reynolds-stress modelling*

$$\underbrace{\frac{\partial\langle u_i u_j\rangle}{\partial t} + \langle U_k\rangle\frac{\partial\langle u_i u_j\rangle}{\partial x_k} + \frac{\partial\langle u_i u_j u_k\rangle}{\partial x_k}}_{\langle d(u_i u_j)\rangle} = \underbrace{-\langle u_i u_k\rangle\frac{\partial\langle U_j\rangle}{\partial x_k} - \langle u_j u_k\rangle\frac{\partial\langle U_i\rangle}{\partial x_k}}_{\textit{correct production term}}$$

$$\langle u_i StM_j\rangle + \langle u_j StM_i\rangle$$

- A stochastic model for **U** requires 3 gradients (for $\nabla\langle P\rangle$)
- A stochastic model for **u** requires 27 gradients (for $\nabla\langle U\rangle$ and $\nabla\langle u_i u_j\rangle$)

Plan

1. General guidelines: Modelling approach and actual models
   - Choice of a modelling approach for single-phase reactive flows
   - Choice of a modelling approach for polydispersed two-phase flows
2. The framework of present Lagrangian two-phase flow models
   - The (one-particle) PDF formalism: from SDEs to Mean fields
   - An reminder on the physical contents
3. Consistency issues in the fluid limit case
   - Correspondence with Reynolds-stress modelling
     - The spurious issue of spurious drifts
     - Various forms of the Langevin equations
   - Consistency issues in the hybrid "Euler/Lagrange" formulation

Consistency issues in the Moment/PDF approach (1)

- In classical hybrid Moment/PDF formulations (Eulerian/Lagrangian), evaluations of fluid and particle statistics may seem well separated
  $\Rightarrow$ fluid mean fields are solved by a Moment Approach based on the choice of a turbulence model ($k-\epsilon$ or RSM): $\langle P \rangle$, k, $\langle \epsilon \rangle$, $\langle \mathbf{U} \rangle_f$, $\langle u_{f,i} u_{f,j} \rangle$
  $\Rightarrow$ particle statistics are solved by the Lagrangian approach based on the choice of a stochastic model for $\mathbf{Z} = (\mathbf{x}_p, \mathbf{U}_p, \mathbf{U}_s, \ldots)$

$$
\begin{cases}
d\mathbf{x}_p = \mathbf{U}_p \, dt \\
d\mathbf{U}_p = \dfrac{\mathbf{U}_s - \mathbf{U}_p}{\tau_p} \, dt + \mathbf{g} \, dt \\
d\mathbf{U}_s = \mathbf{\Pi}(\mathbf{Z}, \langle \mathbf{H}_p \rangle, \langle \mathbf{U}_f \rangle^E, \langle \mathbf{H}_f \rangle) \, dt \\
\qquad\qquad - \dfrac{\mathbf{U}_s - \langle \mathbf{U}_f \rangle^E}{T_L^*} \, dt + \mathbf{B}(\mathbf{Z}, \langle \mathbf{H}_p \rangle, \langle \mathbf{U}_f \rangle^E, \langle \mathbf{H}_f \rangle) \, d\mathbf{W}
\end{cases}
$$

  $\Rightarrow$ Monte Carlo estimations give particle mean values: $\langle \mathbf{U}_p \rangle$, $\langle u_{p,i} u_{p,j} \rangle$.

Consistency issues in the Moment/PDF approach (2)

- When $\tau_p \to 0$, the particle stochastic model reverts to the fluid one

$$\begin{cases} d\mathbf{x}_f = \mathbf{U}_f \, dt \\ d\mathbf{U}_f = -\dfrac{1}{\rho_f}\dfrac{\partial \langle P \rangle}{\partial \mathbf{x}}\, dt - \dfrac{\mathbf{U}_f - \langle \mathbf{U}_f \rangle^E}{T_L}\, dt + \sqrt{C_0 \langle \epsilon \rangle}\, d\mathbf{W} \end{cases}$$

- The Lagrangian solver yield mean fields: $\langle \mathbf{U}_f \rangle^L$, $\langle u_{f,i} u_{f,j} \rangle^L$
- We are now dealing with **duplicate mean fields**!
- The **consistency issue** requires: $\langle \mathbf{U}_f \rangle^L = \langle \mathbf{U}_f \rangle^E$, $\langle u_{f,i} u_{f,j} \rangle^L = \langle u_{f,i} u_{f,j} \rangle^E$.
- the fluid Langevin model is consistent with a Rotta RSM

$$\frac{\partial \langle u_i u_j \rangle}{\partial t} + \langle U_k \rangle \frac{\partial \langle u_i u_j \rangle}{\partial x_k} + \frac{\partial \langle u_i u_j u_k \rangle}{\partial x_k} = -\langle u_i u_k \rangle \frac{\partial \langle U_j \rangle}{\partial x_k} - \langle u_j u_k \rangle \frac{\partial \langle U_i \rangle}{\partial x_k}$$
$$- (1 + \frac{3}{2} C_0) \frac{\langle \epsilon \rangle}{k} \left(\langle u_i u_j \rangle - \frac{2}{3} k \delta_{ij} \right) - \frac{2}{3} \delta_{ij} \langle \epsilon \rangle$$

Consistency issues in the Moment/PDF approach (3)

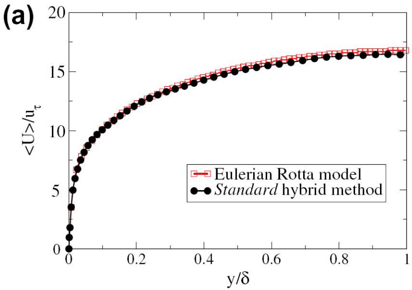
- **<u>Issue</u>**: What happens when two different, and possible inconsistent, turbulence models are used in the Fluid Description (Moment or Eulerian phase) and in the Particle Description (PDF or Lagrangian phase)?
- "*A better $\langle \mathbf{U}_f \rangle^E$ fed into the Langevin model gives better outcomes...*". **Is that really so when consistency issues are disregarded?**
- this question is best assessed in the fluid-limit case by considering various $\langle \mathbf{U}_f \rangle^E$ taken as input into the Langevin model

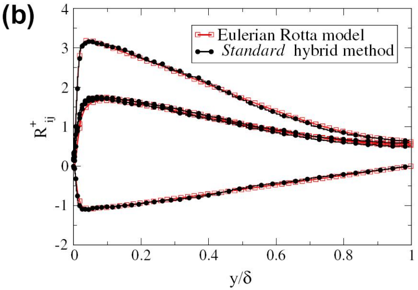
$$\begin{cases} d\mathbf{x}_f = \mathbf{U}_f \, dt \\ d\mathbf{U}_f = -\dfrac{1}{\rho_f} \dfrac{\partial \langle P \rangle}{\partial \mathbf{x}} \, dt - \dfrac{\mathbf{U}_f - \langle \mathbf{U}_f \rangle^E}{T_L} \, dt + \sqrt{C_0 \langle \epsilon \rangle} \, d\mathbf{W} \end{cases}$$

- Potential discrepancies are also present for non-zero inertia particles.

Numerical assesments (1)

- Numerical tests were performed in a channel with various $\langle \mathbf{U}_f \rangle^E$ ("A note on the consistency of hybrid Eulerian/Lagrangian approach to multiphase flows" S. Chibbaro and J.-P. Minier, IJMF, 37, 293-297, 2011)





Numerical assesments (2)