Quadrature-based moment methods for multiphase flows

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Warwick Fluid Dynamics Seminar

Collaborators

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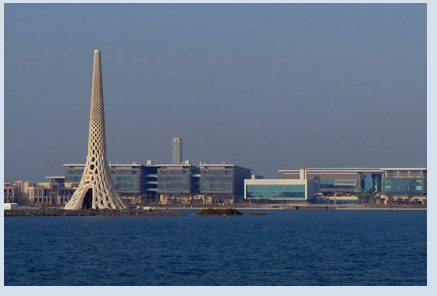

ICES, The University of Texas at Austin

- Serge Prudhomme (now at EP Montreal)
- Ivo Babuska
- Masha Prodanovic (Petrol. Eng.)

Complex flow regimes

Need of upscaled models and efficient methods

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Dimensionless numbers

- Reynolds number (fluid or particles) $\mathrm{Re} = \frac{U^{f,r} L}{\nu}$
- Particles Stokes number $\mathrm{St} = \frac{\tau^p}{\tau_f} = \frac{\tau^p U^f}{L}$
- Knudsen number $\mathrm{Kn} = \frac{\lambda}{L}$

$\mathrm{Re} >> 1 \rightarrow$ transition to turbulence
small scale and collisions, $\mathrm{Kn} > 10^{-3} \rightarrow$ non-equilibrium effects
poly-dispersity, different St, evolving size $\rightarrow$ differential segregation

Problem	Model	Tool
Turbulence	Large Eddy Simulation (LES)	
Poly-dispersity	Population Balance Eq. (PBE)	QBMM[1]
Collisions	Boltzmann Eq.	QBMM
Multi-phase	Eulerian/Mixture	Algebraic Slip
Random heterogeneous materials	DNS + upscaling	

[1]QBMM=Quadrature-Based Moment Method

Open and recent projects

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Fluid dynamics and porous media - Applications

- **Pore-scale simulations (single and multi-phase)**
- Microfluidics, drop impacts on structured surfaces
- Particulate processes in turbulent flows, colloid deposition
- Momentum transfer closures for polydispersed flows

Multiscale simulations - Numerics

- Numerical studies on convergence properties of flow in complex geometries
- **Upscaling/model reduction of PDEs in subsurface flows and in Lithium-ion batteries**
- **Multilevel Monte Carlo sampling for flows with random geometry/parameters**
- Discretization of PDF equations by quadrature-based moment methods

UQ and Stochastic Modelling

- **Bayesian inference for calibration and validation of macro-scale models**
- Dynamic and static data assimilation with mean-field Ensemble Kalman Filter
- High-dimensional interpolation and surrogates for machine learning in MD
- **PDF closures for turbulent and porous media flows**

Outline

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- Gaussian quadrature
- QMOM and DQMOM
- EQMOM
- Multivariate case
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- Gas-liquid flows
- Non-equilibrium and granular flows / non-smooth kernels
- Turbulent reactive flows / PDF as modelling tool
- Porous media
- UQ and other applications

References

- D. Marchisio and R. Fox, Computational Models for Polydisperse Particulate and Multiphase Systems (Cambridge Univ, 2012)
- Rodney Fox, Computational Models for turbulent reacting flows (Cambridge Univ, 2003)
- H. Struchtrup, Macroscopic Transport Equations for Rarefied Gas Flows (Springer, 2005)
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- my PhD thesis (2012)
- O. Le Maitre and O. Knio, Spectral Methods for Uncertainty Quantification (Springer, 2010)
- C.W. Gardiner, Handbooks of Stochastic Methods (Springer, 2004)
- Articles and reviews of R. Fox, D. Marchisio, A. Passalacqua, P. Vedula, L. Massot, ...

Notation

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Please keep in mind the following notation:

- Probability Density function (PDF): f or P
- Number Density Function (NDF): n
- Space coordinates **x**, velocity U
- Subscripts: p for particles, f for fluid
- Statistical moments: M or μ
- Particle mass: m
- Polynomial of order α: P_α
- Internal variables: general ξ (or ξ), size L, species concentration ϕ
- Quadrature nodes denoted by the internal variable with subscript i
- Quadrature weights denoted by w_i
- Ω_ξ (or simply $\mathbb{R}$): support for variable ξ

NO Einstein summation convention

This is just a modelling and numerical overview. Sorry but there will be no mathematical details (spaces, BCs, probability spaces, proofs, etc...), use your intuition (and ask if needed)!!

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Smoluchowski coagulation equation

Smoluchowski, 1916

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Describe particle aggregation/coagulation

$$\frac{\partial n(L,t)}{\partial t} = \frac{1}{2}\int_0^L K(L-\tilde{L},\tilde{L})n(L-\tilde{L},t)n(\tilde{L},t)\,d\tilde{L} - \int_0^\infty K(L,\tilde{L})n(L,t)n(\tilde{L},t)\,d\tilde{L}$$

- Not to be confused with the Smoluchowski equation (drift-diffusion equation)
- Integro-differential equation
- Number density n of particles with size L
- No spatial dependence
- RHS (Q) has a gain and a loss term written in terms of the aggregation frequency K
- K is usually very complex and non-linear

Very interesting mathematical topic (stability, linearization, large-time asymptotics), see works of Klemens Fellner (Graz)

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Population Balance Equation (PBE)

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Extension of the Smoluchowski coagulation equation, very popular in Chemical Engineering, Biology and Social Models

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \cdot (Un) + \frac{\partial}{\partial \xi} \cdot (Gn) = \mathcal{Q}$$

- $n = n(\xi; x, t)$ number of particles per unit volume
- ξ_i generic internal variables (volume, size, area, composition, other properties)
- U given advection velocity field
- $\mathcal{Q}$ describe the generic particulate process with Birth (nucleation), Breakage (Fragmentation) and Aggregation (Coagulation)[2]

$$\mathcal{Q} = \mathcal{Q}_0 + \mathcal{Q}_1(n) + \mathcal{Q}_2(n, n)$$

- G describe growth of particles (velocity in phase space ξ)
- Usually written for spatially inhomogeneous systems and coupled with CFD to simulate dispersed bubbles and particles

[2]with frequency kernels that can be seen as upscaled jump processes

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The physical basis of Boltzmann eq.
Binary collisions

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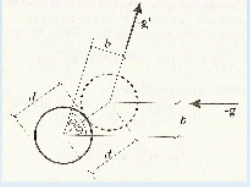
Molecular encounters for hard-spheres potential



- d is the molecular diameter
- $g = U - U_*$ is the pre-collision velocity difference
- $g' = U' - U'_*$ is the post-collision velocity difference

Number and momentum are conserved during a collision

$$m + m_* = m' + m'_*; \qquad U + U_* = U' + U'_*$$

as well as kinetic energy (in the case of elastic collisions)

$$U \cdot U + U_* \cdot U_* = U' \cdot U' + U'_* \cdot U'_*$$

Boltzmann Equation (BE)

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From the Liouville n-particles equation, assuming indistinguishable particle and the "Stosszahlansatz" (molecular chaos[3] hypothesis), the Boltzmann equation is obtained

$$\frac{\partial n(U)}{\partial t} + \frac{\partial}{\partial x} \cdot (Un(U)) + \frac{\partial}{\partial U} \cdot (An(U)) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^+} \left[n(U')n(U'_*) - n(U)n(U_*) \right] \beta(g, x) \, \mathrm{d}s \, \mathrm{d}U_*$$

- A is the acceleration,
- $\mathbb{S}^+$ is the solid angle
- $\beta(g, x)$ is the collision kernel

Equations with similar structure: Vlasov (no collisions), Williams-Boltzmann spray equation, ...

[3] particles are uncorrelated, two-particles PDF is product of one-particle PDF

Boltzmann Equation and Equilibrium

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Most of the studies and methods for BE are based on the concept of **Equilibrium Distribution**

- The equilibrium distribution f_{eq} is such that $\mathcal{Q}(f_{eq}, f_{eq}) = 0$
- Also called "Maxwell-Boltzmann" or "Maxwellian" distribution, a Gaussian in the standard case
- Fixing the first 2 moments (3 in case of NDF), only one Gaussian exist
- If one wants to study non-equilibrium phenomena, more moments must be studied
- Grad's moment method is based on small deviations from equilibrium

$$f \approx f_{eq}(1 + a_1 H_1(v) + a_2 H_2(v) + \dots)$$

- Other methods (such as Lattice Boltzmann) rely on a linearized collision term (BGK, Bhatnagar-Gross-Krook approximation)

$$\mathcal{Q} \approx \frac{1}{\tau_r}(f - f_{eq})$$

All these methods require the prior knowledge of the equilibrium distribution!

Flow regimes

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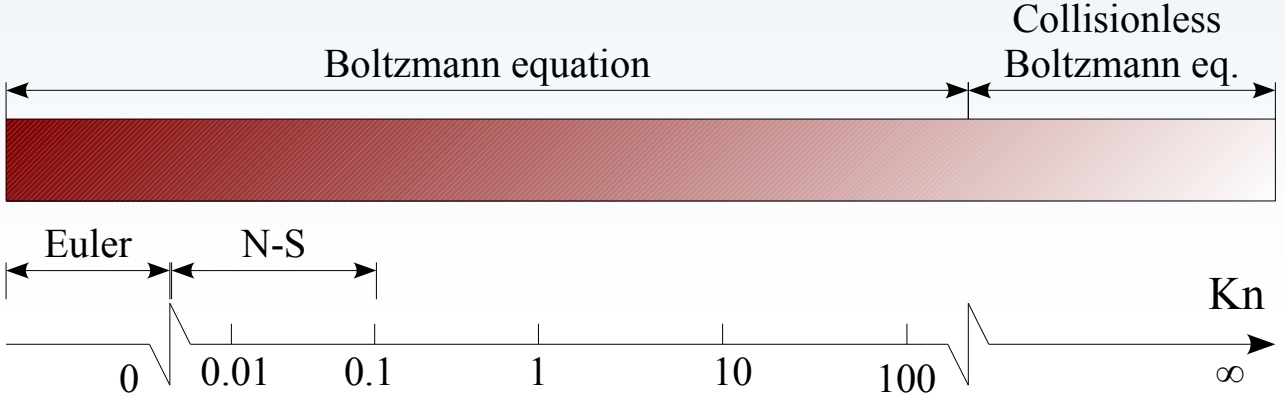
The Boltzmann Equation is not only for rarefied gases!

- The flow regime of a granular gas depends on Knudsen number $Kn = \frac{\lambda}{L_0}$
- The hydrodynamic description based on the Navier-Stokes-Fourier (NSF) equation is valid only for low Kn:
- Continuous regime $(Kn < 0.01)$: NSF with no-slip BC.
- Slip regime $(0.01 < Kn < 0.1)$: NSF and partial slip BC at walls.
- For $Kn > 0.1$: Full Boltzmann equation.



Adapted from: G. A. Bird (1994)

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The Method of Moments

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- MOM originates in kinetic theory of gases[4]: $n(t, x, U)$
- The moment of order zero is related to the density:

$$\rho(t,x) \equiv m M_{0,0,0}(t,x) = m \iiint_{-\infty}^{+\infty} n(t,x,U)\, \mathrm{d}U$$

- The moment of order one is used to define the average velocity:

$$\langle U \rangle = \left(\frac{M_{1,0,0}}{M_{0,0,0}}, \frac{M_{0,1,0}}{M_{0,0,0}}, \frac{M_{0,0,1}}{M_{0,0,0}} \right)$$

- By applying the MOM to the Boltzmann equation, an infinite system of equations (cascade) appears
- Euler, Navier-Stokes and Burnett equations are obtained by with the Chapman-Enskog method (asymptotic expansions at different orders)

[4]The same name however may refer to many different methods in different fields

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The GPBE fluid-particle systems

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- $n(t, x, U_p, \xi_p, U_f, \xi_f)$, represents the number of particles (per unit volume) with velocity equal to U_p, internal coordinate ξ_p and see a continuous phase with velocity U_f and internal coordinate ξ_f.
- The evolution of the NDF is dictated by the GPBE:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \cdot \left(U_p n\right) + \frac{\partial}{\partial U_p} \cdot \left[\left(A_{fp} + A_p\right) n\right] + \frac{\partial}{\partial \xi_p} \cdot \left(G_p n\right) + \frac{\partial}{\partial U_f} \cdot \left[\left(A_{pf} + A_f\right) n\right] + \frac{\partial}{\partial \xi_f} \cdot \left(G_f n\right) = \mathcal{Q} \quad (1)$$

- phase-space velocity for particle velocity: $A_{fp} + A_p$ (average particle acceleration $\rightarrow$ acceleration model (drag, lift, ...)
- phase-space velocity for particle internal coordinate: G_p (e.g. particle growth rate)
- Discontinuous jump term: $\mathcal{Q}$ (e.g. particle collision, aggregation, breakage, nucleation, etc.)

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GPBE and QBMM

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Generalized Population Balance Equation can be used for various applications

- Poly-dispersed[5] multiphase flows
- Bubbly flows, Particle-laden flows
- Granular flows, fluidized beds
- Rarefied gases

Classical CFD models such as Mixture model, two-fluid model can be recovered

In general the idea of quadrature-based moment methods (QBMM) can be used for generic kinetic/PDF equations

- Statistical description of turbulence and turbulent reactive flows (Pope)
- Mean field limit in models of social behavior (crowd, swarms, traffic, opinion)
- Mean field equations of stochastic processes
- Fokker-Planck equation

[5]Fluid or solid particles of different size immersed in a continuous fluid phase

Numerical methods developed

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The mesoscale/kinetic models are highly dimensional (1 time + 3 spatial coordinates + 1 size + 3 velocities + ...)

A plethora of methods have been generated:

- Interesting ways to solve it are Lagrangian / Monte Carlo methods (DSMC) or to high-dimensional adaptive DG methods
- In PBE the distribution is often discretized into classes or sections (FD)
- Widely used among practitioners in multiphase CFD is the multiple-size-group (MUSIG) method
- For the BE it is equivalent to the discrete-velocity method
- The method of moments (MOM) has been used for the solution of both PBE and BE, but the resulting closure problem is overcome by different strategies (e.g. Grad method, other functional assumptions, method of moments with interpolative closure, MOMIC)

Method of Moments

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- Important advantage is that the moments correspond to quantities that have meaningful physical interpretations and are therefore directly measurable
- This is a crucial point, since in many applications the NDF is not directly measured, but is inferred from measurements of integral quantities
- Two main issues arise when using MOM: number of moments to be tracked and closure problem
- The closure problem is the impossibility of writing a term as a function of a finite set of moments
- When the kinetic equation contains a derivative with respect to an internal variable, we have a cascade of equations for the moments (M_i depends on M_{i+1})
- Often integral source terms also need closure

The issues of the number of moments to be tracked and the closure adopted both affect overall accuracy $\Rightarrow$ connected and addressed together

Closure problem

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When applying the moment transform (i.e. integral) closures must be assumed

The closure problem appears always in the following form:

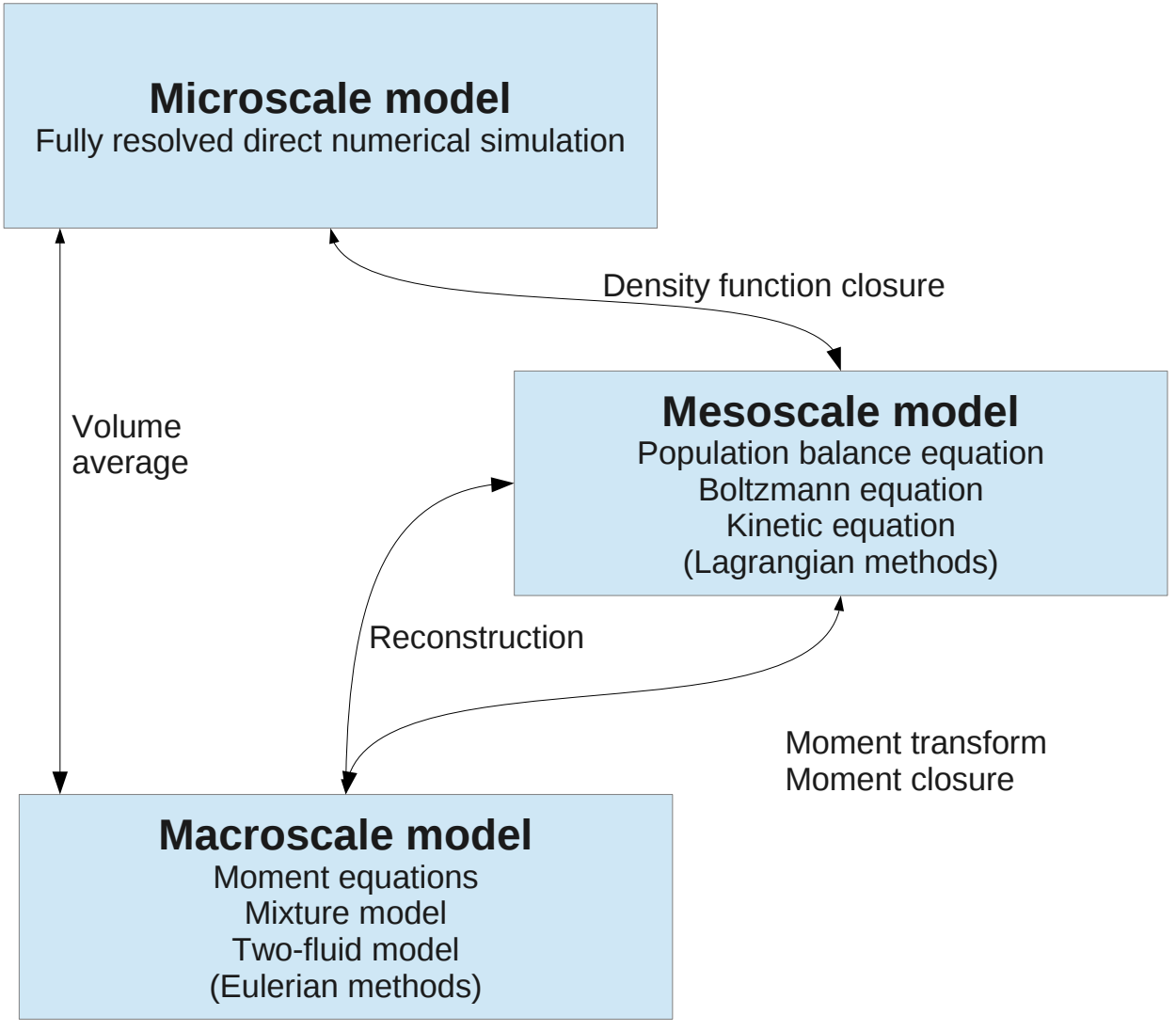
$$I = \int_{\Omega_\xi} g(\xi) n(\xi) \, \mathrm{d}\xi, \tag{2}$$

where $n(\xi)$ is the univariate NDF to be approximated and g a generic function to be closed

Presumed-PDF approaches

- A possible approach is to simply to assume a shape for the PDF/NDF
- This is reasonable when there is a fast relaxation towards equilibrium (e.g., in Boltzmann equations the Maxwellian equilibrium is a Gaussian)
- There are many cases when the actual NDF is far from equilibrium
- How to find the best closure?

The problem is multiscale in nature!



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Gaussian quadrature
Basic idea behind QBMM

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- The closure problem can be overcome by using the following quadrature formula:

$$\int_{\Omega_\xi} n(\xi) g(\xi) \, \mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha g(\xi_\alpha), \tag{3}$$

  where w_α and ξ_α are the weights and the nodes/abscissas of the quadrature formula, and N is the number of nodes
- The degree of accuracy is equal to d if the interpolation formula is exact when the integrand is a polynomial of order less than or equal to d and there exists at least one polynomial of order $d+1$ that makes the interpolation formula inexact.

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Basic idea behind QBMM

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- The closure problem can be overcome by using the following quadrature formula:

$$\int_{\Omega_\xi} n(\xi) g(\xi)\, \mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha g(\xi_\alpha), \tag{4}$$

where w_α and ξ_α are the weights and the nodes/abscissas of the quadrature formula, and N is the number of nodes

QBMM use a Gaussian quadrature

The NDF is the weight function or measure; the moments

$$M_k = M(k) = \langle \xi^k \rangle = \int_{\Omega_\xi} n(\xi) \xi^k \, \mathrm{d}\xi, \quad k = 0, 1, 2, \ldots \tag{5}$$

are used to compute a Gaussian quadrature rule with a degree of accuracy of $2N - 1$,.

Gaussian quadrature

A set of polynomials $\{P_0(\xi), P_1(\xi), \dots, P_\alpha(\xi), \dots\}$ with $P_\alpha(\xi) = k_{\alpha,0}x^\alpha + k_{\alpha,1}x^{\alpha-1} + \cdots + k_{\alpha,\alpha}$, is said to be orthogonal in the integration interval Ω_ξ, with respect to the weight function, if

$$\int_{\Omega_\xi} n(\xi)P_\alpha(\xi)P_\beta(\xi)\,\mathrm{d}\xi \begin{cases} = 0 & \text{for } \alpha \neq \beta, \\ > 0 & \text{for } \alpha = \beta, \end{cases} \tag{6}$$

and, of course, is said to be orthonormal if

$$\int_{\Omega_\xi} n(\xi)P_\alpha(\xi)P_\beta(\xi)\mathrm{d}\xi = \begin{cases} 0 & \text{for } \alpha \neq \beta, \\ 1 & \text{for } \alpha = \beta. \end{cases} \tag{7}$$

Any set of orthogonal polynomials $\{P_\alpha(\xi)\}$ has a recurrence formula relating any three consecutive polynomials in the following sequence:

$$P_{\alpha+1}(\xi) = (\xi - a_\alpha)P_\alpha(\xi) - b_\alpha P_{\alpha-1}(\xi), \quad \alpha = 0, 1, 2, \ldots \tag{8}$$

with $P_{-1}(\xi) \equiv 0$ and $P_0(\xi) \equiv 1$ and where

$$a_\alpha = \frac{\int_{\Omega_\xi} n(\xi)\xi P_\alpha(\xi)P_\alpha(\xi)\,\mathrm{d}\xi}{\int_{\Omega_\xi} n(\xi)P_\alpha(\xi)P_\alpha(\xi)\,\mathrm{d}\xi}, \quad \alpha = 0, 1, 2, \ldots \tag{9}$$

$$b_\alpha = \frac{\int_{\Omega_\xi} n(\xi)P_\alpha(\xi)P_\alpha(\xi)\,\mathrm{d}\xi}{\int_{\Omega_\xi} n(\xi)P_{\alpha-1}(\xi)P_{\alpha-1}(\xi)\,\mathrm{d}\xi}, \quad \alpha = 1, 2, \ldots. \tag{10}$$

One can calculate a_0, then $P_1(\xi)$, then a_1 and b_1 and so on...

- The coefficients a_α and b_α can be written in terms of the moments
- The coefficients necessary for the construction of a polynomial of order N can be calculated from the first $2N-1$ moments of the NDF
- For example with M_0, M_1, M_2 and M_3, it is possible to calculate the following coefficients:

$$
\begin{aligned}
a_0 &= \frac{M_1}{M_0}, \\
a_1 &= \frac{M_3 M_0^2 + M_1^3 - 2M_2 M_1 M_0}{M_2 M_0 + M_1^2 - 2M_1^2 M_0}, \\
b_1 &= \frac{M_2 M_0 + M_1^2 - 2M_1^2 M_0}{M_0^2},
\end{aligned}
\tag{11}
$$

which suffice for the calculation of the polynomial $P_2(\xi)$

GAUSSIAN QUADRATURE

The necessary and sufficient condition for the following formula:

$$\int_{\Omega_\xi} n(\xi) g(\xi)\, \mathrm{d}\xi = \sum_{\alpha=1}^{N} g(\xi_\alpha) w_\alpha + R_N(g), \tag{12}$$

to be a Gaussian quadrature approximation is that its nodes $\{\xi_\alpha\}$ coincide with the N roots of the polynomial $P_N(\xi)$ of order N orthogonal in Ω_ξ with respect to the weight function $n(\xi)$.

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History of quadrature-based moment methods

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- McGraw (1997) introduced the Quadrature Method Of Moments (QMOM) in the context of Population Balance Equation
- Marchisio and Fox (2005) developed the Direct Quadrature Method of Moments (DQMOM) that became very popular in the Chemical Engineering community because very **easy to implement in CFD codes**
- Different extensions to **multivariate** cases have been proposed. The more general one is the Conditional QMOM (CQMOM) (Yuan and Fox, 2011)
- Kernel density type reconstruction have been incorporated in QMOM with the Extended QMOM (EQMOM) (Yuan, Laurent, Fox, 2012)
- Different applications have been studied: particulate processes, dispersed flows (gas-liquid, gas-solid, fluid-solid), turbulent micro-mixing, rarefied gases, generic kinetic/Fokker-Planck equations, non-linear filtering, ...
- Recently proposed for **Uncertainty Quantification** (Passalacqua and Fox, 2012; Attar and Vedula, 2012)
- A large number of variants have been proposed (FCMOM, TBMM, DuQMoGeM, SQMOM , ...)

All the closures based on Gaussian quadratures computed directly from moments took the name of **QUADRATURE-BASED MOMENT METHODS (QBMM)**

Quadrature-based moment methods

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- For univariate problems things are simple: with QMOM, transport equations for the first $2N$ moments are solved, the closure problem is overcome by using a quadrature approx.
- The quadrature is very accurate in approximating integrals of smooth functions in which the NDF appears (such as the collision integrals)
- The method implicitly assumes that the NDF is a summation of Dirac delta functions centered on the nodes and weighted by the weights of the quadrature approximation
- The quadrature approximation of order N is calculated from the first $2N$ moments with direct inversion algorithms: product-difference or Wheeler algorithms

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HOW DO WE COMPUTE THE GAUSSIAN QUADRATURE APPROX?

The N weights and N abscissas can be determined by solving the following non-linear system:

$$\begin{aligned} M_0 &= \sum_{\alpha=1}^{N} w_\alpha, \\ &\vdots \\ M_{2N-1} &= \sum_{\alpha=1}^{N} w_\alpha \xi_\alpha^{2N-1}. \end{aligned} \tag{13}$$

using the Newton-Raphson method, or any other non-linear equation solver (very expensive, ill-posed and very good initial guess needed)

Much more efficient are the product-difference or Wheeler algorithms

Quadrature method of moments

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- Let us consider the following example (continuous rate of change of the internal coordinate $\dot{\xi} = G_{\mathrm{p}}$):

$$\frac{\mathrm{D}n}{\mathrm{D}t} = S = -\frac{\partial}{\partial \xi}\left(G_{\mathrm{p}} n\right) + h, \tag{14}$$

- We solve transport equations for the moment set:

$$\frac{\mathrm{D}M_k}{\mathrm{D}t} = \overline{S}_k, \tag{15}$$

with $k = 0, 1, 2, \ldots, 2N-1$ and with an initial condition $M_k(0) = \int_{\Omega_\xi} n(0,\xi)\xi^k \,\mathrm{d}\xi$

- Integration of the system requires the evaluation of the source term through the quadrature approximation

Quadrature method of moments

WARWICK

- Moment equations

$$\frac{\mathrm{D}M_k}{\mathrm{D}t} = k\int_0^\infty \langle G_\mathrm{p}|\xi\rangle \xi^{k-1} n(\xi)\,\mathrm{d}\xi \tag{16}$$

- The closure problem is overcome as follows:

$$\frac{\mathrm{D}M_k}{\mathrm{D}t} = k\sum_{\alpha=1}^{N} \langle G_\mathrm{p}|\xi_\alpha\rangle (\xi_\alpha)^{k-1} w_\alpha \tag{17}$$

- where as already mentioned weights w_α and nodes ξ_α are calculated from the PD or Wheeler algorithm from the moments
- This method is called Quadrature Method of Moments (the variables are the moments)

Quadrature method of moments

WARWICK

In the case of standard nucleation, (positive) growth, growth dispersion, aggregation and breakage, application of QBMM to the source term yields

$$\frac{\mathrm{D}M_k}{\mathrm{D}t} = \overline{J}_k + k\sum_{\alpha=1}^{N}\xi_\alpha^{k-1}G_\alpha w_\alpha + k(k-1)\sum_{\alpha=1}^{N}\xi_\alpha^{k-2}D_\alpha w_\alpha$$

$$+\frac{1}{2}\sum_{\alpha=1}^{N}\sum_{\gamma=1}^{N}\left[(\xi_\alpha+\xi_\gamma)^k-\xi_\alpha^k-\xi_\gamma^k\right]\beta_{\alpha,\gamma}w_\alpha w_\gamma+\sum_{\alpha=1}^{N}b_\alpha\bar{N}_\alpha^k w_\alpha-\sum_{\alpha=1}^{N}\xi_\alpha^k b_\alpha w_\alpha$$

where $G_\alpha = \langle G_\mathrm{p}|\xi_\alpha\rangle$, $D_\alpha = D(\xi_\alpha)$, $\beta_{\alpha,\gamma} = \beta(\xi_\alpha,\xi_\gamma)$ and $b_\alpha = b(\xi_\alpha)$ and the moments of the daughter distribution function are $\bar{N}_\alpha^k = \int \xi^k N(\xi|\xi_\alpha)\,\mathrm{d}\xi$.

Direct quadrature method of moments

WARWICK

- The fact that the closure problem is overcome with the quadrature approximation:

$$\int_{\Omega_\xi} n(\xi) g(\xi) \, \mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha g(\xi_\alpha), \tag{19}$$

- Is equivalent to the assumption that the NDF is as follows:

$$n(\xi) = \sum_{\alpha=1}^{N} w_\alpha \delta\left(\xi - \xi_\alpha\right), \tag{20}$$

- Instead of tracking the evolution for the moments, the evolution of the weights and nodes in the quadrature approximation could be directly tracked:
  Direct quadrature method of moments

Direct quadrature method of moments

WARWICK

- Assuming that the weights and nodes are differentiable in space/time the following transport equation is obtained:

$$\sum_{\alpha=1}^{N} \delta(\xi - \xi_\alpha) \left(\frac{\mathrm{D}w_\alpha}{\mathrm{D}t} \right) - \sum_{\alpha=1}^{N} \delta'(\xi - \xi_\alpha) \left(w_\alpha \frac{\mathrm{D}\xi_\alpha}{\mathrm{D}t} \right) = S(\xi), \quad (21)$$

- If the weighted nodes (or weighted abscissas) $\varsigma_\alpha = w_\alpha \xi_\alpha$ are introduced:

$$\sum_{\alpha=1}^{N} \delta(\xi - \xi_\alpha) \left(\frac{\mathrm{D}w_\alpha}{\mathrm{D}t} \right) - \sum_{\alpha=1}^{N} \delta'(\xi - \xi_\alpha) \left(-\xi_\alpha \frac{\mathrm{D}w_\alpha}{\mathrm{D}t} + \frac{\mathrm{D}\varsigma_\alpha}{\mathrm{D}t} \right) = S(\xi). \quad (22)$$

Direct quadrature method of moments

WARWICK

- We now define a_α and b_α to be the source terms:

$$\frac{\mathrm{D}w_\alpha}{\mathrm{D}t} = a_\alpha, \quad \frac{\mathrm{D}\varsigma_\alpha}{\mathrm{D}t} = b_\alpha. \tag{23}$$

- Using these definitions Eq. (22) can be rewritten in a simpler form:

$$\sum_{\alpha=1}^{N} \left[\delta(\xi-\xi_\alpha) + \delta'(\xi-\xi_\alpha)\xi_\alpha\right] a_\alpha - \sum_{\alpha=1}^{N} \delta'(\xi-\xi_\alpha) b_\alpha = S(\xi). \tag{24}$$

- This equation can now be used to determine the unknown functions a_α and b_α by applying the moment transformation.

Direct quadrature method of moments

WARWICK

- DQMOM can be applied for any independent set of moments (number of moments MUST be equal the number of unknown functions)
- Knowing that:

$$\int_{-\infty}^{+\infty} \xi^k \delta(\xi - \xi_\alpha)\,\mathrm{d}\xi = (\xi_\alpha)^k, \qquad \int_{-\infty}^{+\infty} \xi^k \delta'(\xi - \xi_\alpha)\,\mathrm{d}\xi = -k(\xi_\alpha)^{k-1}, \tag{25}$$

- The moment transform of Eq. (24) yields

$$(1-k)\sum_{\alpha=1}^{N} \xi_\alpha^k a_\alpha + k\sum_{\alpha=1}^{N} \xi_\alpha^{k-1} b_\alpha = \overline{S}_k, \tag{26}$$

with $k = k_1, k_2, \ldots, k_{2N}$.

Direct quadrature method of moments

WARWICK

- The linear system in Eq. (26) can be written in matrix form:

$$A\alpha = d. \tag{27}$$

where

$$\alpha = \begin{bmatrix} a_1 & \cdots & a_N & b_1 & \cdots & b_N \end{bmatrix}^T = \begin{bmatrix} a \\ b \end{bmatrix}, \tag{28}$$

$$d = \begin{bmatrix} \overline{S}_{k_1} & \cdots & \overline{S}_{k_{2N-1}} \end{bmatrix}^T, \tag{29}$$

- The components of the matrix A are

$$a_{ij} = \begin{cases} (1-k_i)\,\xi_j^{k_i} & \text{if } 1 \leq j \leq N, \\ k_i \xi_j^{k_i - 1} & \text{if } N+1 \leq j \leq 2N. \end{cases} \tag{30}$$

Direct quadrature method of moments

WARWICK

- If (as in QMOM) the first $2N$ integer moments are chosen (i.e., $k = 0, \ldots, 2N-1$), the matrix of the linear system is

$$A = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & \cdots & 1 \\ -\xi_1^2 & \cdots & -\xi_N^2 & 2\xi_1 & \cdots & 2\xi_N \\ \vdots & & \vdots & \vdots & & \vdots \\ 2(1-N)\xi_1^{2N-1} & \cdots & 2(1-N)\xi_N^{2N-1} & (2N-1)\xi_1^{2N-2} & \cdots & (2N-1)\xi_N^{2N-2} \end{bmatrix}$$

- A does not depend on the weights w_α and if the abscissas ξ_α are unique, then A will be full rank.

Direct quadrature method of moments

WARWICK

- This method is called Direct quadrature method of moments and follows this procedure:
- The evolution equations for weights and nodes of the quadrature approximation are solved:

$$\frac{\mathrm{D}w_\alpha}{\mathrm{D}t} = a_\alpha, \quad \frac{\mathrm{D}w_\alpha\xi_\alpha}{\mathrm{D}t} = b_\alpha. \tag{32}$$

- The source terms are calculated by inverting the linear system and by using the following initial condition:

$$w_\alpha(0) = w_\alpha^0, \quad \varsigma_\alpha(0) = w_\alpha^0\xi_\alpha^0 \quad \text{for } k = 1, \dots, N. \tag{33}$$

in turn calculated from the initial moments

QMOM & DQMOM

WARWICK

- QMOM & DQMOM are very accurate in tracking the evolution of the moments of the NDF: 4-8 moments do the same job of many (e.g. 100) classes or sections (see for example the work of Marchisio et al., 2003 and Vanni,2000)
- The Wheeler algorithm is very robust (if the moments are realizable) and for particular cases the Wheeler algorithm is successful when PD fails
- QMOM & DQMOM are identical for spatially homogeneous systems (if the nodes are distinct and if the problem is continuous in time)
- Important differences arise when treating spatially inhomogeneous systems (discussed next)
- In general increasing the number of nodes of the quadrature approximation and of moments to be tracked increases the accuracy
- Problems can appear when kernels and NDFs are discontinuous or when they are localized in the phase-space (e.g. fine dissolution)

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WARWICK

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- EQMOM
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- Poly-dispersed flows / coupling with turbulence and multiphase models
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Extended QMOM

WARWICK

- only integral representation, no localized processes in phase space, smoothness of kernels β, G,...
- It fails in the computation of the entropy $\int_{\Omega_\xi} f log f \mathrm{d}\xi$
- However smooth basis functions can be used instead of delta functions (Extended Quadrature Method of Moments, EQMOM)
- PDF reconstructed as a mixture of Gaussians (or other distributions) like the Kernel Density Estimation
- The choice of basis functions can be done arbitrarily or with additional unknown parameters (e.g., mean and variance of normal distribution)
- Additional parameters must be found by additional equations (i.e., more moments must be solved)
- The inversion problems can become difficult to solve

An alternative is the reconstruction through Maximum Entropy Method or the reconstruction through the orthogonal polynomials

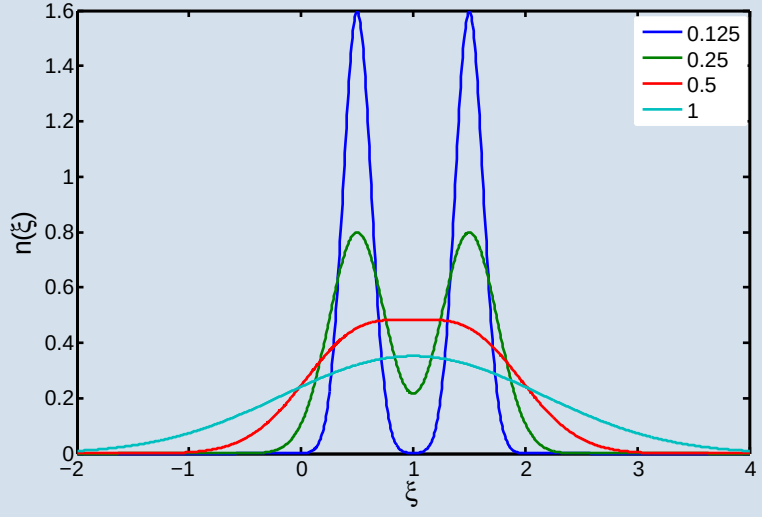
REMARK: An underlying kinetic representation and the reconstruction of the PDF of the velocity are also the basis of the so-called **Kinetic schemes** and **Asymptotic Preserving schemes** (see very interesting works of S. Jin, P. Degond, ...)

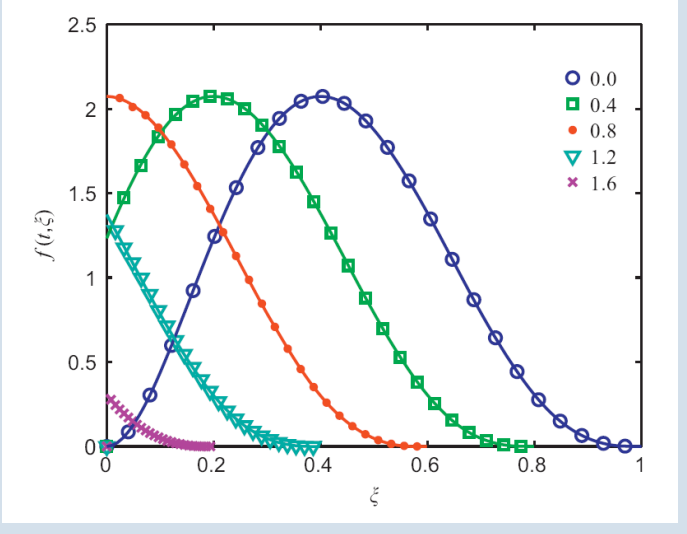
Quadrature-based moment methods

WARWICK

EQMOM for a dissolution problem

Gaussian distr. Solution with $N = 4$ beta distr.





[a]

[a]Yuan, C., Laurent, F., Fox, R.O. An extended quadrature method of moments for population balance equations (2012) Journal of Aerosol Science, 51, pp. 1-23.

$$\delta_\sigma = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\xi-\xi_\alpha)^2}{2\sigma^2}\right); \delta_\sigma = \frac{\xi^{\frac{\xi_\alpha}{\sigma}-1}(1-\xi)^{\frac{(1-\xi_\alpha)}{\sigma}-1}}{B(\xi_\alpha,\sigma)}$$

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QBMM - multivariate case

WARWICK

The original multiivariate GPBE for M-dimensional phase space:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \cdot \left(U_p n\right) = \frac{\partial}{\partial x} \cdot \left(D \frac{\partial n}{\partial x}\right) - \frac{\partial}{\partial \xi} \cdot \left(G n\right) + \mathcal{Q}, \tag{34}$$

is solved with DQMOM with the following $(M+1)N$ equations:

$$\frac{\partial w_\alpha}{\partial t} + \frac{\partial}{\partial x} \cdot \left(U_{p,\alpha} w_\alpha\right) = \frac{\partial}{\partial x} \cdot \left(D_\alpha \frac{\partial w_\alpha}{\partial x}\right) + a_\alpha, \tag{35}$$

$$\frac{\partial w_\alpha \xi_\alpha}{\partial t} + \frac{\partial}{\partial x} \cdot \left(U_{p,\alpha} w_\alpha \xi_\alpha\right) = \frac{\partial}{\partial x} \cdot \left(D_\alpha \frac{\partial w_\alpha \xi_\alpha}{\partial x}\right) + b_\alpha \tag{36}$$

with $\alpha \in 1, \ldots, N$ and where the source terms are calculated by solving the following linear system:

$$\sum_{\alpha=1}^{N} \left[\left(1 - \sum_{\beta=1}^{M} k_\beta\right) \prod_{\beta=1}^{M} \xi_{\beta,\alpha}^{k_\beta} \right] a_\alpha + \sum_{\alpha=1}^{N} \sum_{\beta=1}^{M} \frac{\partial}{\partial \xi_{\beta,\alpha}} \left(\prod_{\gamma=1}^{M} \xi_{\gamma,\alpha}^{k_\gamma} \right) b_{\beta,\alpha}$$

$$= \sum_{\alpha=1}^{N} \sum_{\beta=1}^{M} \sum_{\gamma=1}^{M} \frac{\partial^2}{\partial \xi_{\beta,\alpha} \partial \xi_{\gamma,\alpha}} \left(\prod_{\delta=1}^{M} \xi_{\delta,\alpha}^{k_\delta} \right) + \overline{S}_{k_1,\ldots,k_M}, \tag{37}$$

QBMM - multivariate case

WARWICK

Whereas with QMOM after having defined a generic moments :

$$M_k \equiv \int_{\Omega_\xi} \xi_1^{k_1} \cdots \xi_M^{k_M} n(t,\xi)\, \mathrm{d}\xi \tag{38}$$

equivalent notations $M_{k_1,\ldots,k_M} = M_k = M(k_1,\ldots,k_M) = M(k)$, we solve the resulting transport equations:

$$\frac{\partial M_k}{\partial t} + \frac{\partial}{\partial x}\cdot\left(U_p^k M_k\right) - \frac{\partial}{\partial x}\cdot\left(D^k \frac{\partial M_k}{\partial x}\right) = \overline{\mathcal{S}}_k = \int_{\Omega_\xi} \xi^k \left[-\frac{\partial}{\partial \xi}\cdot\left(\langle G_p|\xi\rangle n\right) + \mathcal{S}\right] \mathrm{d}\xi \tag{39}$$

and the closure problem is overcome by using the quadrature approximation.

QBMM - multivariate case

WARWICK

For multivariate problems $N(M+1)$ moments (optimal moment set) are used to determine the quadrature approximation
Brute-force QMOM: direct solution of the following non-linear system

$$M_{k_{i1},k_{i2},\ldots,k_{iM}} = M(\mathsf{k}_i) = \sum_{\alpha=1}^{N} w_\alpha \prod_{\beta=1}^{M} \xi_{\beta,\alpha}^{k_{i\beta}}, \quad 1 \le i \le N(M+1)$$

by employing the Newton-Raphson iterative scheme:

$$Z_{n+1} = Z_n - A^{-1}(K, X_n)F(Z_n).$$

The Jacobian A is identical to the matrix of the linear system of DQMOM!
Alternatively the Tensor-Product QMOM can be used

Optimal moment set

WARWICK

- To perform calculations with both multivariate QMOM[6] and DQMOM the matrix A must be non-singular (or full rank)
- For $M = 1$ (univariate) problems this requirement is satisfied if the nodes are distinct
- For multivariate cases, having distinct abscissas does not guarantee that A will be full rank
- It can be shown that for fixed N and M, certain distinct moments are linearly dependent when $M \geq 1$ for all possible sets of abscissas
- It is therefore necessary to identify a moment set for which A is always non-singular for all non-degenerate points in phase space for given values of M and N.
- This definition is useful also when other inversion algorithms are used (e.g. Tensor-Product QMOM)

[6] If the Brute-Force inversion algorithm is used.

Optimal moment set

WARWICK

OPTIMAL MOMENT SET

1. An optimal moment set consists of $N(M+1)$ distinct moments.
2. An optimal moment set will result in a full-rank square matrix *A* for all possible sets of N distinct, non-degenerate abscissas.
3. An optimal moment set includes all linearly independent moments of a particular order γ_i before adding moments of higher order.
4. An optimal moment set must result in a perfectly symmetric treatment of the internal coordinates.

Optimal moment set

Table: Moments used to build a bivariate quadrature approximation ($M = 2$) for $N = 2$. In this case $M_{0,3}$ is chosen as the third-order moment to saturate the degrees of freedom.

M(2,0)			
M(1,0)			
M(0,0)	M(0,1)	M(0,2)	M(0,3)

Table: Moments used to build a bivariate quadrature approximation ($M = 2$) for $N = 3$. In this case $M_{2,1}$, $M_{1,2}$ and $M_{0,3}$ are chosen among the third-order moments to saturate the degrees of freedom.

M(2,0)	M(2,1)		
M(1,0)	M(1,1)	M(1,2)	
M(0,0)	M(0,1)	M(0,2)	M(0,3)

Optimal moment set

Table: Optimal moment set used to build a bivariate quadrature approximation ($M = 2$) for $N = 4$. Only when $N^{1/M}$ is an integer, there exists an optimal moment set (that fulfills the symmetry requirement).

M(3,0)	M(3,1)		
M(2,0)	M(2,1)		
M(1,0)	M(1,1)	M(1,2)	M(1,3)
M(0,0)	M(0,1)	M(0,2)	M(0,3)

Table: Optimal moment set used to build a bivariate quadrature approximation ($M = 2$) for $N = 9$.

M(5,0)	M(5,1)	M(5,2)			
M(4,0)	M(4,1)	M(4,2)			
M(3,0)	M(3,1)	M(3,2)			
M(2,0)	M(2,1)	M(2,2)	M(2,3)	M(2,4)	M(2,5)
M(1,0)	M(1,1)	M(1,2)	M(1,3)	M(1,4)	M(1,5)
M(0,0)	M(0,1)	M(0,2)	M(0,3)	M(0,4)	M(0,5)

Multivariate Conditional QMOM

WARWICK

- Methods based on conditional density functions:
  $n(\xi_1, \xi_2) = n_1(\xi_1) f_{21}(\xi_2|\xi_1) = n_2(\xi_2) f_{12}(\xi_1|\xi_2)$
- Univariate quadrature (N_1) calculated from the first $2N_1 - 1$:

$$\begin{pmatrix} M_{0,0,\ldots,0,0} \\ \vdots \\ M_{2N_1-1,0,\ldots,0,0} \end{pmatrix} \xrightarrow{\text{PD/Wheeler}} \begin{pmatrix} w_1 \\ \vdots \\ w_{N_1} \end{pmatrix} \begin{pmatrix} \xi_{1;1} \\ \vdots \\ \xi_{1;N_1} \end{pmatrix}.$$

  resulting for example in: $n(\xi_1, \xi_2) = \sum_{\alpha_1=1}^{N_1} w_{\alpha_1} \delta\left(\xi_1 - \xi_{1;\alpha_1}\right) f_{21}(\xi_2|\xi_1)$

- The generic moment becomes:

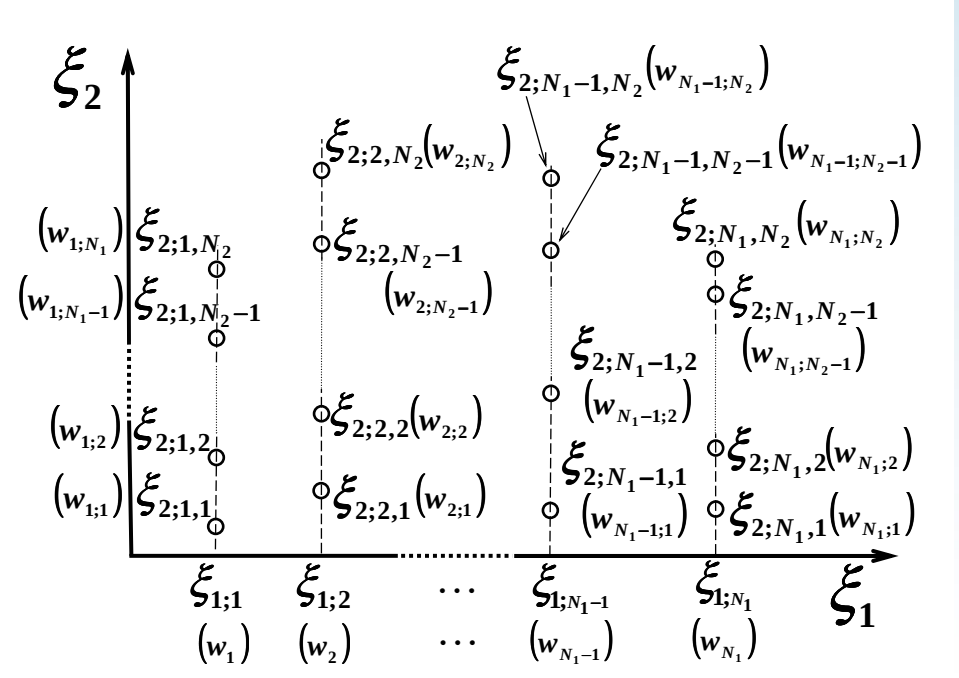
$$\begin{aligned} M_{k_1,k_2} &= \iint n(\xi_1, \xi_2) \xi_1^{k_1} \xi_2^{k_2} \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \\ &= \sum_{\alpha_1=1}^{N_1} w_{\alpha_1} \xi_{1;\alpha_1}^{k_1} \int f_{21}(\xi_2|\xi_{1;\alpha}) \xi_2^{k_2} \, \mathrm{d}\xi_2 \end{aligned}$$

- Conditional moment: $\left\langle \xi_2^{k_2} \right\rangle_{\alpha_1} = \int f_{12}(\xi_2|\xi_{1;\alpha_1}) \xi_2^{k_2} \, \mathrm{d}\xi_2$

Multivariate Conditional QMOM

WARWICK

For each of these N_1 nodes, $2N_2 - 1$ conditional moments are calculated, and univariate quadratures N_2 are determined (in direction ξ_2): Conditional QMOM or CQMOM



Multivariate Conditional QMOM

WARWICK

Table: Moments used to build a bivariate quadrature approximation ($M = 2$) for $N_1 = N_2 = 3$ using CQMOM with ξ_2 conditioned on ξ_1 (top) and ξ_1 conditioned on ξ_2 (bottom).

M(5,0)					
M(4,0)					
M(3,0)					
M(2,0)	M(2,1)	M(2,2)	M(2,3)	M(2,4)	M(2,5)
M(1,0)	M(1,1)	M(1,2)	M(1,3)	M(1,4)	M(1,5)
M(0,0)	M(0,1)	M(0,2)	M(0,3)	M(0,4)	M(0,5)

M(5,0)	M(5,1)	M(5,2)			
M(4,0)	M(4,1)	M(4,2)			
M(3,0)	M(3,1)	M(3,2)			
M(2,0)	M(2,1)	M(2,2)			
M(1,0)	M(1,1)	M(1,2)			
M(0,0)	M(0,1)	M(0,2)	M(0,3)	M(0,4)	M(0,5)

QBMM - multivariate case

WARWICK

Bivariate Gaussian distr. with $\rho = 0.0$ and $N = 9$; **BF-QMOM** (diamond), **TP-QMOM** (circle) and CQMOM (square)

QBMM - multivariate case

WARWICK

Bivariate Gaussian distr. with $\rho = 0.5$ and $N = 9$; **BF-QMOM** (diamond), **TP-QMOM** (circle) and CQMOM (square)

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Quadrature Method of Moments

WARWICK

- The spatially inhomogeneous GPBE operating on $n(\xi)$ reads as follows:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \cdot \left(\langle U_p | \xi \rangle n \right) = \frac{\partial}{\partial x} \cdot \left(D(\xi) \frac{\partial n}{\partial x} \right) - \frac{\partial}{\partial \xi} \left(\langle G_p | \xi \rangle n \right) + \mathcal{S} \quad (40)$$

- The application of the moment transform, $M_k = \int n(\xi) \xi^k \, \mathrm{d}\xi$, generates several closure problems:

$$\frac{\partial M_k}{\partial t} + \frac{\partial}{\partial x} \cdot \left(U_p^k M_k \right) = \frac{\partial}{\partial x} \cdot \left(D^k \frac{\partial M_k}{\partial x} \right) + \overline{S}_k \quad (41)$$

  where of course $U_p^k = \frac{\int \langle U_p | \xi \rangle n(\xi) \xi^k \, \mathrm{d}\xi}{M_k}$ (similarly D^k) and $\overline{\mathcal{S}}_k = \int \left(\frac{\partial}{\partial \xi} \left(\langle G_p | \xi \rangle n \right) + \mathcal{S} \right) \xi^k \, \mathrm{d}\xi$.

- The solution with QMOM is as usual ...

Quadrature Method of Moments

WARWICK

- From $\{M_0, M_1, \dots, M_{2N-1}\}$ the Gaussian quadrature with N nodes is constructed resulting in the following approximation

$$M_k(t,x) = \int_{\Omega_\xi} n(t,x,\xi)\xi^k \, \mathrm{d}\xi \approx \sum_{\alpha=1}^{N} w_\alpha(t,x) \left(\xi_\alpha(t,x)\right)^k \tag{42}$$

- that can be used to overcome the different closure problems, for example:

$$U_{\mathrm{p}}^k(t,x) = \frac{\int_{\Omega_\xi} \langle U_{\mathrm{p}}|\xi\rangle n(t,x,\xi)\xi^k \, \mathrm{d}\xi}{M_k} \approx \frac{\sum_{\alpha=1}^{N} \langle U_{\mathrm{p}}|\xi_\alpha\rangle w_\alpha \xi_\alpha^k}{M_k} \tag{43}$$

- By using different velocities, $U_{\mathrm{p}}^k(t,x)$, for the different moments, we can describe mixing and segregation patterns

Direct quadrature method of moments

WARWICK

Moreover if w_α and ξ_α are continuous functions of space and time, DQMOM can also be applied (slightly different now due to the diffusion term):

$$\frac{\partial w_\alpha}{\partial t} + \frac{\partial}{\partial x} \cdot \left(\langle U_p | \xi_\alpha \rangle w_\alpha \right) = \frac{\partial}{\partial x} \cdot \left(D(\xi_\alpha) \frac{\partial w_\alpha}{\partial x} \right) + a_\alpha \tag{44}$$

$$\frac{\partial w_\alpha \xi_\alpha}{\partial t} + \frac{\partial}{\partial x} \cdot \left(\langle U_p | \xi_\alpha \rangle w_\alpha \xi_\alpha \right) = \frac{\partial}{\partial x} \cdot \left(D(\xi_\alpha) \frac{\partial w_\alpha \xi_\alpha}{\partial x} \right) + b_\alpha \tag{45}$$

with $\alpha \in 1, \ldots, N$ and where the source terms are as usual determined by solving the following linear system:

$$(1-k) \sum_{\alpha=1}^{N} \xi_\alpha^k a_\alpha + k \sum_{\alpha=1}^{N} \xi_\alpha^{k-1} b_\alpha = \overline{S}_k + \overline{C}_k, \tag{46}$$

where

$$\overline{C}_k = k(k-1) \sum_{\alpha=1}^{N} \xi_\alpha^{k-2} C_\alpha, \quad C_\alpha = w_\alpha D \left(\frac{\partial \xi_\alpha}{\partial x} \cdot \frac{\partial \xi_\alpha}{\partial x} \right), \tag{47}$$

Spatial discretization and moment corruption

- A moment set is said to be valid or realizable, if the Hankel-Hadamard determinants are all non-negative:

$$\Delta_{k,l} = \begin{vmatrix} M_k & M_{k+1} & \cdots & M_{k+l} \\ M_{k+1} & M_{k+2} & \cdots & M_{k+l+1} \\ \vdots & \vdots & \vdots & \vdots \\ M_{k+l} & M_{k+l+1} & \cdots & M_{k+l+l} \end{vmatrix} \geq 0, \quad k = 0, 1, \quad l \geq 0 \tag{48}$$

  for $k = 0, 1$ and $l \geq 0$.

- For $l = 1$ we get:

$$M_k M_{k+2} - M_{k+1}^2 \geq 0 \quad k = 0, 1, 2, \ldots . \tag{49}$$

  which for $k = 0$ becomes the constraint of positive variance

- Equivalently this becomes:

$$\frac{\square\square(M_k) + \square\square(M_{k+2})}{2} \geq \square\square(M_{k+1}) \quad k = 0, 1, 2, \ldots ; \tag{50}$$

  or in other words convexity of the function $\square\square(M_k)$ with respect to k

Spatial discretization and moment corruption

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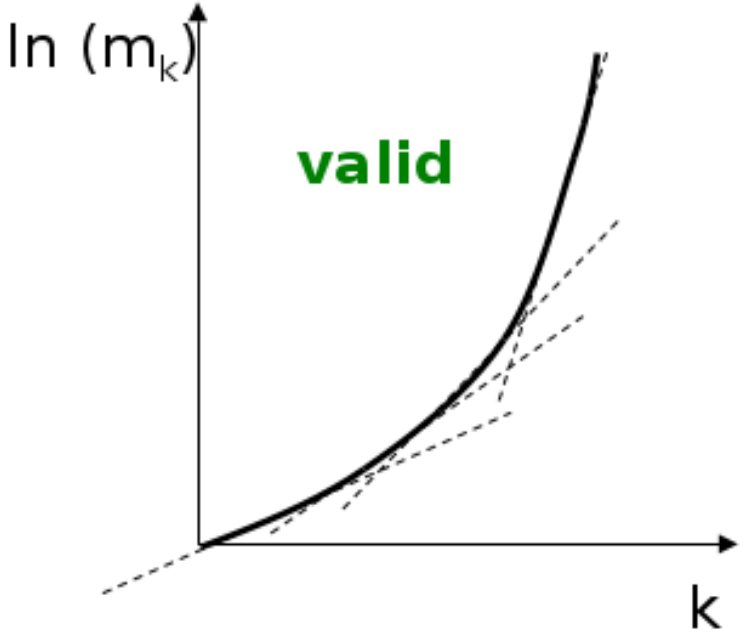
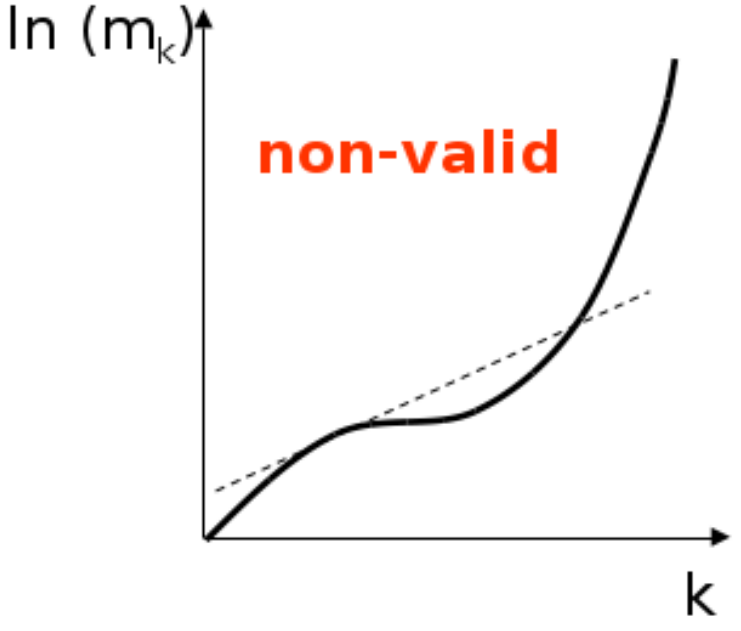
Less stringent condition: convexity of function (M_k) with respect to k

$$m_k m_{k-2} - m_{k-1}^2 \geq 0$$





Ad-hoc correction algorithms are needed!

Spatial discretization in QMOM

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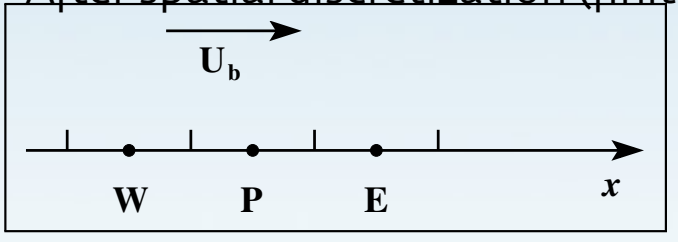
An alternative is to solve the transport equation for a generic moment M_k with discretization schemes that PRESERVE the moments ("Realizable schemes"):

$$\frac{\partial M_k}{\partial t} + \cancel{U_p \frac{\partial M_k}{\partial x}} = \overline{S}_k - U_p \frac{\partial M_k}{\partial x}$$

After spatial discretization (finite-volume):



$$\frac{dM_k^P}{dt} = \overline{S}_k^P - \frac{U_p}{\Delta x}\left(M_k^e - M_k^w\right)$$

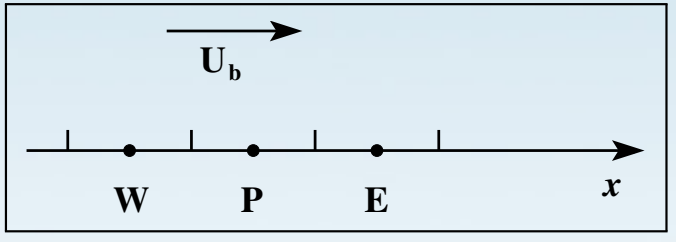
With first-order upwind $M_k^e = M_k^P$ and $M_k^w = M_k^W$

Spatial discretization schemes based on first-order upwind always result in VALID moments. Higher-order schemes (CDS, second-order upwind, QUICK, MUSCL) can result in INVALID moments.

Spatial discretization in QMOM

WARWICK

- One solution would be to evaluate the moments at the faces M_k^e and M_k^w through the quadrature approximation
- We know the value of the moments at the center of the cells M_k^W, M_k^P, M_k^E



- From these moments we can evaluate the corresponding weights w_α^P and abscissas ξ_α^P
- If weights at the center of the face are interpolated with p^{th}-order spatial reconstruction and the abscissas are interpolated 1^{st}-order spatial the resulting moments will be valid
- This allows to improve the numerical accuracy preserving the moments!
- Alternatively one can use semi-Lagrangian schemes (Attili and Bisetti, 2013)

Spatial discretization in DQMOM

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- In QMOM the governing equations are for the moments that are 'conserved' variables
- In DQMOM the governing equations are for weights and weighted abscissas that are 'primitive' variables
- When QMOM is used (if proper discretization schemes are used) only the transported $2N$ moments are preserved and conserved (and their linear combination)
- When DQMOM is used only weights and weighted abscissas are conserved and their linear combination: M_0 and M_1
- One disadvantage of DQMOM is that only two moments (of the $2N$ selected) are conserved and saved from numerical errors!
- Another way to look at the problem is to consider that the equations in finite-volume codes are solved with an error called numerical diffusion whose coefficient is unknown!

Spatial discretization in DQMOM

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- The original DQMOM requires the solution of these equations:

$$\begin{aligned} \frac{\partial w_\alpha}{\partial t} + U_\mathrm{p}\frac{\partial w_\alpha}{\partial x} &= a_\alpha \\ \frac{\partial w_\alpha \xi_\alpha}{\partial t} + U_\mathrm{p}\frac{\partial w_\alpha \xi_\alpha}{\partial x} &= b_\alpha \\ &\Updownarrow \\ \frac{\partial M_k}{\partial t} + U_\mathrm{p}\frac{\partial M_k}{\partial x} &= \overline{S}_k \end{aligned}$$

- When the finite-volume discretization is applied:

$$\begin{aligned} \frac{\mathrm{d}w_\alpha^P}{\mathrm{d}t} + \frac{U_\mathrm{p}}{\Delta x}\left(w_\alpha^e - M_k^w\right) &= a_\alpha^P \\ \frac{\mathrm{d}(w_\alpha \xi_\alpha)^P}{\mathrm{d}t} + \frac{U_\mathrm{p}}{\Delta x}\left((w_\alpha \xi_\alpha)^e - (w_\alpha \xi_\alpha)^w\right) &= b_\alpha^P \\ &\Updownarrow \\ \frac{\mathrm{d}M_k^P}{\mathrm{d}t} + \frac{U_\mathrm{p}}{\Delta x}\left(M_k^e - M_k^w\right) &= \overline{S}_k^P \end{aligned}$$

failing in conserving higher-order moments ($k \geq 2$)

Spatial discretization in DQMOM

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- Solution: fully conservative version of DQMOM (DQMOM-FC):

$$\begin{aligned}
\frac{\mathrm{d}M_k^P}{\mathrm{d}t} &= -\frac{U_\mathrm{p}}{\Delta x}\left(M_k^e - M_k^w\right) + \overline{S}_k^P \\
&\Updownarrow \\
\frac{\mathrm{d}w_\alpha^P}{\mathrm{d}t} &= -a_{c,\alpha}^P + a_\alpha^P \\
\frac{\mathrm{d}(w_\alpha \xi_\alpha)^P}{\mathrm{d}t} &= -b_{c,\alpha}^P + b_\alpha^P
\end{aligned}$$

  now successfully conserving all the moments of the NDF

- Alternatively one can use semi-Lagrangian schemes (Attili and Bisetti, 2013)
- Summarizing if the equations for the moments have large physical diffusion terms DQMOM can be safely used (numerical diffusion will be smaller than real diffusion and the solution will contain no discontinuities and no shocks)
- When only the equation for the moments do not contain any physical diffusion term than DQMOM-FC should be used

Outline

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- Poly-dispersed flows / coupling with turbulence and multiphase models
- Gas-liquid flows
- Non-equilibrium and granular flows / non-smooth kernels
- Turbulent reactive flows / PDF as modelling tool
- Porous media
- UQ and other applications

Turbulence models
DNS, LES, RANS

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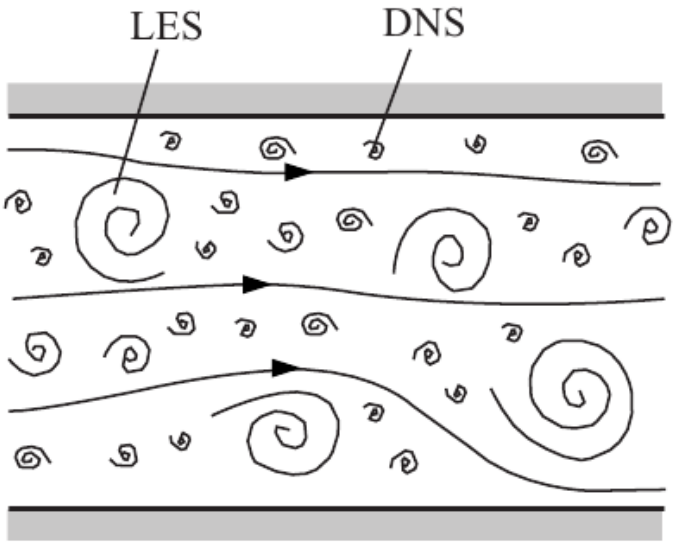

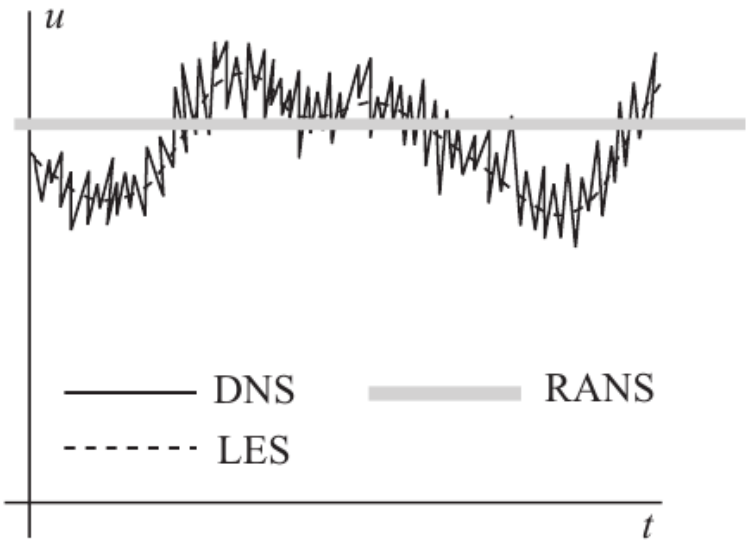

Direct Numerical Simulation (DNS)

All the flow-scales are solved without model ⇒ virtual experiments (3D and unsteady)

Large Eddy Simulation (LES)

Equations are filtered in space (or frequency). Bigger 3D unsteady scales are solved; smaller ones are modelled with sub-grid scale (SGS) models

RANS

Time-averaged equations ⇒ only the mean flow is predicted

Poly-dispersed particles

Particle Size Distribution (PSD) and Population Balance Eq. (PBE)

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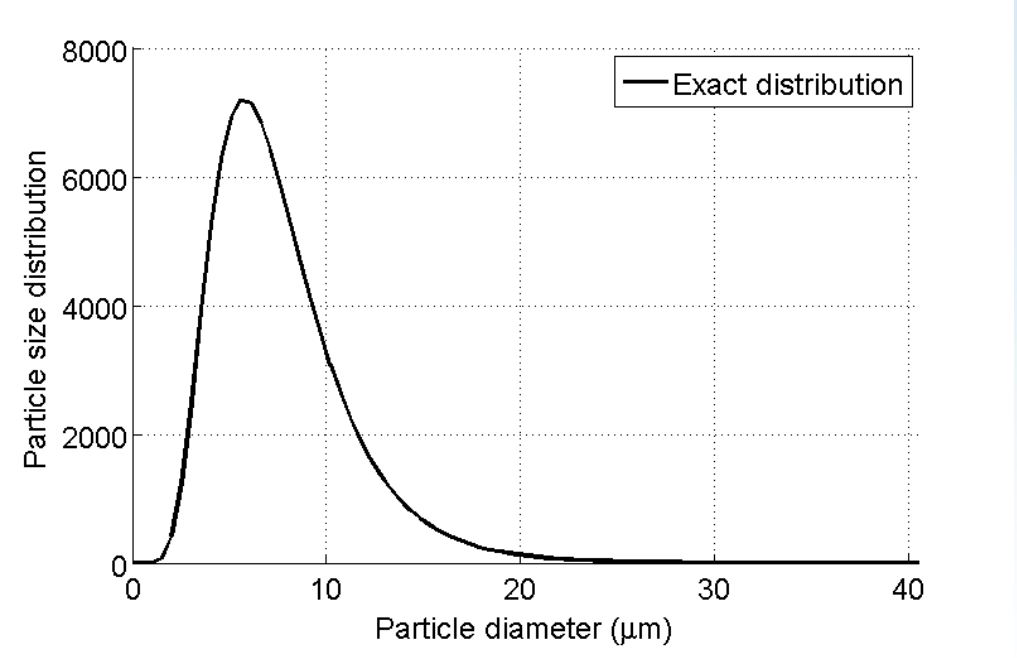
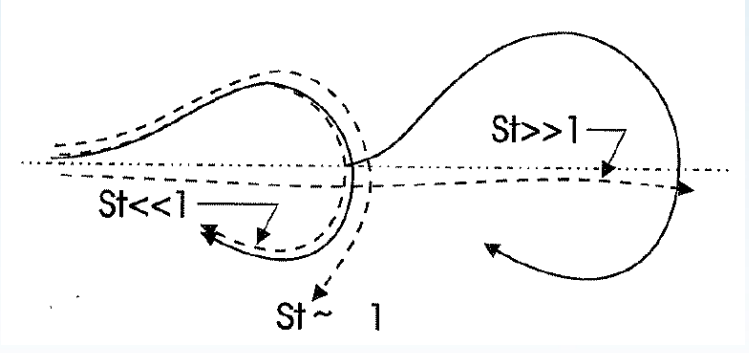
Particle Size Distribution $$n(L;x,t) = \int_{\mathbb{R}^3} n(L, U_p; x, t)\, dU_p$$



$$\mathrm{St} = \frac{\tau_p}{\tau_f} \approx \frac{\rho_p D^2}{18 \mu \tau_f}$$



Particles of different size behave very differently with a non-linear relation between size and relative velocity

Poly-dispersed particles

Log-normal PSD and QBMM approximation

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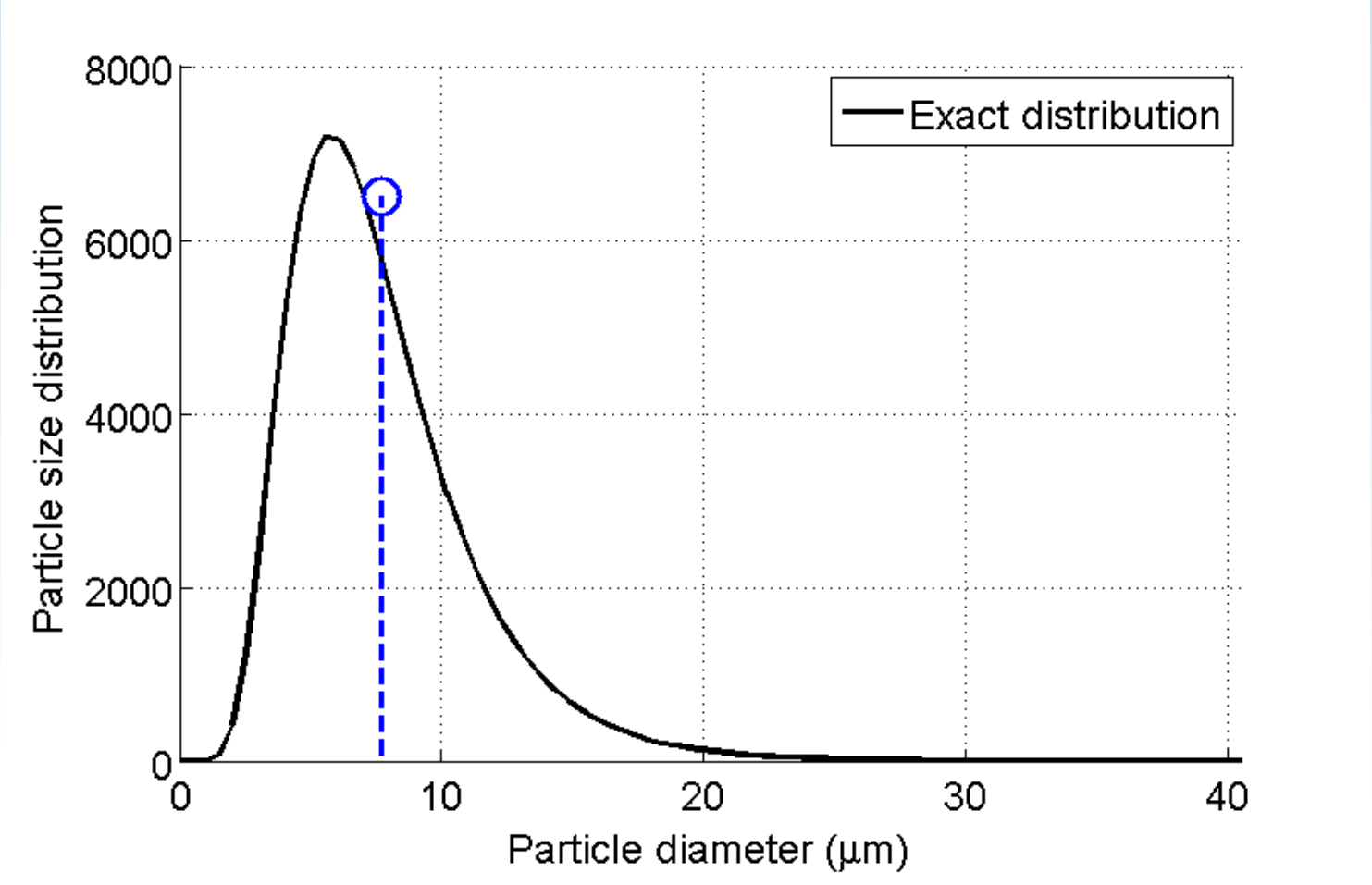
Quadrature-based Moment Method (QBMM)
nodes and weights to approximate $f(L)$



2 moments $\rightarrow$ 1 node, 1 weight
Mean size

Poly-dispersed particles

Log-normal PSD and QBMM approximation

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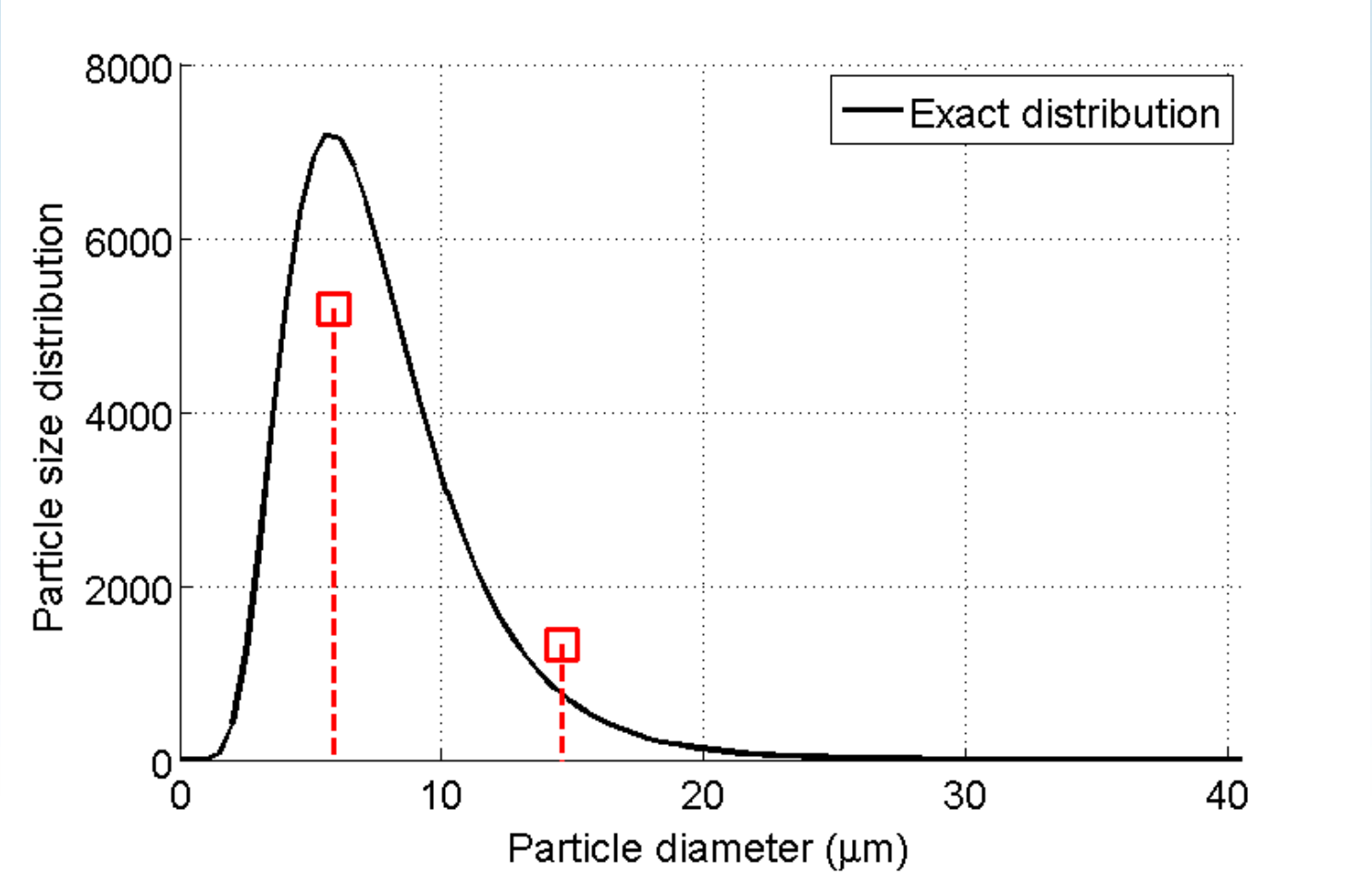
nodes and weights to approximate $f(L)$



4 moments $\rightarrow$ 2 nodes, 2 weights
Volume fraction

Poly-dispersed particles

Log-normal PSD and QBMM approximation

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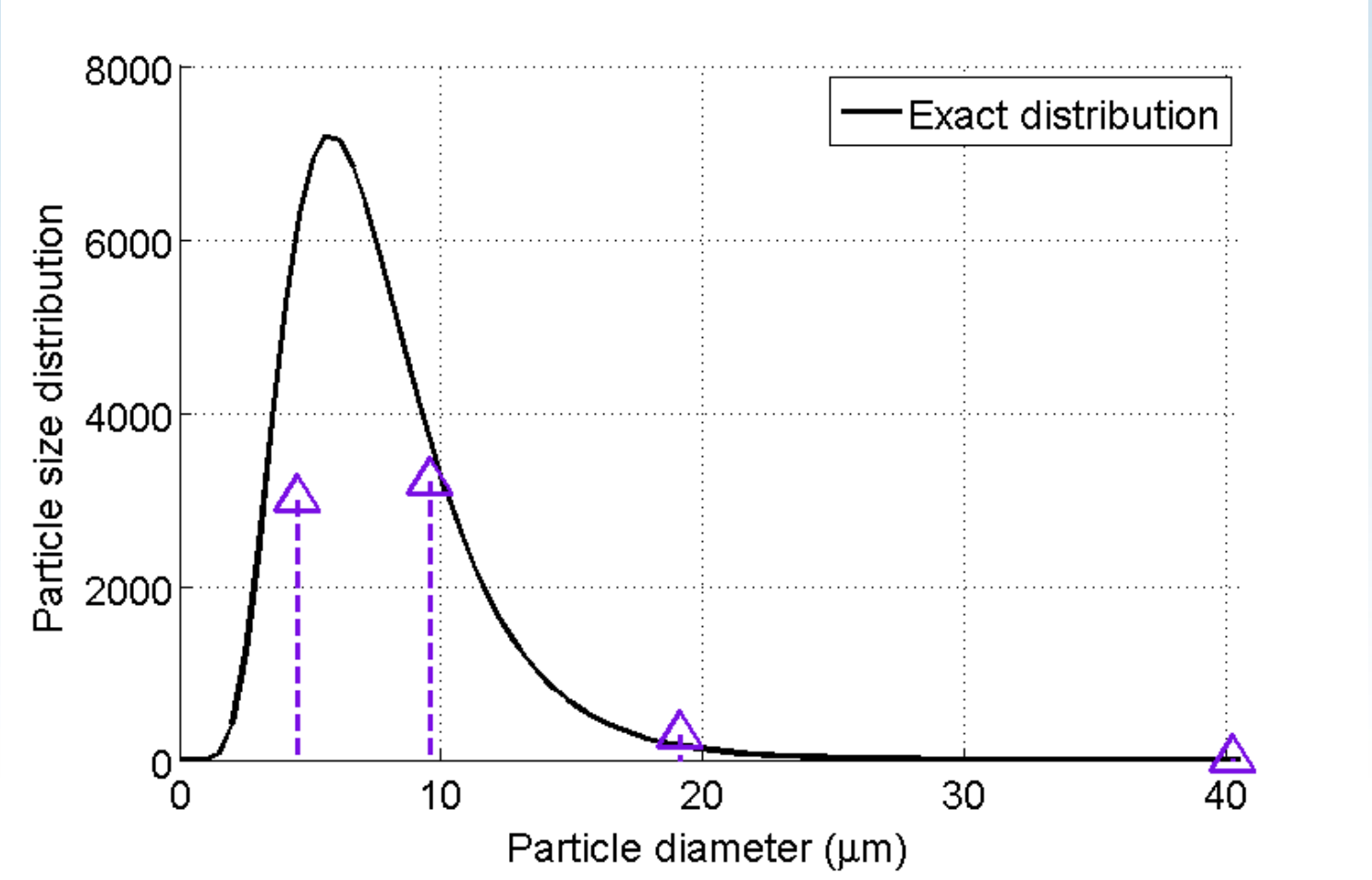
Quadrature-based Moment Method (QBMM)
nodes and weights to approximate $f(L)$



8 moments $\longrightarrow$ 4 nodes, 4 weights

Real-space advection

from homogeneous model to multi-fluid model

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Population balance equation:

$$\partial_t n + \partial_x \langle U_p | L \rangle n + \cancel{\partial_L n G} = \cancel{Q(n,n)}$$

no growth term

no aggregation, breakage, nucleation

Models for conditional velocity $\langle U_p | L \rangle = U_p(L)$

Pseudo-homogeneous model, $St \ll 1$

Particles flow with fluid velocity $U_p(L) = U$

Algebraic models (Mixture), $St \leq 1$

$U_p(L)$ is calculated with algebraic relations from the knowledge of U

Differential models (Multi-fluid), $St > 1$

$U_p(L)$ is solved with a momentum balance equation

Equilibrium Model (Ferry/Balachandar)

Drag forces and gravity

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- similar to the classical Algebraic Slip Model
- expansion of Maxey-Riley equation for small particle response time τ_p

$$U_p \approx U + O(\tau_p) \Rightarrow U_p - U = -\tau_p \left(\frac{DU}{Dt} - g \right)$$

- 1^{st} order correction

$$U_p - U = -\tau_p \left(I + \tau_p \nabla U^T \right)^{-1} \left(\frac{DU}{Dt} - g \right)$$

- High Re_p effects considered using a modified τ_p^*
- can be extended to take into account other forces and two-way coupling

SGS model for particles
Approximate Deconvolution Method

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In Large Eddy Simulation (LES) we have only filtered velocity field $\overline{U}$

Approximate Deconvolution Method (ADM)

To estimate the "real" unfiltered velocity we use an approximate inverse filter

$$U_i^* = \sum_{k=0}^{N_c} (I - G)^k \, \overline{U_i}$$

- G is a test filter
- N_c is the deconvolution order
- if $N_c = 1$ it is like an inverse dynamic model
- considered $N_c = 1, 5$ with Gaussian weights

PBE approximation

Quadrature-Based Moment Method (QBMM) – DQMOM formulation

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- Single momentum equation for the mixture
- Equilibrium model to calculate velocity $U_p(L)$
- Population balance discretized with Quadrature-Based Moment Method (QBMM)
- Solved directly in terms of nodes L_i and weights w_i (DQMOM formulation)

Single velocity model

All particles flow with an overall mean velocity $U_p(L) = U_p(\overline{L})$

Multiple velocities model

Each node (particle class) considered as a separate phase with its own relative velocity

Turbulent poly-dispersed channel flow

Turbophoresis effects

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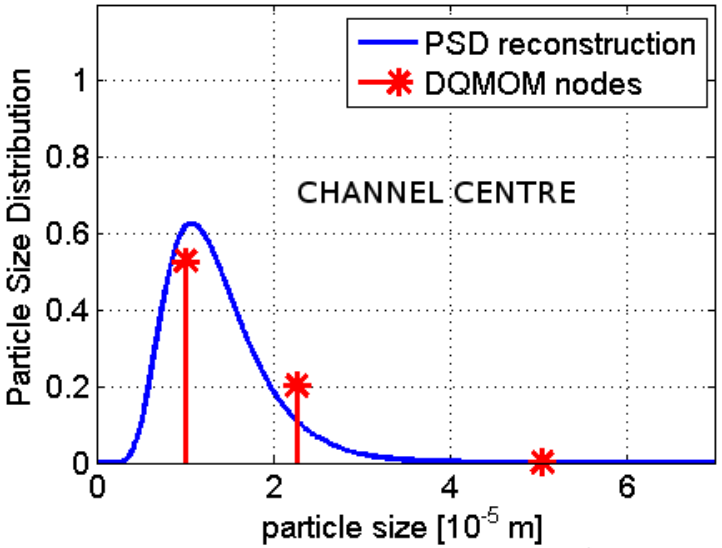

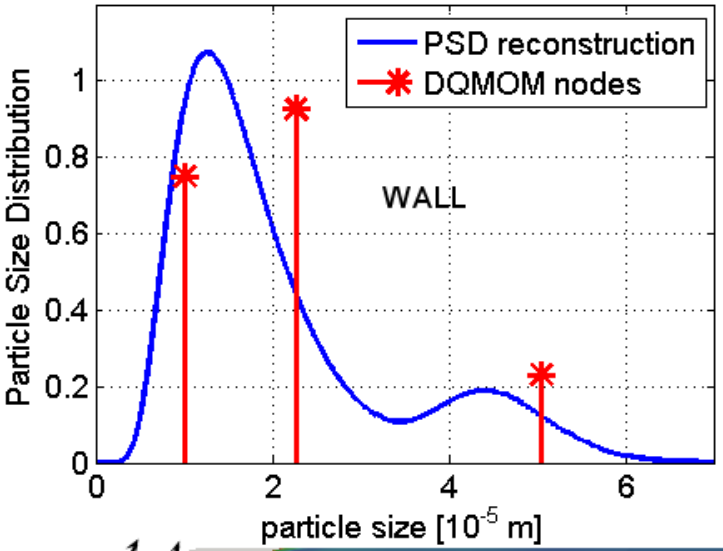

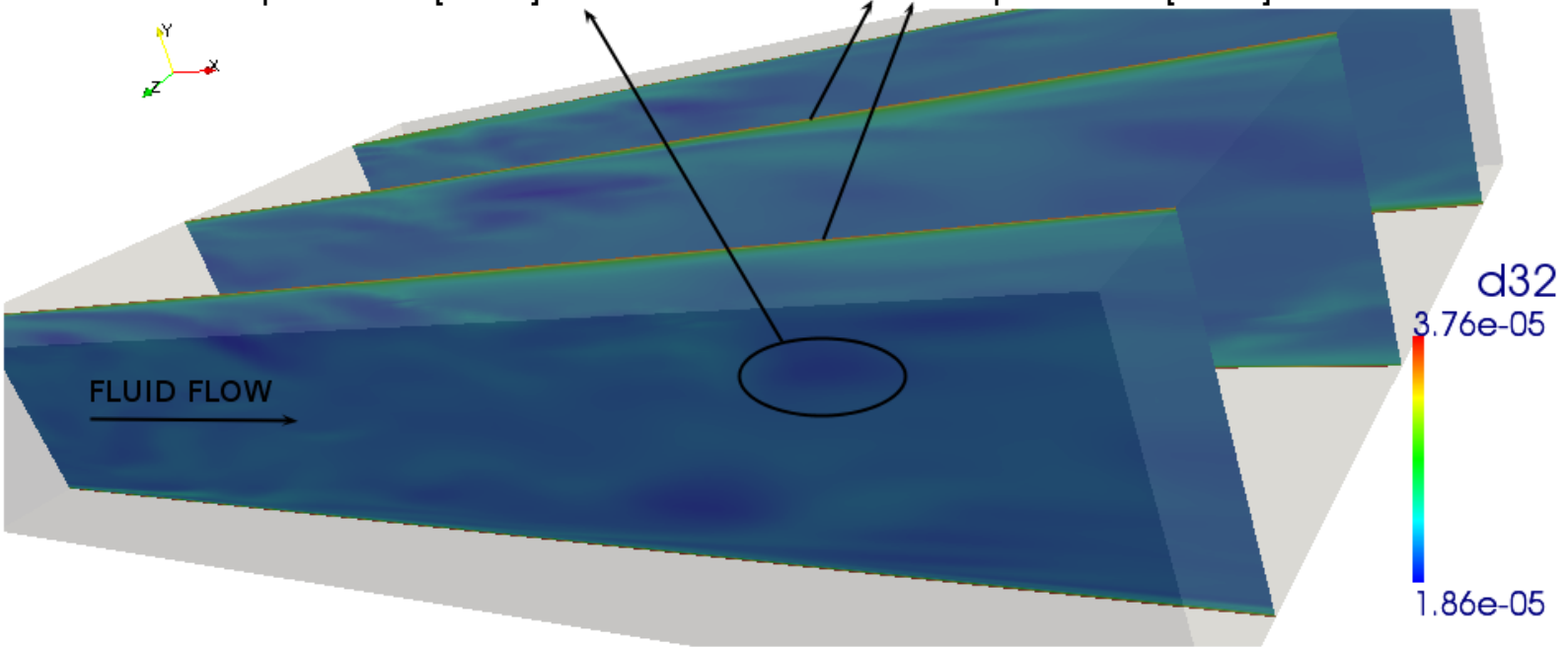

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Relative velocity models
Algebraic slip model

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- Slip velocity (based on the review of Manninen et al., 1996) solved with Newton-Raphson method
- Drag and lift forces
- Tomiyama relations (Tomiyama et al., 2002) for drag and lift coefficients

$$C_D = (1-\alpha_g) max\left[\frac{24}{\mathrm{Re}}\left(1+0.15\mathrm{Re}^{0.687}\right), \frac{8}{3}\frac{Eo}{Eo+4}\right]$$

$$C_L = \begin{cases} \min[0.288\tanh(0.121\mathrm{Re}); 0.00105\mathrm{Eo}^3 - 0.0159\mathrm{Eo}^2 - 0.0204\mathrm{Eo} + 0.474]; & \mathrm{Eo}<4 \\ 0.00105\mathrm{Eo}^3 - 0.0159\mathrm{Eo}^2 - 0.0204\mathrm{Eo} + 0.474; \quad 4 < \mathrm{Eo} < 10 \\ -0.27 \text{ elsewhere} \end{cases}$$

- Lift and drag coefficients depends on Eotvos number (in our case mainly bubble diameter)
- Lift changes sign at about 5.8 mm (for the test case under study)

Another force has been considered close to the wall (wall-lift force) based on the models of Tomiyama et al. (1995), Hosokawa et al. (2002), Antal et al. (1991) (see also review of Rzehak et al., 2012)

Turbulence and collision models

Aggregation and breakage - see also work presented by Buffo et al.

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Turbulence model must be included(either DNS, LES or RANS)

- PBE models are usually expressed only in terms of time-averaged RANS formulation
- Turbulent dispersion force added as isotropic turbulent diffusivity in the DQMOM equations
- Coalescence kernel (Laakkonen, 2007; Prince and Blanch, 1990; Coulaloglou and Tavlarides 1977):

$$\alpha(\lambda, L) = C_A \epsilon^{1/3} (\lambda + L)^2 (\lambda^{2/3} + L^{2/3})^{1/2} \exp\left(-6 \cdot 10^9 \frac{\mu_l \rho_l \epsilon}{\sigma^2} \left(\frac{\lambda L}{\lambda + L} \right)^4 \right)$$

- Breakup kernel (Laakkonen, 2007; Alopaeus et al., 2002):

$$\beta(L) = C_B \epsilon^{1/3} \operatorname{erfc}\left(\sqrt{0.04 \frac{\sigma}{\rho_l \epsilon^{2/3} L^{5/3}} + 0.01 \frac{\mu_l}{\sqrt{\rho_l \rho_g} \epsilon^{1/3} L^{4/3}}} \right)$$

- β—PDF Daughter distribution function (binary)
- constants taken from Laakkonen, 2007 and Buffo et al., 2011

Gas-liquid vertical pipe

Test case description

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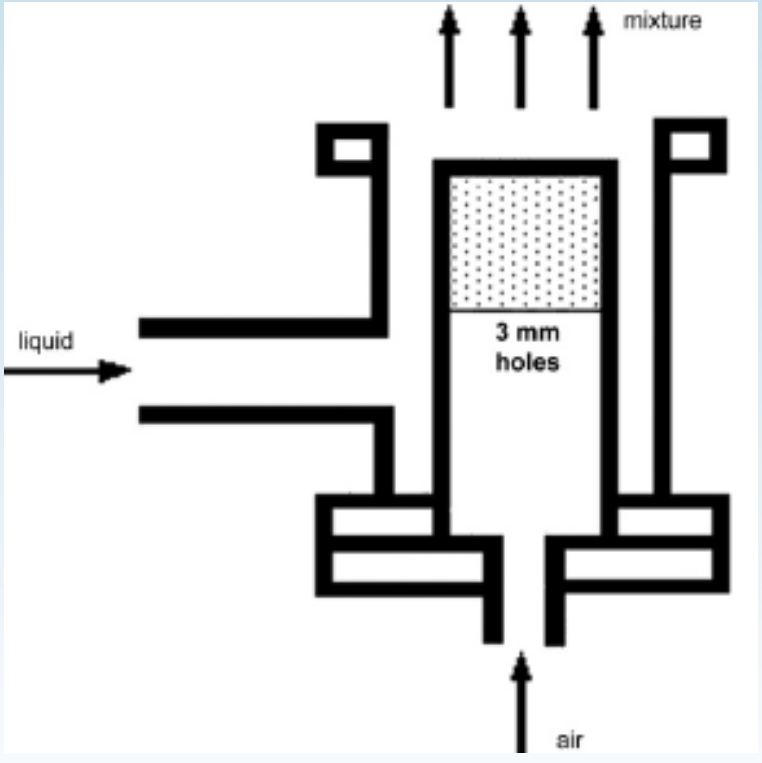


- experimental data (Szalinsky et. al., 2008)
- height 6.0 [m]
- diameter 0.067 [m]

Test Case 1:

- Gas superficial velocity 0.05 [m/s]
- Water superficial velocity 0.25 [m/s]

Test Case 2:

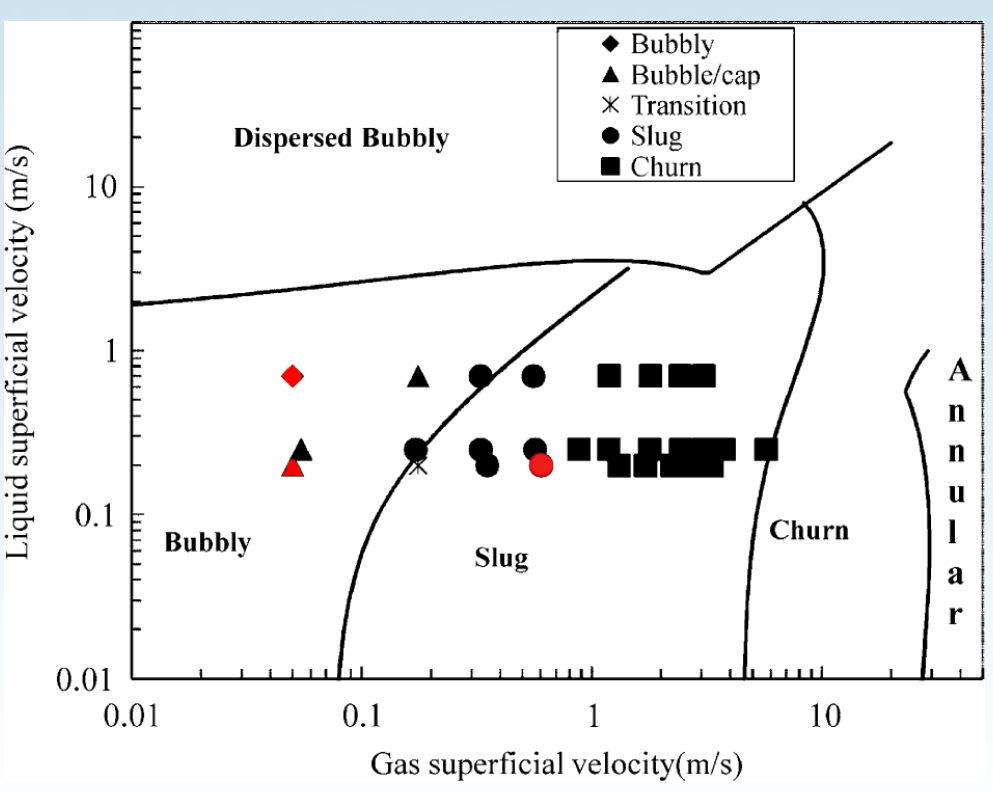
- Gas superficial velocity 0.05 [m/s]
- Water superficial velocity 0.7 [m/s]

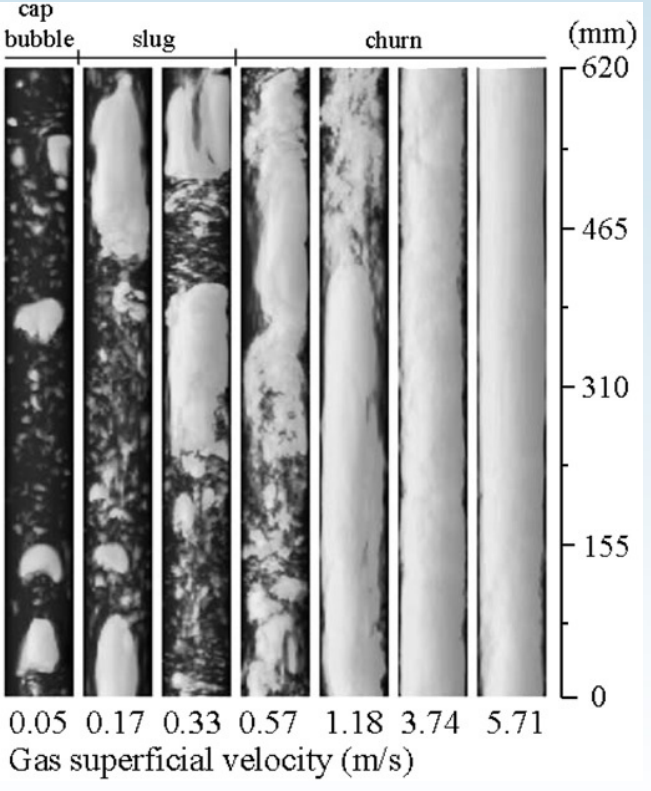
mean void fraction known from experiments

Results analyzed in terms of void fraction profiles at the outlet and bubble size

Flow regimes

Figure taken from Szalinsky et al. (2010)





2 test cases (red points) of bubbly flow with moderate gas fraction (<0.1) and Stokes number (<10)

DQMOM initialization and BCs

DQMOM vs Classic ASM

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Inlet BSD

- The bubbles enter the pipe through 3mm diameter holes
- the model of Miyahara et al. (1983) and Nicholas et al. (1991) has been used to estimate the initial bubble size distribution, based on the system and the sparger properties
- a log-normal distribution has been used with a mean diameter of 7 mm
- inlet lognormal parameters, mean and STD, can have strong influence on the overall results

The "Classic ASM" model (without population balance) instead has a fixed bubble size derived with a fitting procedure

Numerical details
Commercial CFD code TransAT

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- RANS standard $k - \epsilon$ model for mixture phase
- Coarse grid : 307×15
- Fine grid: 620×33
- Steady state 2D axisymmetric domain
- Convection: HLPA scheme

Model validation

- Mesh
- Pipe height (3 m vs 6 m)
- steady VS unsteady formulations

Results

- Experimental profile
- Classic ASM
- ASM + DQMOM 4 moments
- ASM + DQMOM 6 moments

Vertical pipe flow
Results - void fraction

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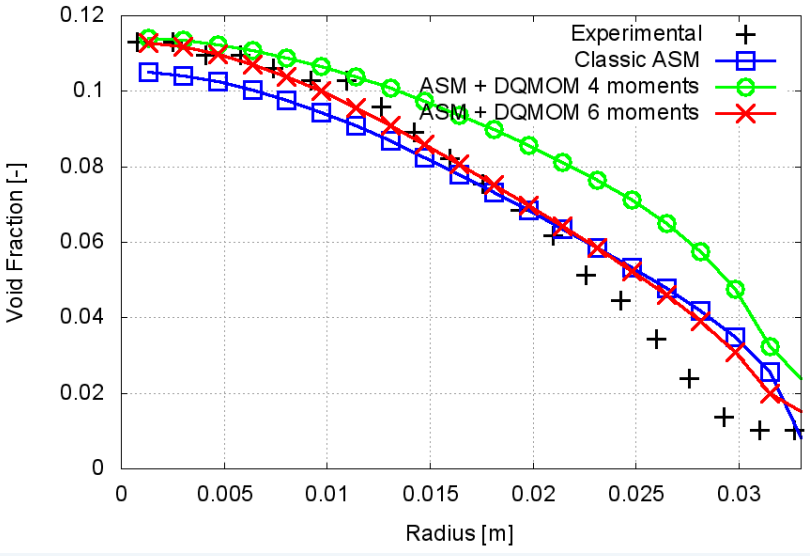
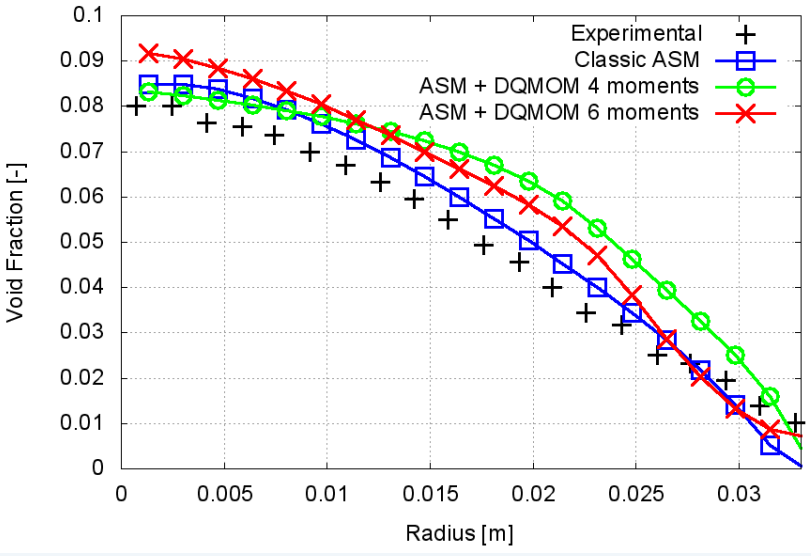
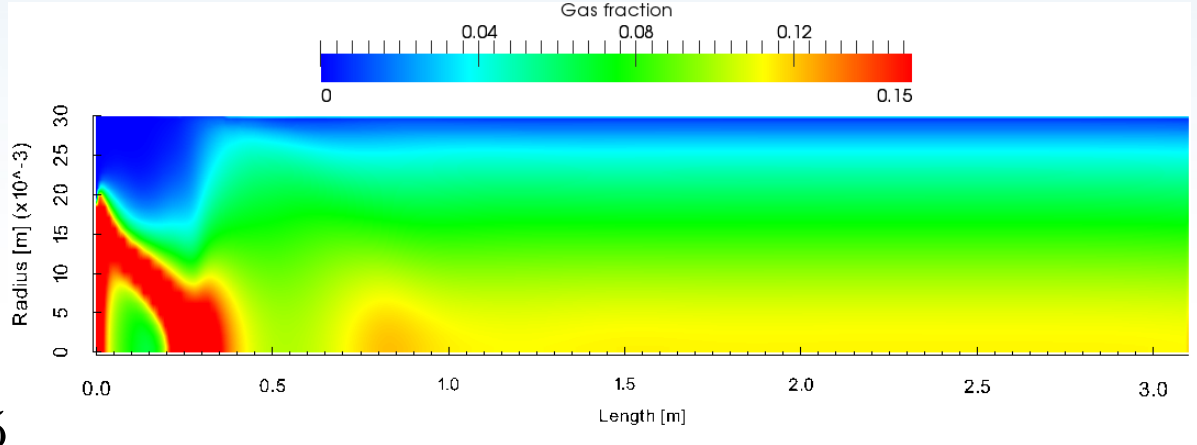
$V_L = 0.25$



$V_L = 0.7$





$V = 0.25$

Vertical pipe flow

Results - Sauter diameter - at wall and in the center

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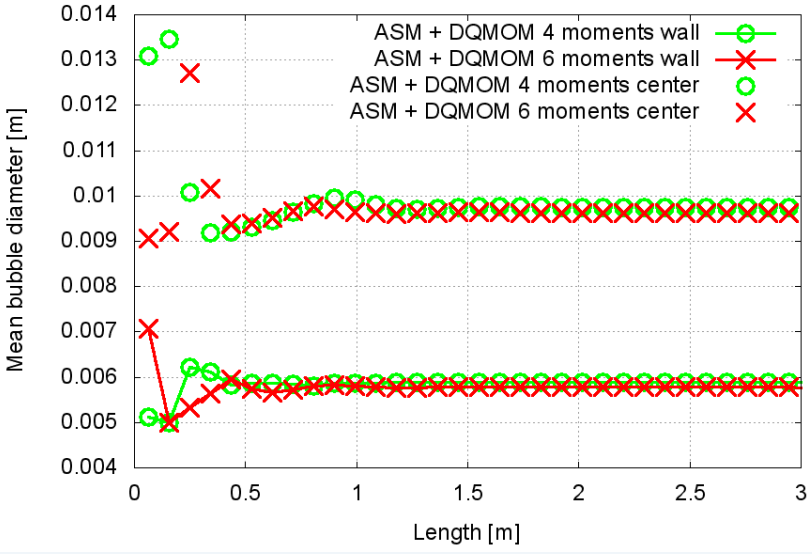
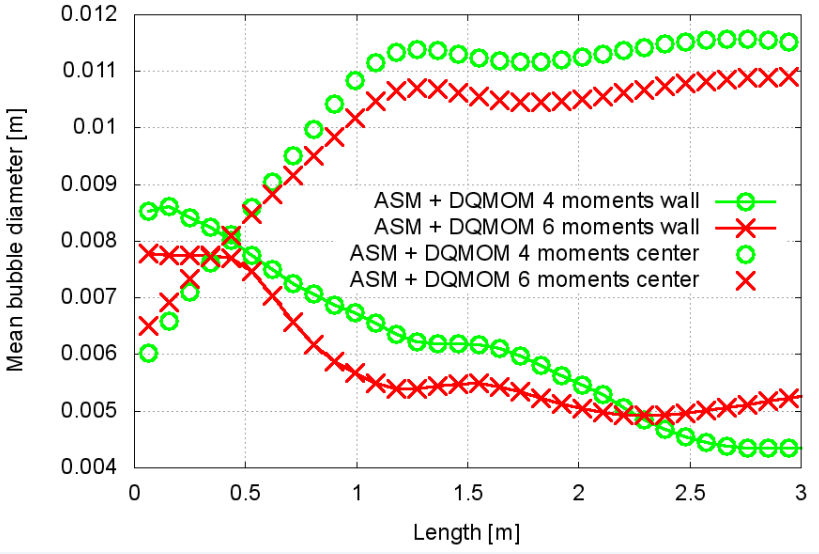
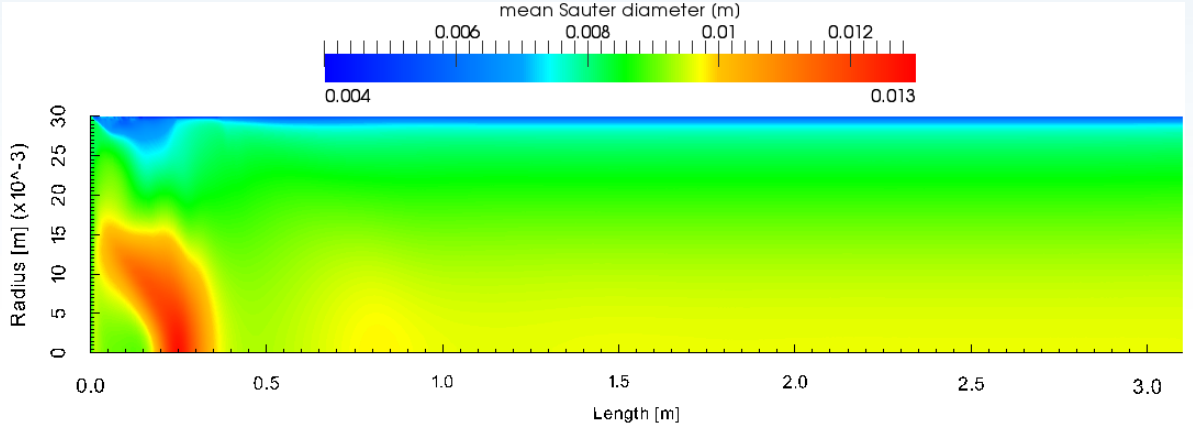
$V_L = 0.25$



$V_L = 0.7$





$V = 0.25$

Vertical pipe flow $V_L = 0.25$

Results - Bubble surface area

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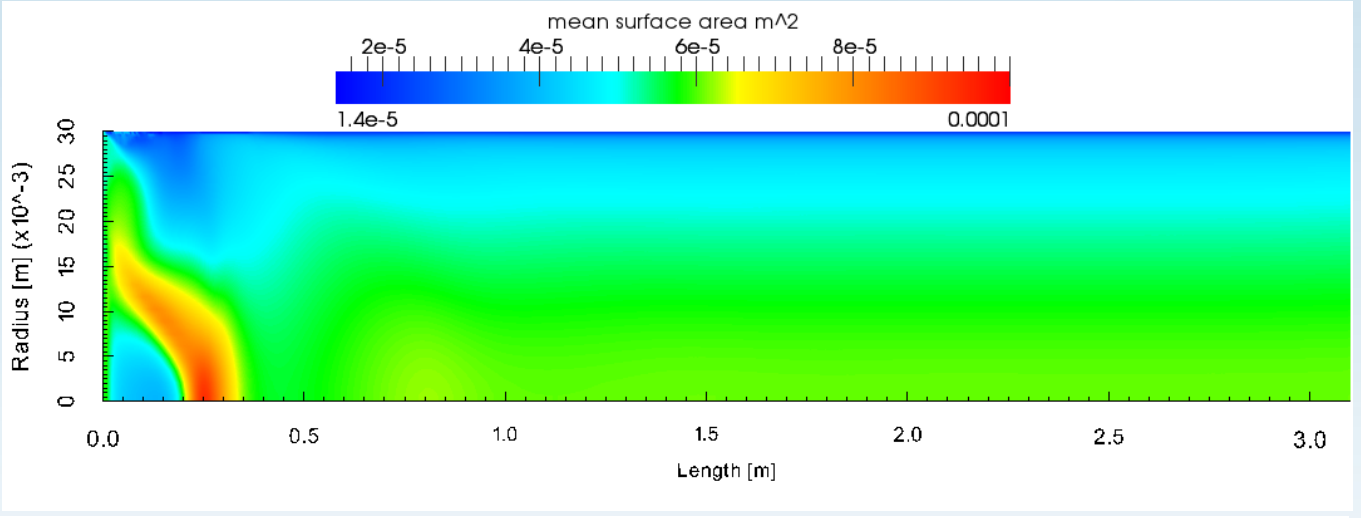
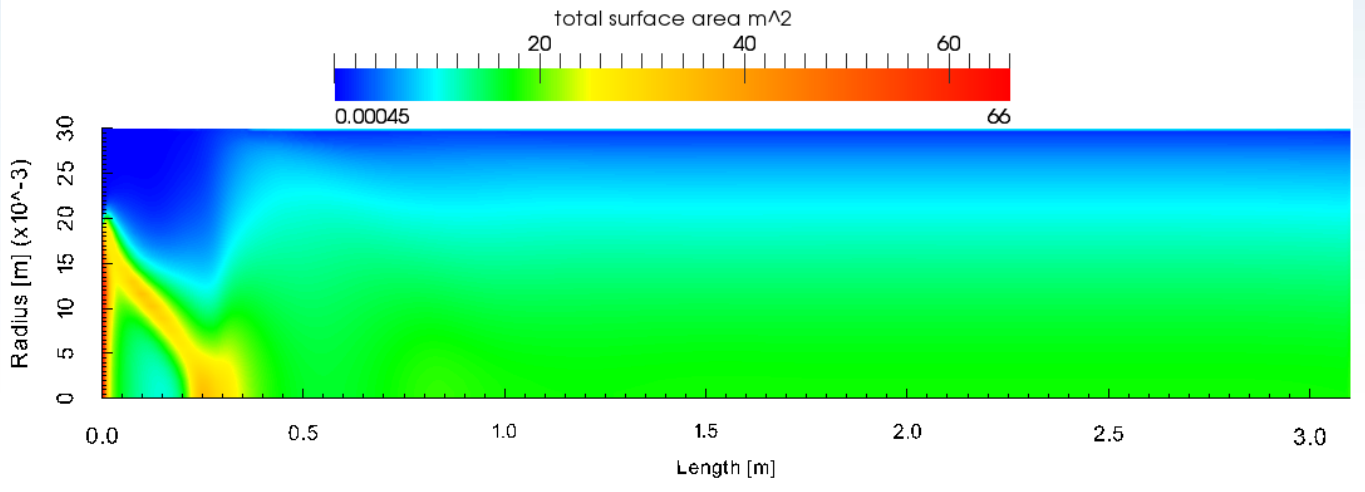
mean



total



Vertical pipe flow $V_G = 0.57$

Slug flow test

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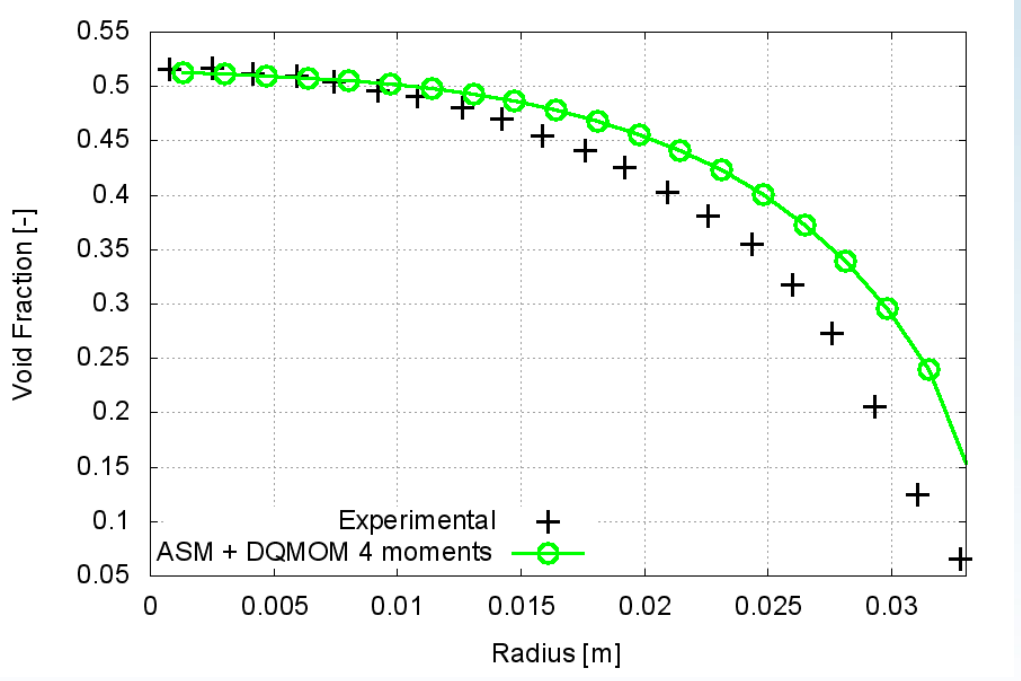
A test for slug flow regime has also been tested



Surprisingly this model gives good results for void fraction but BSD is no more coherent because it cannot include slugs formation

Outline

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Kinetic and PDF equations

- Smoluchowski coagulation equation
- Population balance equation (PBE)
- Boltzmann equation (BE)
- Method of Moments
- Generalized population balance equation (GPBE)

Quadrature-based moment methods

- Numerical Methods and Closure problem
- Gaussian quadrature
- QMOM and DQMOM
- EQMOM
- Multivariate case
- Implementation in CFD codes / spatial inhomogeneity

Applications

- Poly-dispersed flows / coupling with turbulence and multiphase models
- Gas-liquid flows
- Non-equilibrium and granular flows / non-smooth kernels
- Turbulent reactive flows / PDF as modelling tool
- Porous media
- UQ and other applications

Boltzmann equation

Homogeneous isotropic case (HIBE)

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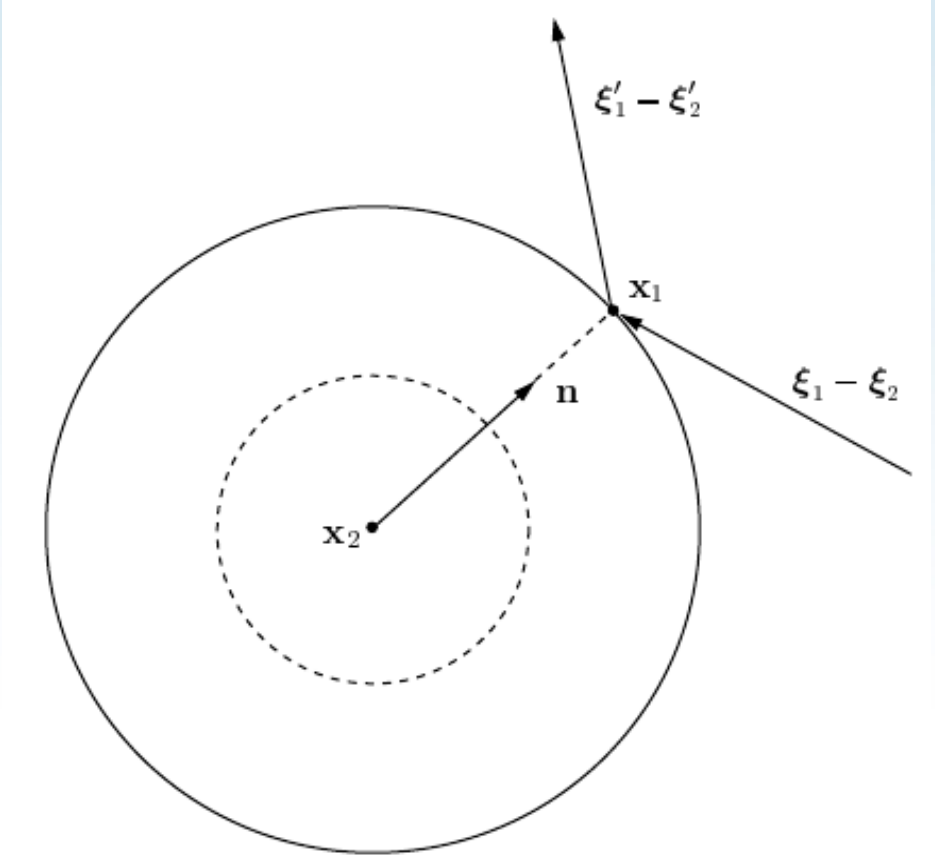
Particle Velocity Distribution $$f(U_p; x, t) = \int_{\mathcal{R}} f(L, U_p; x, t)\, dL$$



Model equation

- scalar molecular speed ξ
- distribution of velocities $f(\xi)$
- no spatial derivatives
- only collisions $\mathcal{Q}(f, f)$
- Hard-sphere model
- $x = \cos(\xi_1 \angle n), \quad y = \cos(\xi_2 \angle n)$
- collision frequency $|\xi_2 y - \xi_1 x|$

Boltzmann equation

Homogeneous isotropic case (HIBE)

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HIBE evolution equation: $\dfrac{df}{dt} = Q(f,f)$

$$Q = 2\,\pi^2\,a^2 \int_0^{+\infty} \xi_2^2 \int_{-1}^{+1}\int_{-1}^{+1} \left(f(\xi_1')f(\xi_2') - f(\xi_1)f(\xi_2)\right)\,|\xi_2 y - \xi_1 x|\,dx\,dy\,d\xi_2$$

Let us introduce the even moments $M_{2p} = \Phi_p$ (density Φ_0, energy Φ_1, etc.).

After change of variable $E = \frac{\xi^2}{2}$ and a few manipulations:

$$\frac{d\Phi_p}{dt} = 4\pi\sqrt{2}\int_0^{\infty} Q(f,f)E^{p+1/2}dE =$$

$$16\pi^3\sqrt{2}\int_0^{\infty}\int_0^{\infty}\int_{-1}^{+1}\int_{-1}^{+1} |q|\left[(C_p^+) - (C_p^-)\right] f(E)f(E_*)(EE_*)^{1/2}dxdydE_*dE$$

$$q = yE_*^{1/2} - xE^{1/2}, \qquad C_p^+ = \left[E(1-x^2) + E_* y^2\right]^p, \qquad C_p^- = E^p$$

Quadrature approximation for HIBE

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Collisional integral

$$\int_0^\infty \int_0^\infty \int_{-1}^{+1} \int_{-1}^{+1} |q| \left[(C_p^+) - (C_p^-)\right] f(E) f(E_*) (EE_*)^{1/2} dx dy dE_* dE$$

$$\sum_{i=0}^{M/2} \sum_{j=0}^{M/2} \int_{-1}^{+1} \int_{-1}^{+1} |q| \left[(C_p^+) - (C_p^-)\right] w_i w_j dx dy dE_* dE$$

Written in terms of pre-collisional quantities only $\rightarrow$ quadrature approximation

$$\tilde{f}(E) \approx \sum_{i=1}^{M/2} \frac{w_i}{4\pi\sqrt{2E}} \delta(E - E_i) \qquad \Rightarrow \frac{d\Phi_p}{dt} \approx \frac{\pi}{\sqrt{2}} \sum_{i=1}^{M/2} \sum_{j=1}^{M/2} w_i w_j \Lambda_{ij,p}$$

at equilibrium $Q = 0 \rightarrow \frac{d\Phi_p}{dt} = 0$ BUT this is not guaranteed with the quadrature approximation

Collisions drive the flows towards the wrong steady state

Quadrature-Based Moment Method (QBMM)

Homogeneous Isotropic Boltzmann Equation (HIBE)

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$$\frac{d\Phi_p}{dt} = \frac{\pi}{\sqrt{2}} \sum_{i=1}^{M/2} \sum_{j=1}^{M/2} w_i w_j \Lambda_{ij,p} = S_p$$

w_i and E_i calculated from Φ_p with inversion algorithms[7]

- QMOM fails to approach the equilibrium $\rightarrow$ source term must be corrected
- Static correction (QMOM+SC):

$$\frac{d\Phi_p}{dt} = S_p - S_p^{eq}$$

- Dynamic correction (QMOM+DC) weighted with a distance from equilibrium:

$$\frac{d\Phi_p}{dt} = S_p - \left| \frac{\Phi_p(t) - \Phi_p(0)}{\Phi_p^{eq}(t) - \Phi_p(0)} \right|^h S_p^{eq}, \qquad h = 1.5$$

[7] Product-Difference or Wheeler algorithms

QMOM approximation vs DVM, Grad, oLBM

Homogeneous Isotropic Boltzmann Equation (HIBE)

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Let us consider a closed box of particles far from equilibrium (initial velocity distribution NOT Gaussian):

QMOM approximation selecting M moments ($M/2$ nodes and weights)

Comparison with:

- Discrete Velocities Method (DVM): reference results with 400 discrete velocities - HomIsBoltz open-source Matlab code (Asinari, 2010)
- Grad expansion method (GM) of order M with generalized Laguerre polynomials
- Quadrature approximation with M fixed Laguerre nodes $\rightarrow$ Lattice Boltzmann Method (LBM) with off-lattice prescribed velocities

QMOM approximation vs DVM, Grad, oLBM [1]

Homogeneous Isotropic Boltzmann Equation (HIBE)

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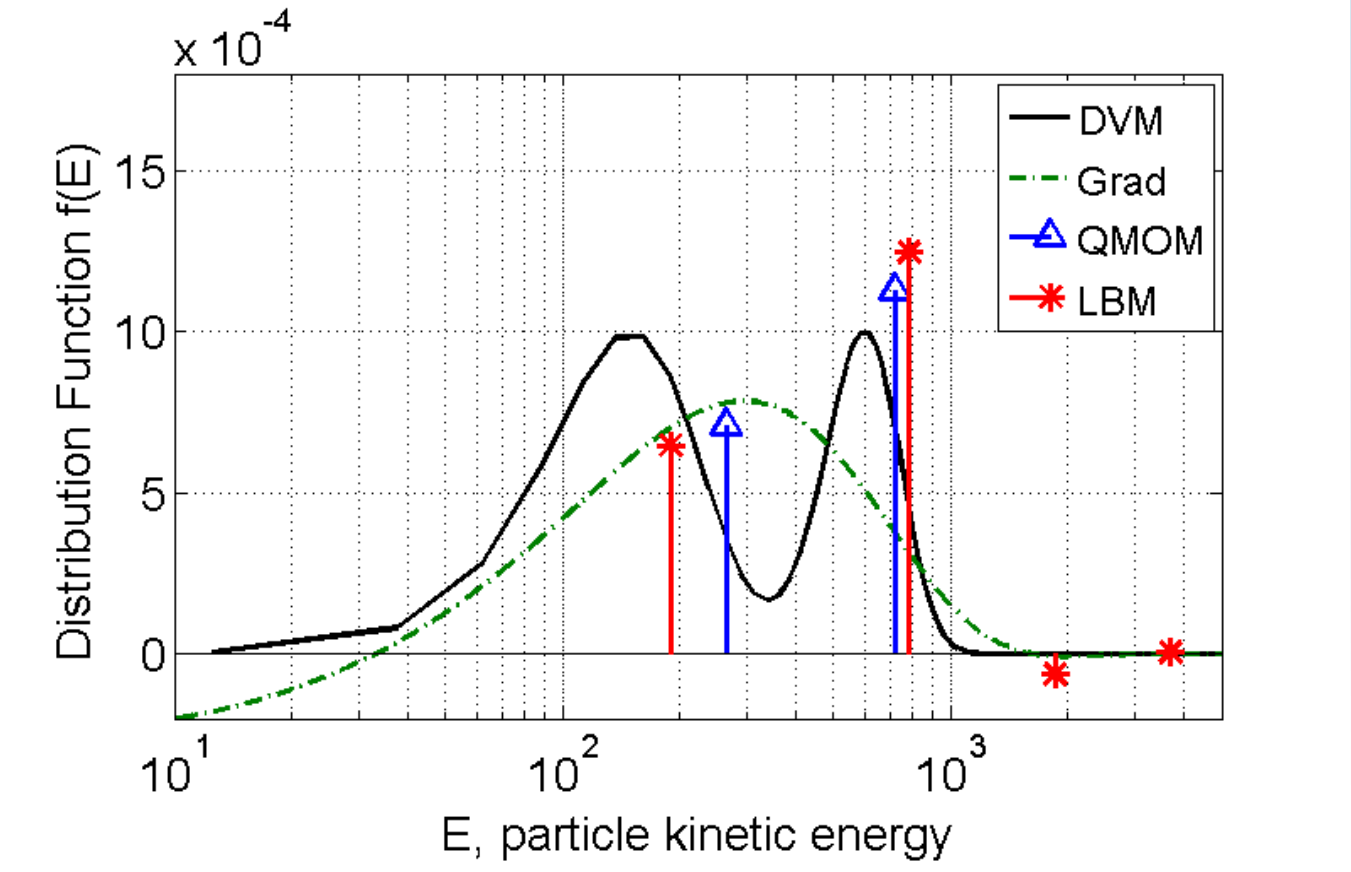
$$M = 4$$

Initial condition

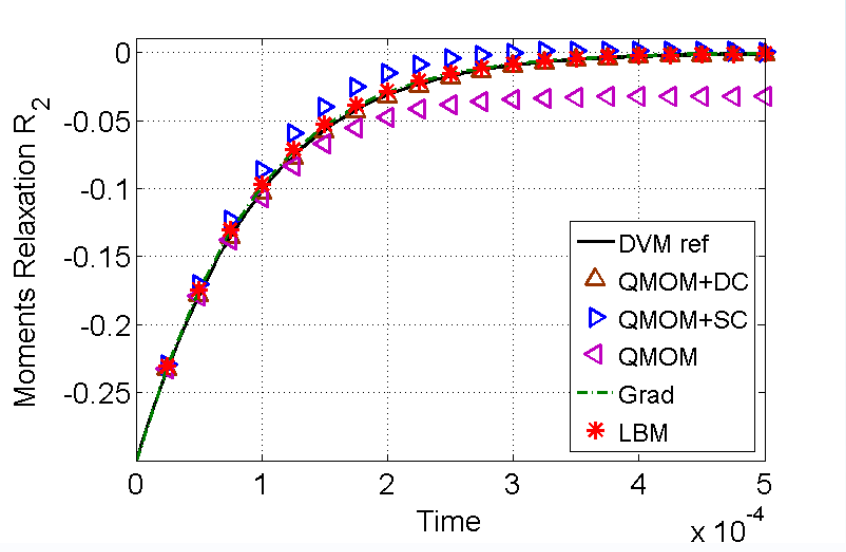


QMOM approximation vs DVM, Grad, oLBM – 2

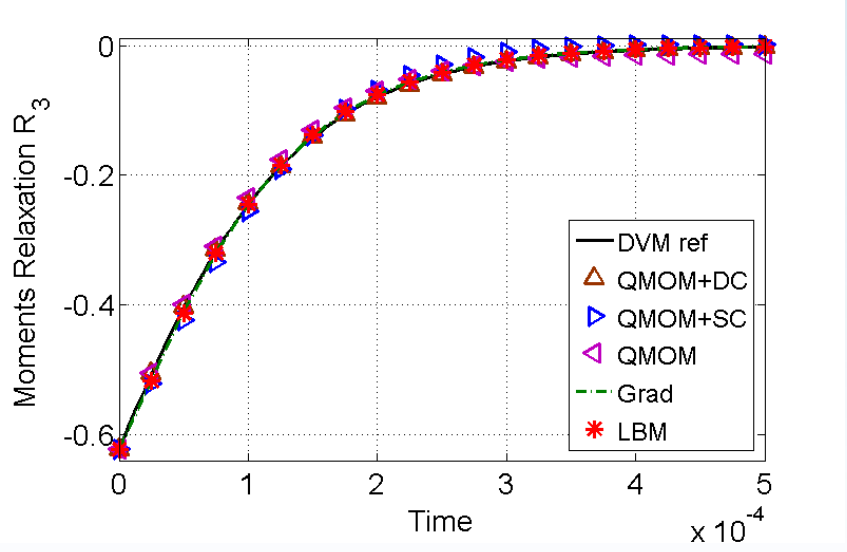
Homogeneous Isotropic Boltzmann Equation (HIBE)

$$M = 4$$

Relaxation to equilibrium $R_p = \frac{\Phi_p - \Phi_p^{eq}}{\Phi_p^{eq}}$



2nd energy moment



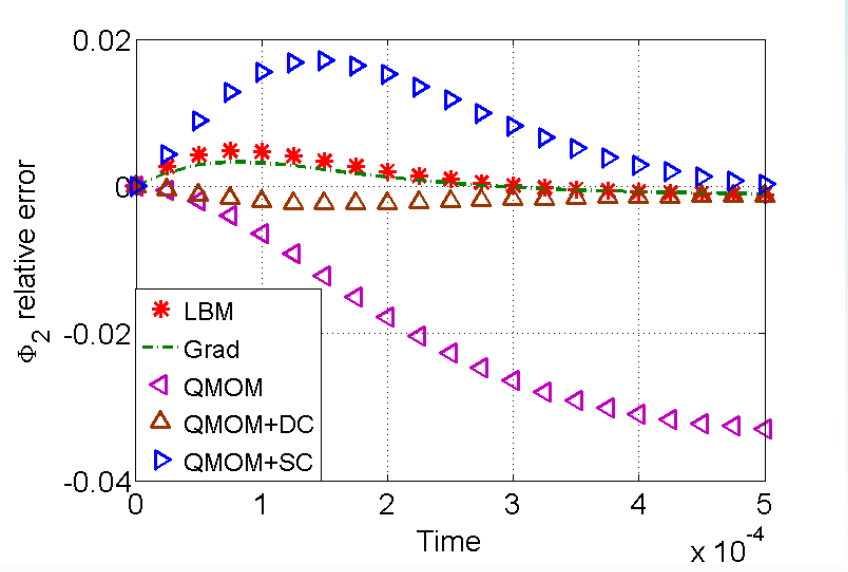
3rd energy moment

QMOM approximation vs DVM, Grad, oLBM – 3

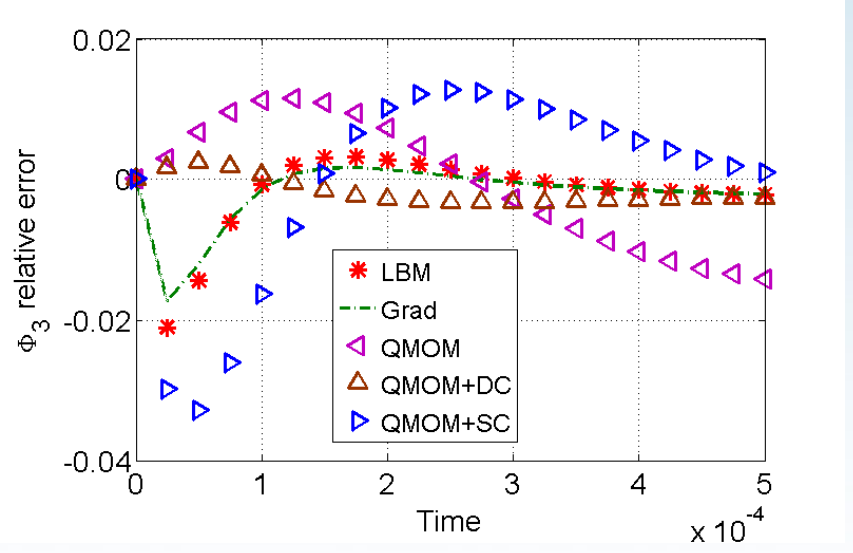
Homogeneous Isotropic Boltzmann Equation (HIBE)

$$M = 4$$

Relative error on Φ_p



2nd energy moment



3rd energy moment

HIBE steady state
Quadrature error

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Comparison of steady-state moments

	$M=4$		$M=6$		$M=8$	
$\times 10^{8}$	Φ_2	%	Φ_2	%	Φ_2	%
Grad (exact)	1.0034	0.0	1.0034	0.0	1.0034	0.0
oLBM	1.0033	0.01	1.0034	0.003	1.0034	0.001
QMOM	0.9704	3.29	0.9979	0.55	1.0022	0.12
QMOM+SC/DC	1.0034	0.0	1.0034	0.0	1.0034	0.0
$\times 10^{11}$	Φ_3	%	Φ_3	%	Φ_3	%
Grad (exact)	1.4921	0.0	1.4921	0.0	1.4921	0.0
oLBM	1.4919	0.02	1.4921	0.004	1.4921	0.002
QMOM	1.4707	1.44	1.4874	0.31	1.4910	0.08
QMOM+SC/DC	1.4921	0.0	1.4921	0.0	1.4921	0.0
$\times 10^{14}$			Φ_4	%	Φ_4	%
Grad (exact)	-	-	2.8529	0.0	2.8529	0.0
oLBM	-	-	2.8527	0.005	2.8528	0.002
QMOM	-	-	2.8302	0.80	2.8478	0.18
QMOM+SC/DC	-	-	2.8529	0.0	2.8529	0.0
$\times 10^{17}$			Φ_5	%	Φ_5	%
Grad (exact)	-	-	6.6666	0.0	6.6666	0.0
oLBM	-	-	6.6662	0.006	6.6665	0.002
QMOM	-	-	6.6244	6.34	6.6548	0.18
QMOM+SC/DC	-	-	6.6666	0.0	6.6666	0.0

HIBE steady state
Quadrature error - 2

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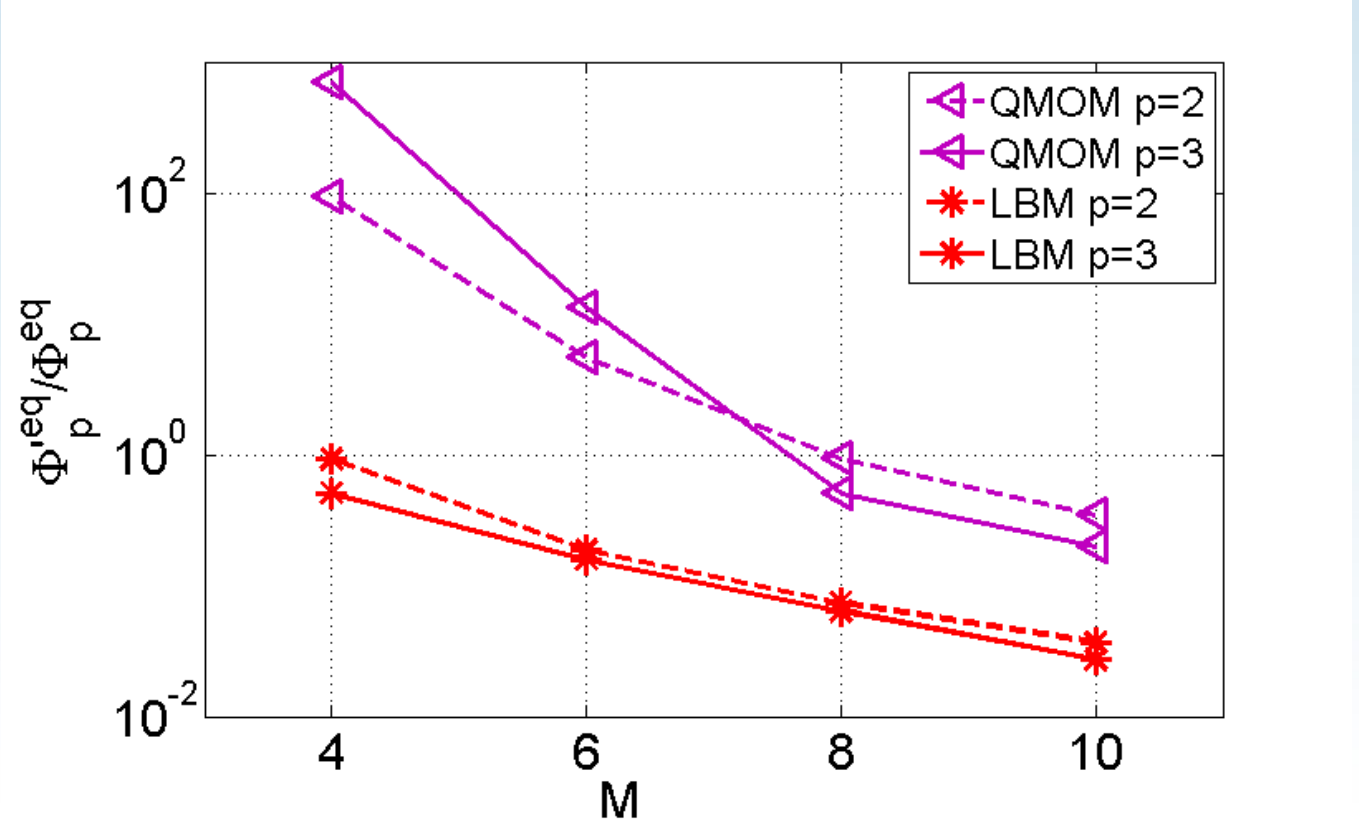
Quadrature error at the true equilibrium



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Turbulence models
DNS, LES, RANS

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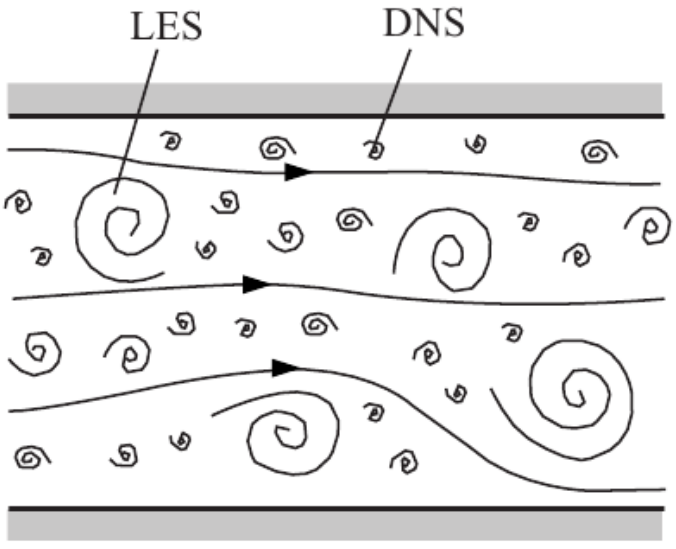

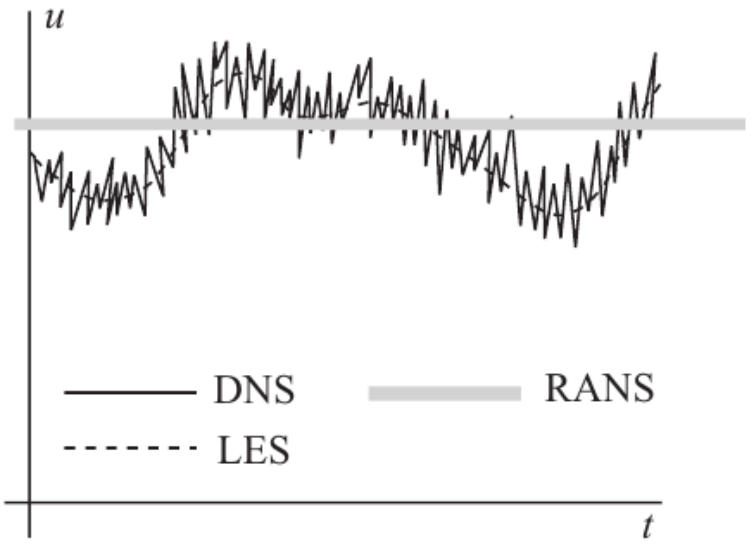

Direct Numerical Simulation (DNS)

All the flow-scales are solved without model ⇒ virtual experiments (3D and unsteady)

Large Eddy Simulation (LES)

Equations are filtered in space (or frequency). Bigger 3D unsteady scales are solved; smaller ones are modelled with sub-grid scale (SGS) models

RANS

Time-averaged equations ⇒ only the mean flow is predicted

Turbulent reactive flows
Closure problem

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- N_s species denoted by capital letters $A, B, C, \dots, R, S$
- Vector of concentrations $\phi = (\phi_1, \dots, \phi_{N_s})$
- Consider a simple reaction

$$A + B \xrightarrow{k} R$$

- Transport equations for concentrations with source terms

$$S_A = -k\phi_A\phi_B = S_B$$

- In turbulent flows a RANS average (in time) or LES filter (in space) is performed

$$\langle S_A \rangle = -k\langle \phi_A\phi_B \rangle \neq -k\langle \phi_A \rangle \langle \phi_B \rangle$$

- In general the term $\langle S(\phi) \rangle \neq S(\langle \phi \rangle)$

Turbulent reactive flows

PDF description (Pope, Fox)

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- The chemical source term can be closed if we assume the existence of a joint probability density function of the concentrations

$$\langle S(\phi) \rangle = \int S(\psi) P(\psi; x, t) d\psi$$

- Rigorously, when using LES we are dealing with a filtered-density function

$$P(\psi; x, t) = \int \delta(\psi - \phi(x, t)) G(r - x) dr$$

where G is the LES filter

- For the box filter this could be no more a PDF so we simply assume a PDF P that represents the spatial dishomogeneity in the cells such that

$$\int \psi P(\psi; x, t) d\psi = \langle \phi \rangle$$

is the filtered scalar and

$$\int (\psi_\alpha^2 - \langle \psi_\alpha \rangle^2) P(\psi_\alpha; x, t) d\psi_\alpha = \langle \phi_\alpha'^2 \rangle$$

the scalar fluctuation

PDF Transport Equation

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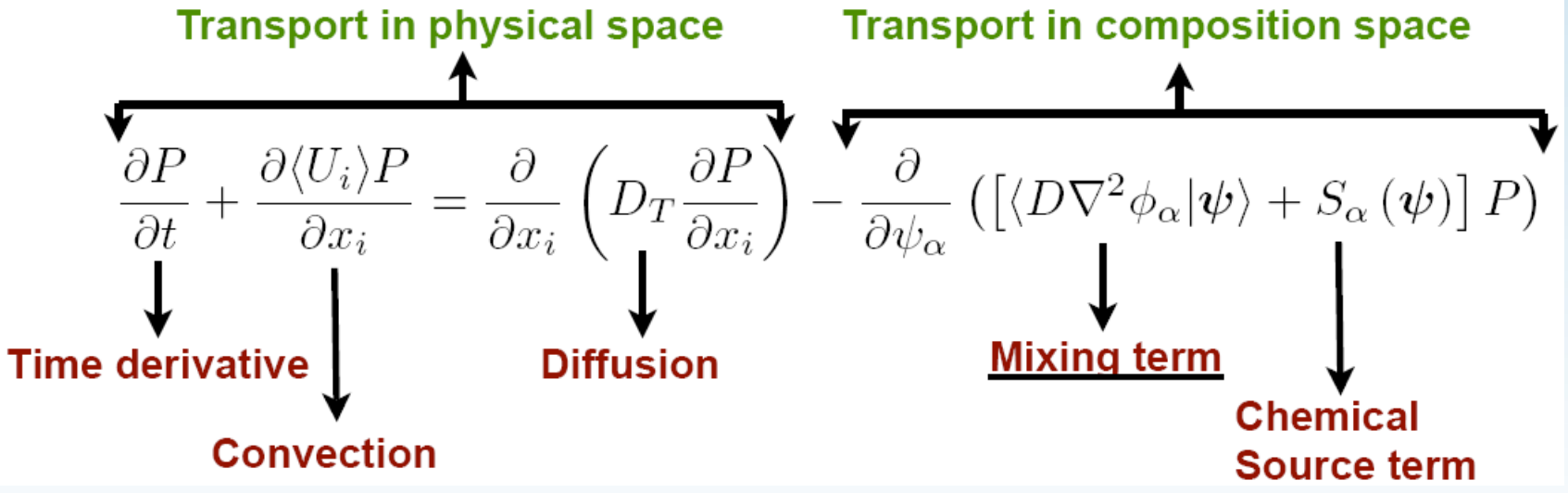
- P can be solved in a advection-reaction-diffusion equation with $N_s + 4$ independent variables



- The turbulent diffusion term comes from the assumption that the conditional fluctuations $\langle U_i' | \psi \rangle P = -D_T \frac{\partial P}{\partial x_i}$
- Molecular mixing term needs to be modeled

Mixing models

Interaction by exchange with the mean (IEM)

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- The most simple and popular model for Eulerian simulations is the IEM

$$\langle D\nabla^2\phi_\alpha|\psi\rangle = -\frac{C_\phi}{\tau}(\psi - \langle\phi\rangle)$$

- It is a linear relaxation of the scalars to the mean value with time scale τ and a parameter C_ϕ
- τ is chosen to be a turbulence time scale, $\frac{2k}{\epsilon}$ for RANS and $\frac{2\Delta^2}{D+D_T}$ where Δ is the filter width
- C_ϕ is the scalar-to-mechanical time-scale ratio and it depends on the local Schmidt and Reynolds numbers (for gases at high $Re\, C_\phi \approx 2$)

PDF discretization

Quadrature Method of Moments - Multi environment formulation

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- In the Quadrature Method of Moments (QMOM) the integrals are approximated using a quadrature rule

$$\int g(\psi)P(\psi;x,t)d\psi \approx \sum_{i=1}^{M} g(\phi_i)w_i$$

where ϕ_i are the abscissas and w_i the weights of the quadrature rule

- For a given set of $2M$ moments, the M abscissas and weights can be calculated using inversion algorithms (Wheeler or Product-Difference)
- This means that we are approximating the exact PDF P with a multi-environment PDF f

$$f_\phi(\psi;x,t) = \sum_{i=1}^{M} w_i(x,t)\delta[\psi - \phi_i(x,t)]$$

where δ is a multi-dimensional delta function

DQMOM-IEM

Direct Quadrature Method of Moments with IEM closure

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- In the DQMOM transport equations for w_i and $w_i\psi_i$ are solved instead of equations for μ_i
- $M(1+N)$ equations with some constraints (e.g. $\sum_{i=1}^{M} w^i = 1$)
- The source term is such that the first $M(1+N)$ moments are coherent with the transported ones
- Let us consider a competitive reaction scheme simplified using a mixture fraction ξ and a reaction progress Y (linear combination of species concentration). This results in $N = M = 2$ and $\phi = (\xi, Y)$

$$\frac{\partial w_1}{\partial t} + \overline{U}_i \frac{\partial w_1}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_1}{\partial x_i} \right) = 0 \,,$$

$$w_2 = 1 - w_1$$

$$\frac{\partial w_1 \xi_1}{\partial t} + \overline{U}_i \frac{\partial w_1 \xi_1}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_1 \xi_1}{\partial x_i} \right)$$
$$= \frac{C_\phi}{\tau} w_1 w_2 [\xi_2 - \xi_1] + \frac{D_T}{\xi_1 - \xi_2}\left(w_1 \frac{\partial \xi_1}{\partial x_i}\frac{\partial \xi_1}{\partial x_i} + w_2 \frac{\partial \xi_2}{\partial x_i}\frac{\partial \xi_2}{\partial x_i} \right) ,$$

$$\frac{\partial w_2 \xi_2}{\partial t} + \overline{U}_i \frac{\partial w_2 \xi_2}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_2 \xi_2}{\partial x_i} \right)$$
$$= \frac{C_\phi}{\tau} w_1 w_2 [\xi_1 - \xi_2] + \frac{D_T}{\xi_2 - \xi_1}\left(w_1 \frac{\partial \xi_1}{\partial x_i}\frac{\partial \xi_1}{\partial x_i} + w_2 \frac{\partial \xi_2}{\partial x_i}\frac{\partial \xi_2}{\partial x_i} \right) ,$$

DQMOM-IEM

Example: set of equations (Marchisio,2009)

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$$\frac{\partial w_1 Y_1}{\partial t} + \overline{U}_i \frac{\partial w_1 Y_1}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_1 Y_1}{\partial x_i} \right)$$
$$= w_1 S(\xi_1, Y_1) + \frac{C_\phi}{\tau} w_1 w_2 [Y_2 - Y_1]$$
$$+ \frac{D_T}{Y_1 - Y_2}\left(w_1 \frac{\partial Y_1}{\partial x_i}\frac{\partial Y_1}{\partial x_i} + w_2 \frac{\partial Y_2}{\partial x_i}\frac{\partial Y_2}{\partial x_i} \right),$$

$$\frac{\partial w_1 Y_2}{\partial t} + \overline{U}_i \frac{\partial w_1 Y_2}{\partial x_i} - \frac{\partial}{\partial x_i}\left(D_T \frac{\partial w_1 Y_2}{\partial x_i} \right)$$
$$= w_2 S(\xi_2, Y_2) + \frac{C_\phi}{\tau} w_1 w_2 [Y_1 - Y_2]$$
$$+ \frac{D_T}{Y_2 - Y_1}\left(w_1 \frac{\partial Y_1}{\partial x_i}\frac{\partial Y_1}{\partial x_i} + w_2 \frac{\partial Y_2}{\partial x_i}\frac{\partial Y_2}{\partial x_i} \right).$$

Only the progress variable Y has a source term S

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Groundwater remediation

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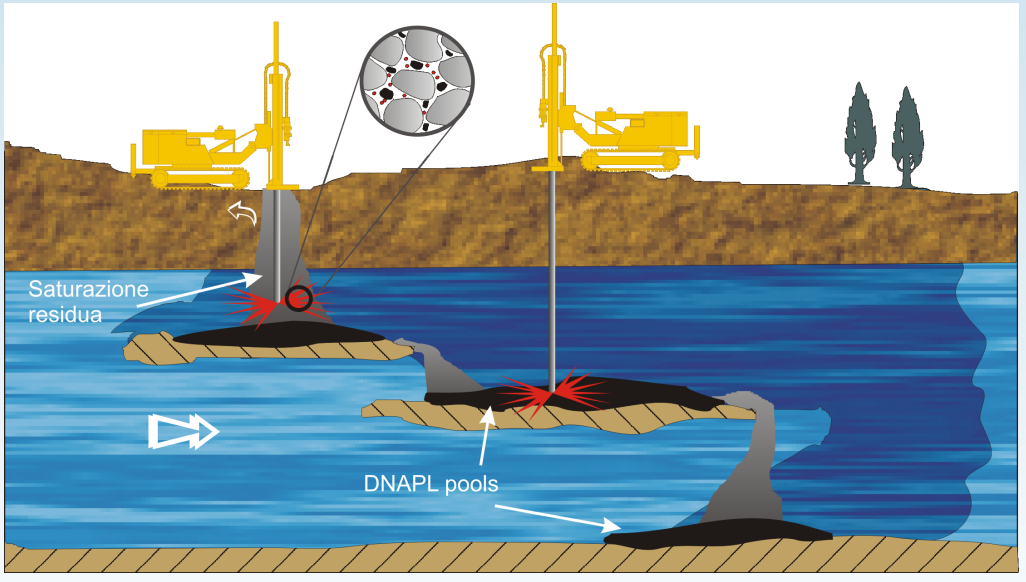
Zero-valent iron nano-particle injection



Objectives

- Develop predictive macro-scale transport and reaction models
- Determine unknown parameters

Challenges

- Limited experimental data
- Multi-scale multi-physics problem

Multi-scale porous media modelling

Subsurface flows

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Length/time scales

- **field/reservoir scale:** large spatial variations of material properties and parameters
- **core/lab scale:** homogenized and averaged equations with constant effective parameters
- **pore/CFD scale:** fluid continuum equations
- **molecular/single-pore scale:** molecular discrete models

Pore scale

- governing equations: Stokes or Navier-Stokes + particle transport (Eulerian or Lagrangian)
- porous matrix is undeformable and represent domain boundaries
- micro-scale parameters and fluid properties are considered known and fixed
- particles can (sometimes) be considered of negligible size

Numerical and simulation difficulties

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1 – Pre-processing

- extraction of porous media properties
- creation of realistic packings
- fix and modify pore geometry (grain contacts, external container)

2 – Setup and simulation

- meshing
- realistic boundary conditions
- numerical schemes for NS and ADR

3 – Post-processing

- mesh convergence analysis, error estimation
- data analysis and model validation
- upscaling and estimation of macroscopic parameters

3D Geometry creation

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Problem: how to get a realistic geometry representative of a generic porous media? Given porosity and grain size distribution, infinite possible realizations exist

REAL SAMPLES

- Images (microCT)
- Detailed representation of the pore spaces
- Segmentation and reconstruction of a surface mesh not trivial
- Process is hardly automatised and result is not "unique"

ALGORITHMIC RECONSTRUCTION

- From simple models to (quasi)-realistic porous media
- Easier to build different test cases and compute statistics
- No need of expensive instrumentation
- Choice of parameters not trivial

PACKING ALGORITHMS:
ballistic sedimentation $\longrightarrow$ DEM, rigid body
dynamic/collective rearrangement $\longrightarrow$ MD, random placing

Virtual porous media – Random packing

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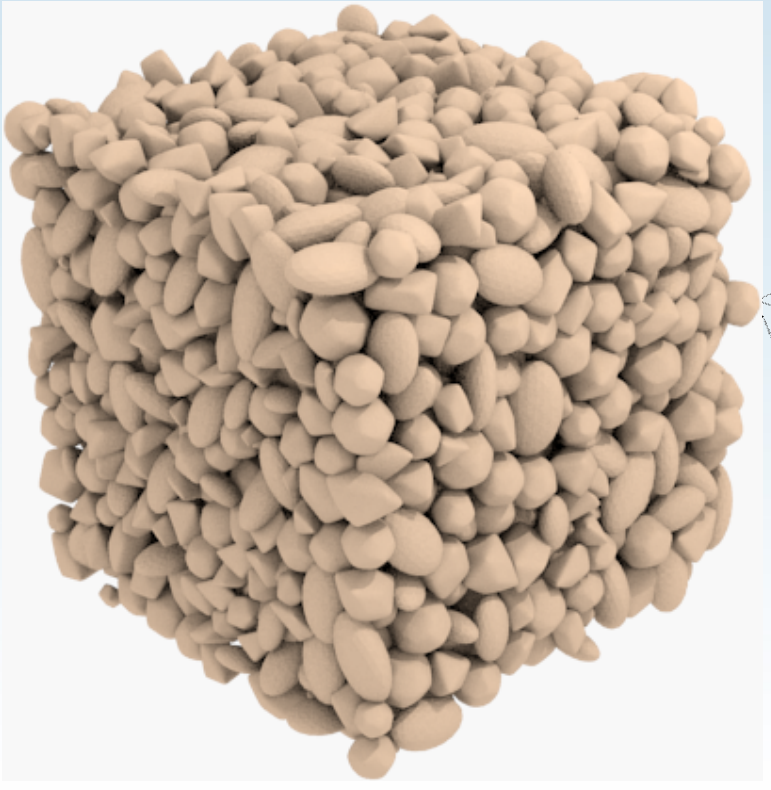
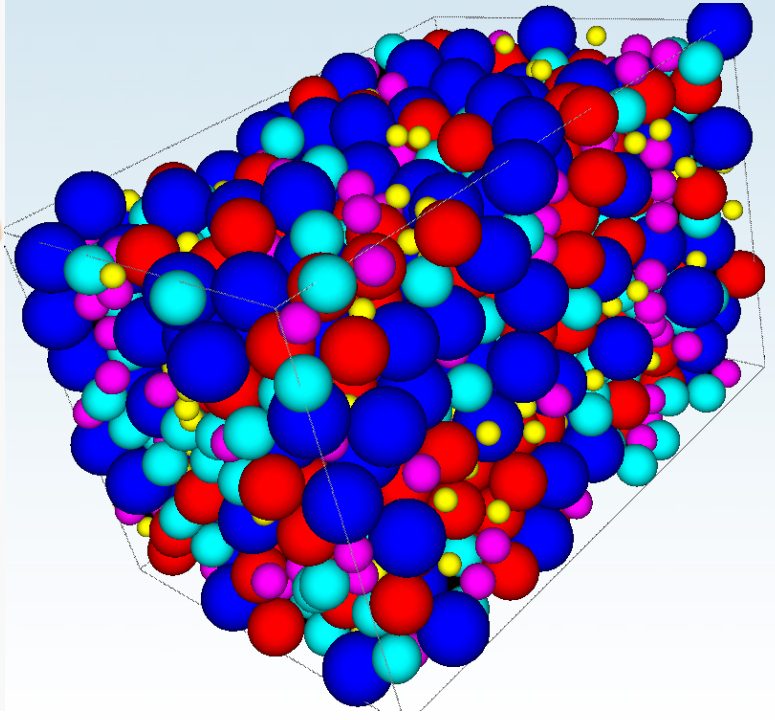


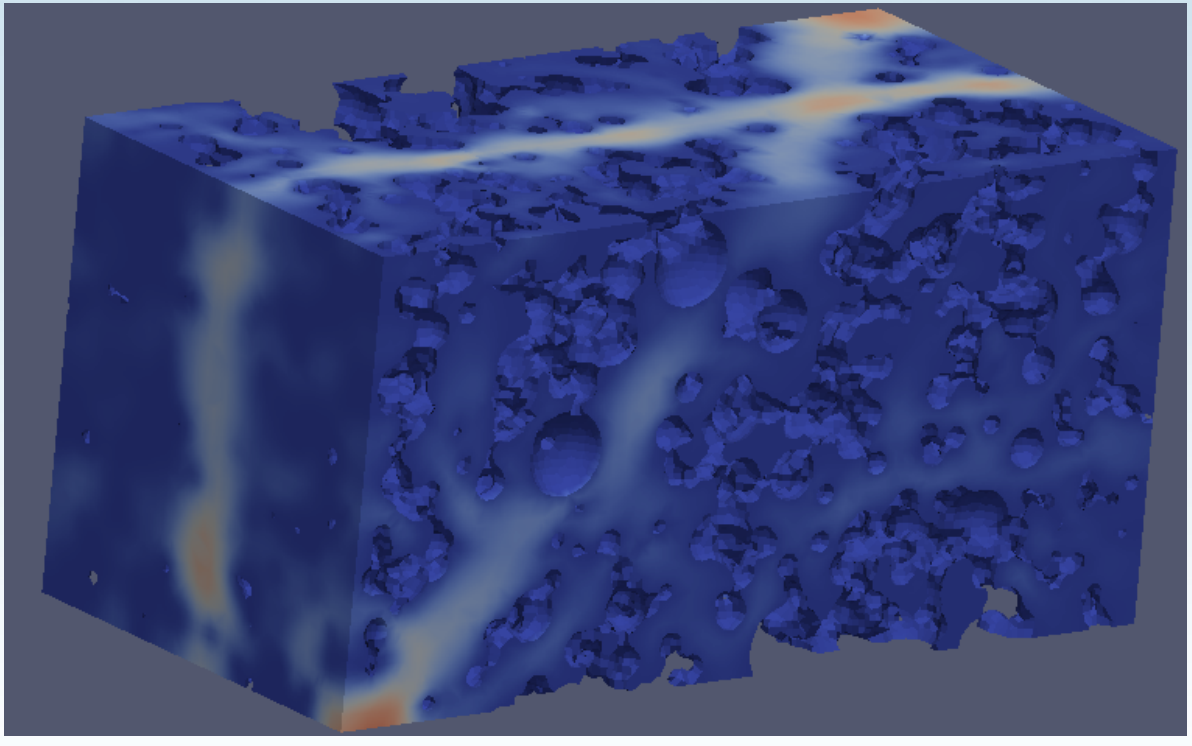
Bullet physics (Blender)



MD-like (A. Donev)

Nice YouTube animations: "Porous medium packing (blender visualization)"

Virtual porous media – Random with overlaps



- Fully random independent placement from distribution $f(x, y, z)$
- Post-processing with Jodrey-Tory algorithm to reduce overlapping
- Randomization of the surfaces

Further manual post-processing

1 – Pre-processing

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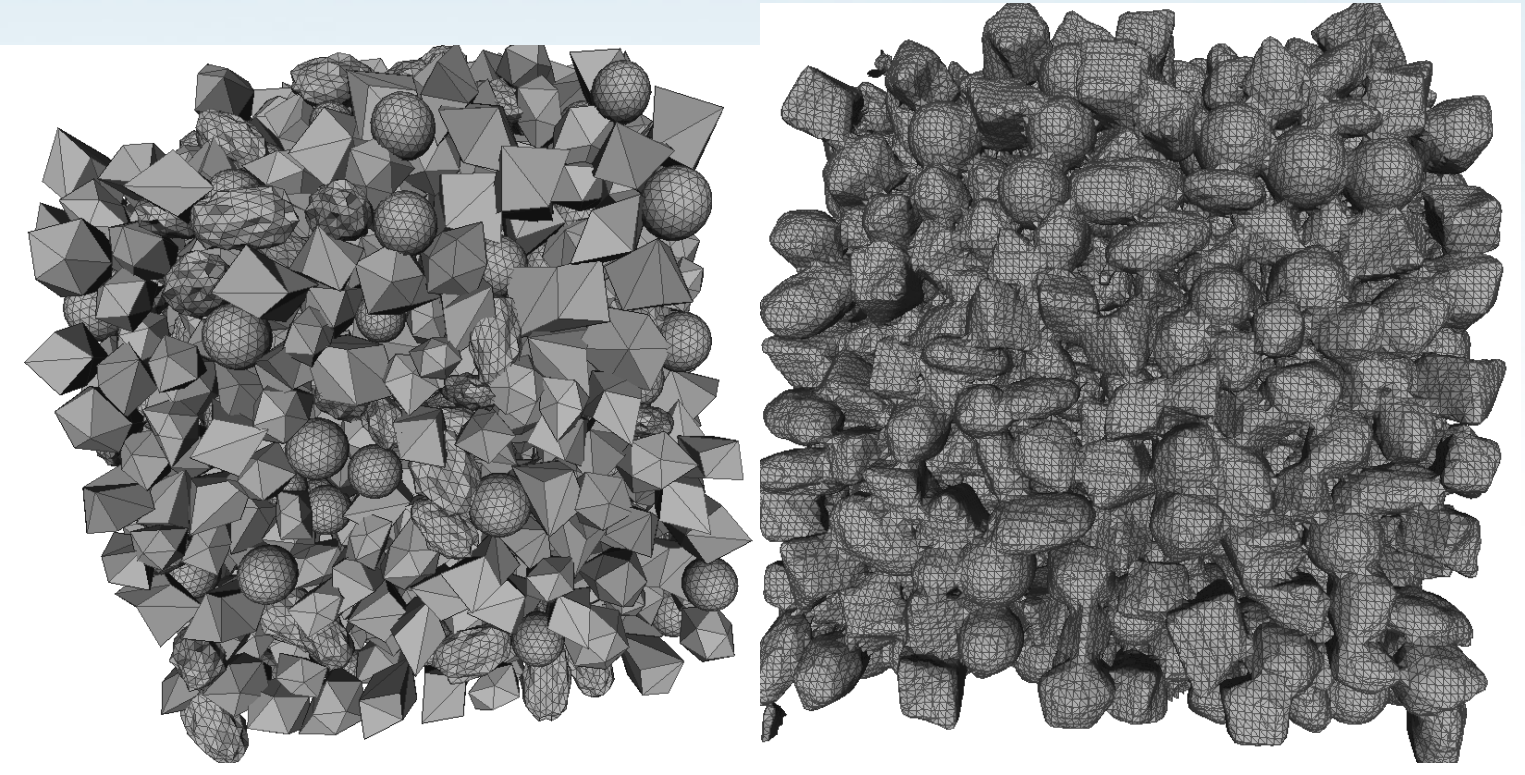
Surface triangular mesh (e.g., STL)

- Porosity: must be calculated a posteriori
- Contacts: if the packing algorithm is not exact there can be overlapping or non-touching grains
- Non-realistic features: too sharp or smooth edges

Mesh resampling with Marching Cubes algorithms



Mathematical models

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Assumptions: Newtonian fluids, undeformable porous media, isothermal, ...

Micro-scale models

- u velocity
- p pressure
- c concentration/ volume fraction/ phase-field
- D_0 molecular diffusion

Macro/Meso-scale models

- V Darcy flux
- P pressure
- C concentration/ saturation/ phase-field
- K permeability
- D dispersivity

$$\partial_x p = -\frac{\mu}{K} V \qquad \text{Darcy's law}$$

$$\partial_x P = -\frac{\mu}{K} V - \rho\beta V^2 \qquad \text{Darcy-Forchheimer}$$

$$\partial_x P = -\frac{\mu}{K} V - \mu_{eff}\Delta V \qquad \text{Brinkman}$$

$$\rho\partial_t V + \partial_x P = -\frac{\mu}{K} V \qquad \text{Unsteady Darcy}$$

$$\dots$$

Solute transport

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Two miscible incompressible fluids, $\rho_1 \approx \rho_2, \mu_1 \approx \mu_2$, one-way coupling.

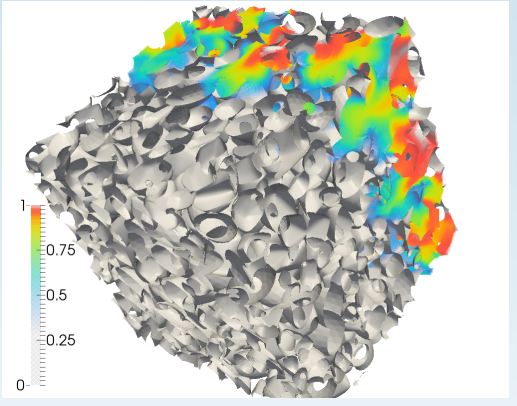
Pore-scale model

Steady Navier Stokes equations in the pore space, $\mu = \mu_1, \rho = \rho_1$

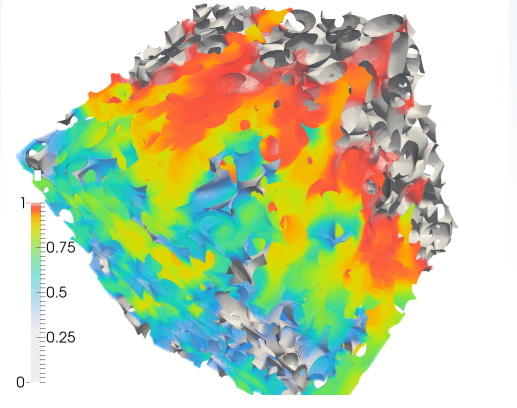
$$\nabla \cdot u = 0 \qquad u \cdot \nabla u = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\Delta u$$

Advection Diffusion Reaction:

$$\frac{\partial c}{\partial t} + \nabla \cdot (uc + D_0 \nabla c) = r$$



Pore-scale simulation of solute transport (Icardi et. al, Phys. Rev. E, 2014)



Darcy-scale model

$$\nabla \cdot v = 0 \qquad v = -\frac{K}{\mu}\nabla P$$

Advection-Dispersion-Reaction:

$$\frac{\partial C\phi}{\partial t} + \nabla \cdot (vC + D\phi \nabla C) = R$$

Two phase immiscible model

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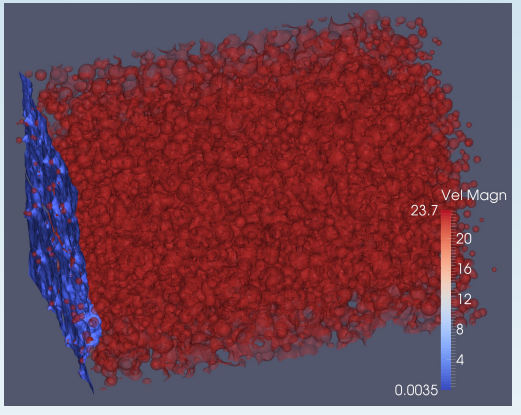
Pore-scale model:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho u) = 0$$

$$\rho\frac{\partial}{\partial t}(u)+\rho u\cdot\nabla(u) = -\nabla p+\mu\Delta u+\nabla\cdot(\tau_m)+\kappa\sigma n\delta(\Gamma)$$

Advection Diffusion Reaction (unsteady):

$$\frac{\partial c}{\partial t} + \nabla \cdot (uc) = r$$



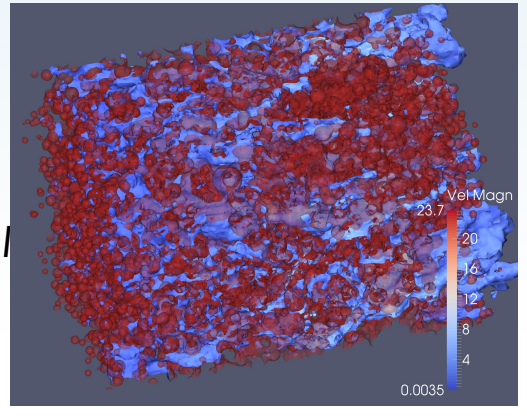
Pore-scale simulation of CO_2 injection (Icardi et. al, in preparation)

Darcy-scale model (mixture)

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho V)=0 \qquad V=-\frac{K}{\mu}(\nabla P-\rho\frac{\partial V}{\partial t}) \qquad K=K_r(C)I$$

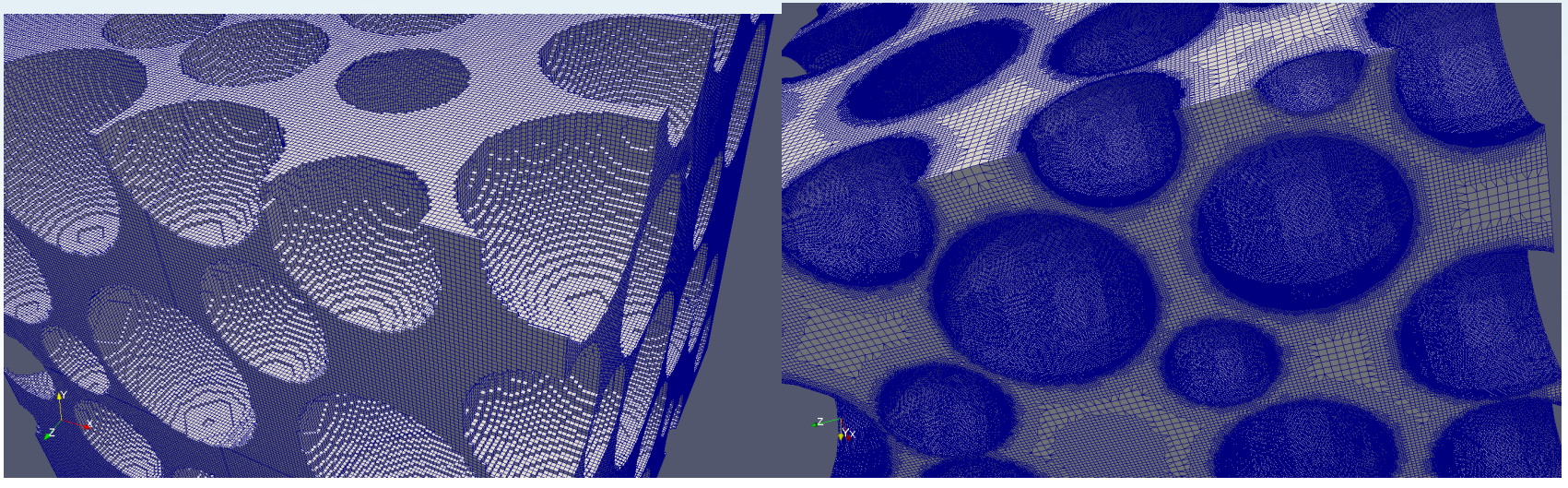
Advection-Dispersion-Reaction (saturation equation):

$$\frac{\partial C\phi}{\partial t} + \nabla \cdot (V_c C + D\phi\nabla C) = R$$



Immersed boundaries VS body-fitted grids

- IB are accurate but not adaptable and first order near the wall
- BF are fully adaptable but difficult to build high quality elements
- Octree refinement with adaptation on the surface (cut-cell)



Boundary conditions

2 – Setup and simulation

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To estimate macro-scale parameter, we have to choose the simplest possible scenario: Quasi-1D flow

Flow boundary conditions

- Total pressure (or periodic BC with uniform body force) imposed at the inlet/outlet
- Symmetry (no normal flow) or periodic on the lateral boundaries (infinite medium)
- Wall conditions to simulate experimental columns (confined medium)

Scalar boundary conditions

- Constant Dirichlet (=1) on inlet (or mixed Danckwerts condition)
- Homogeneous Neumann on outlet and on the grains
- Ad-hoc mixed BCs on the grain could be derived from micro-scale deposition models

$$\partial_n C = \frac{(1 - \eta(C))}{\eta(C)}$$

3D tests – Convergence study with IB

Random spheres packing; porosity 0.6; 600k–80M cells; $\frac{\Delta P}{\Delta x} = 6 \cdot 10^{-5}$

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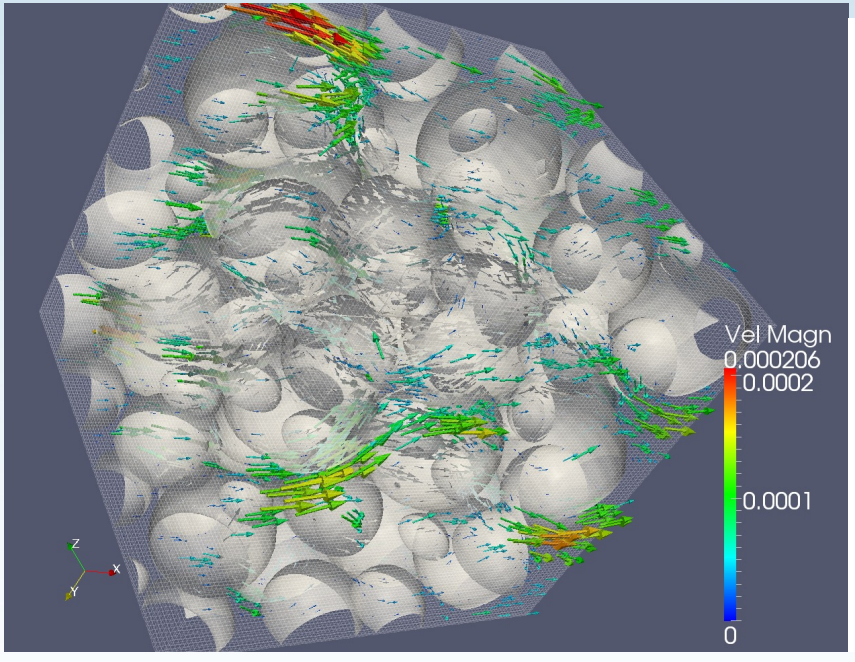
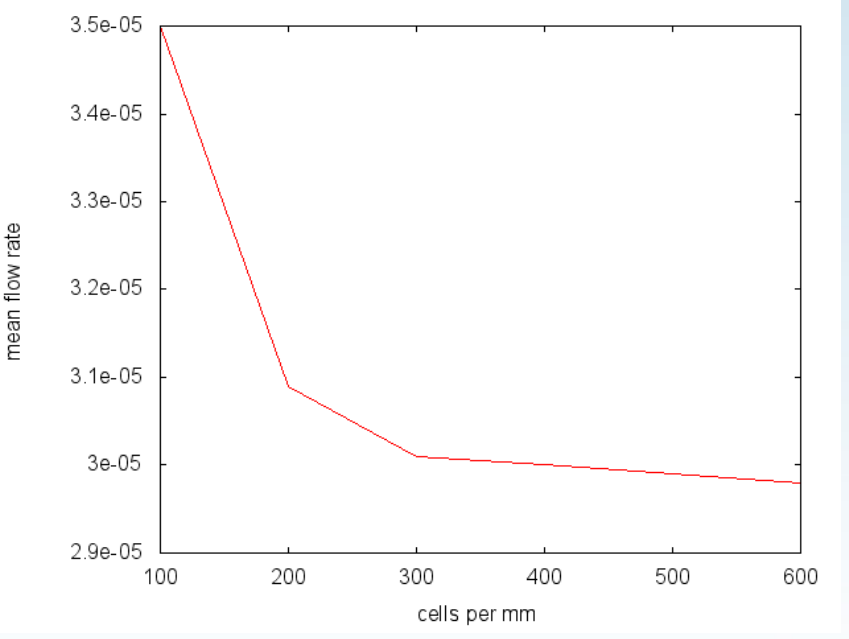
Sphere packing, 100 grains, high porosity

Tolerance on permeability set to 3%



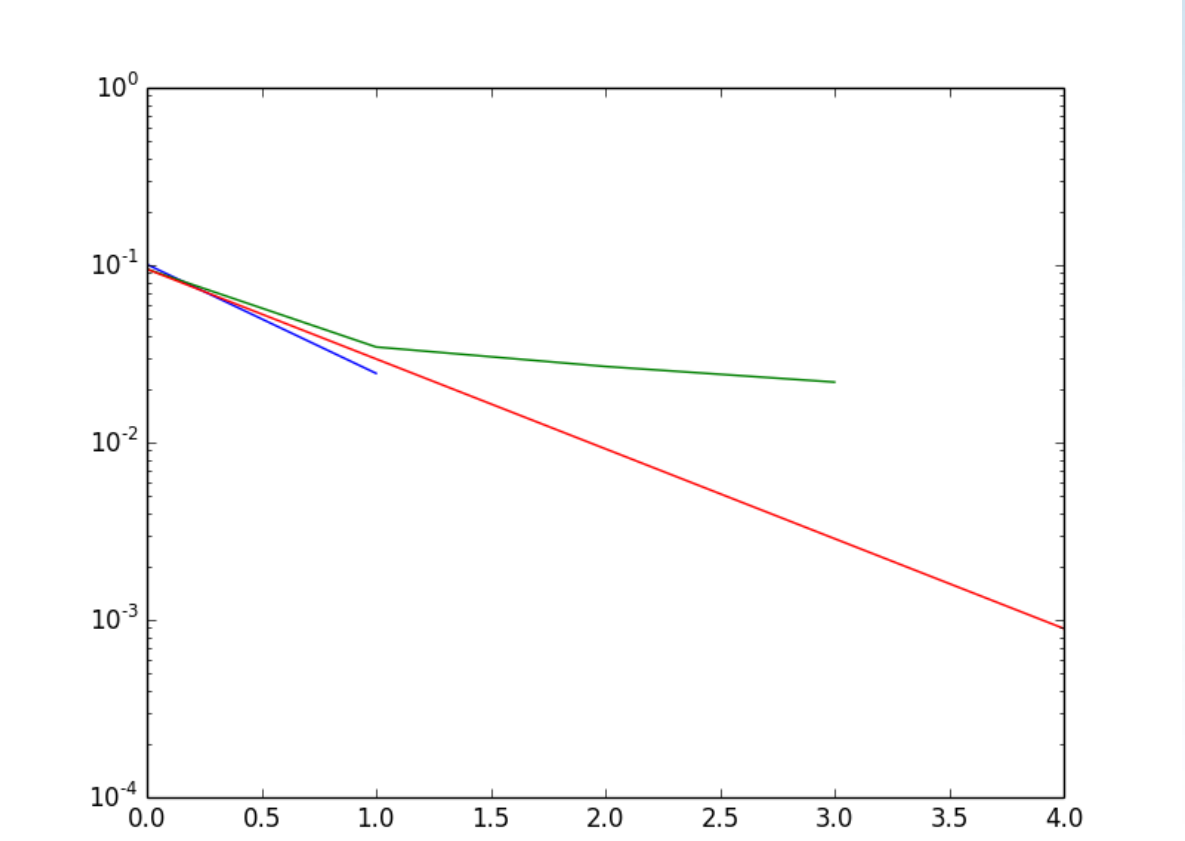


Convergence with standard Immersed Boundary (IB) is not satisfactory (more finite size effects), adapted meshes converge faster

This is confirmed by convergence studies on BCC regular periodic sphere packing

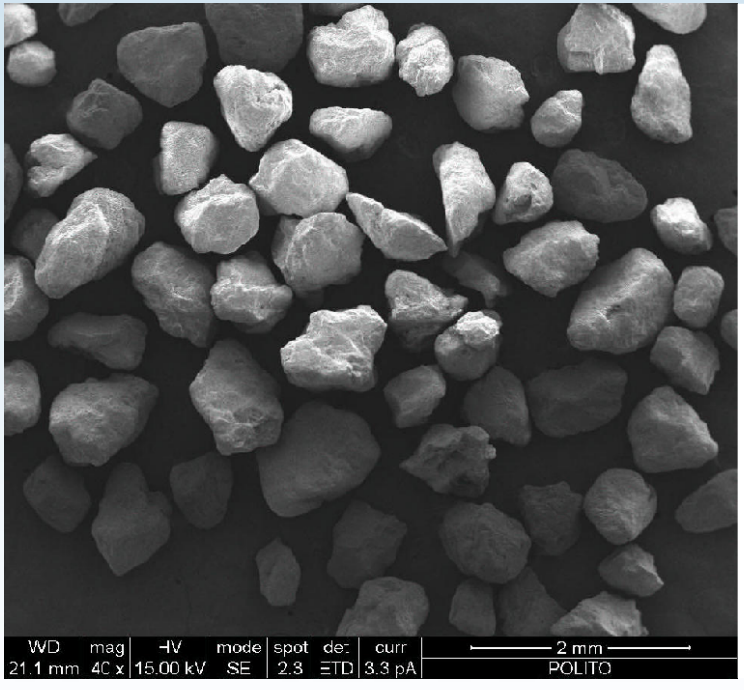
3D tests – Convergence study with adapted mesh

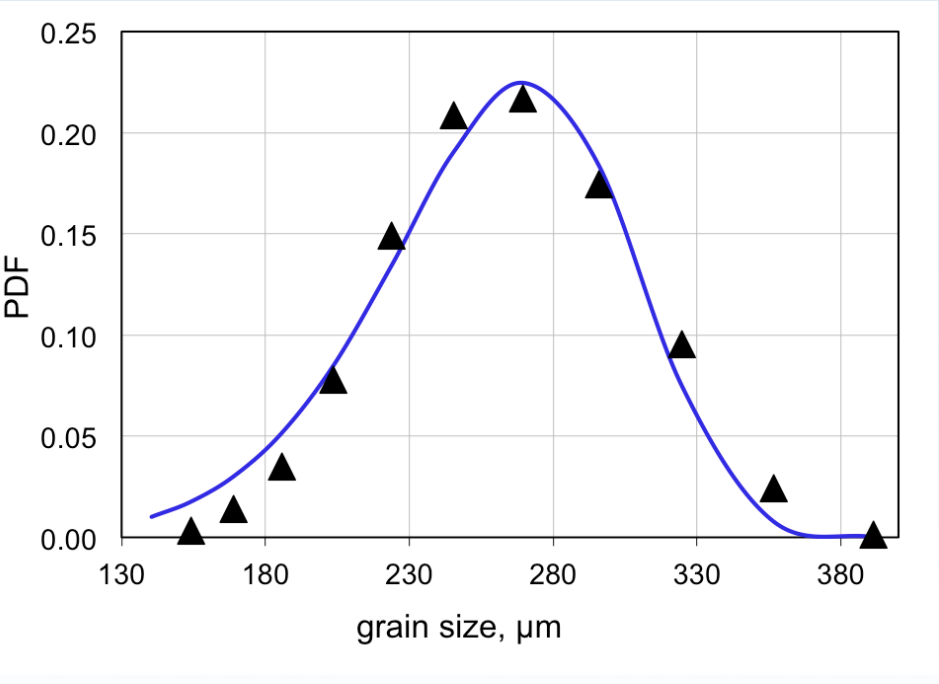
Relative error VS refinement level
uniform refinement (blue), 1:1 refinement (green), 1:2 refinement (red)



Convergence with adapted mesh faster if the refinement is done correctly

Realistic geometry – experimental sand





3D results – Realistic geometries

Irregular packing; porosity 0.35; >2000 grains

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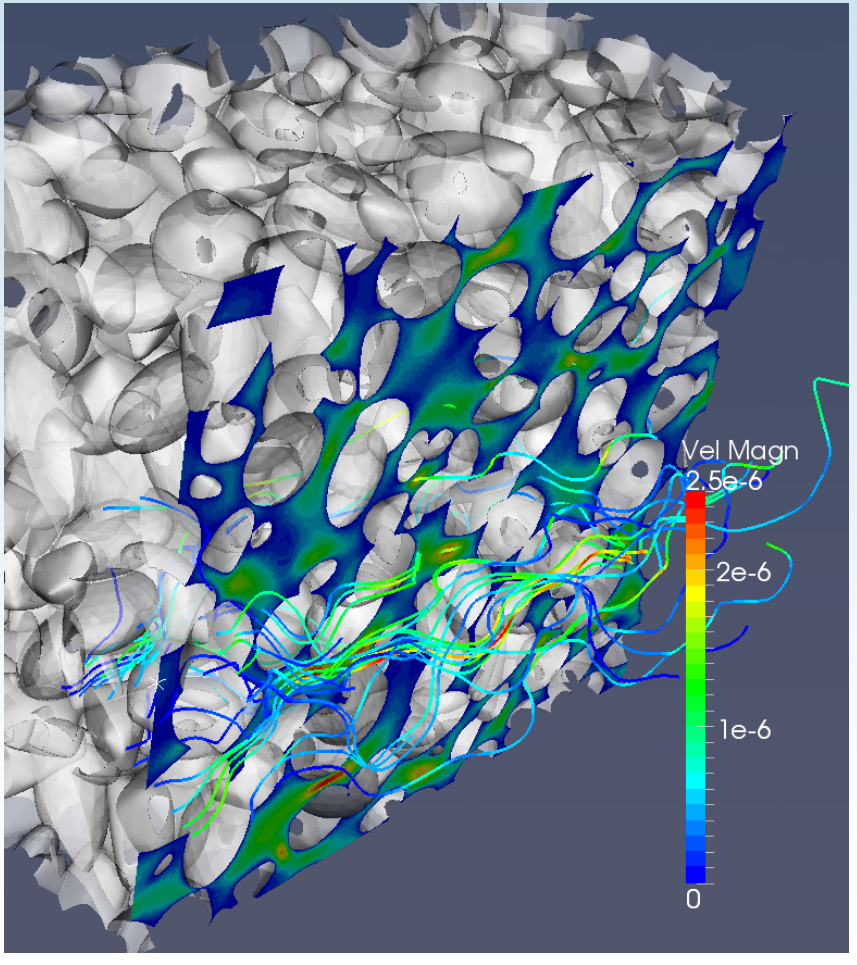
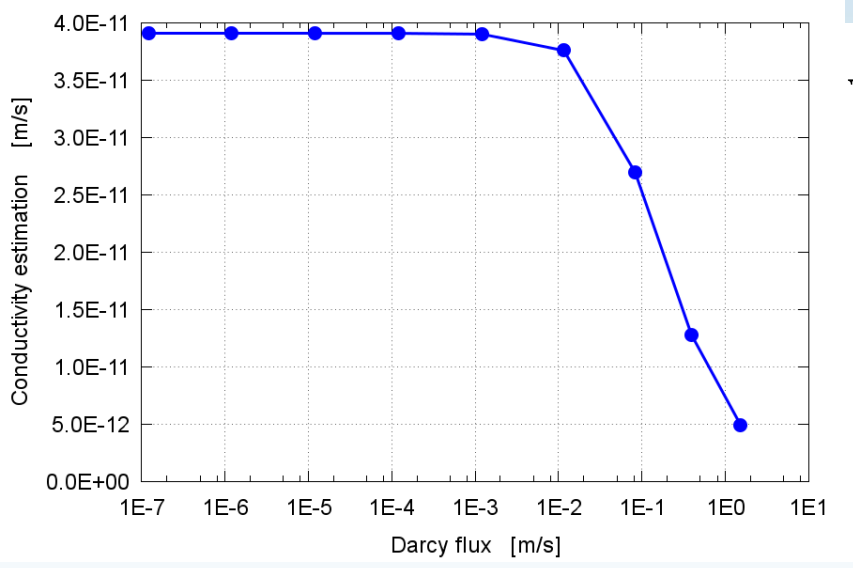
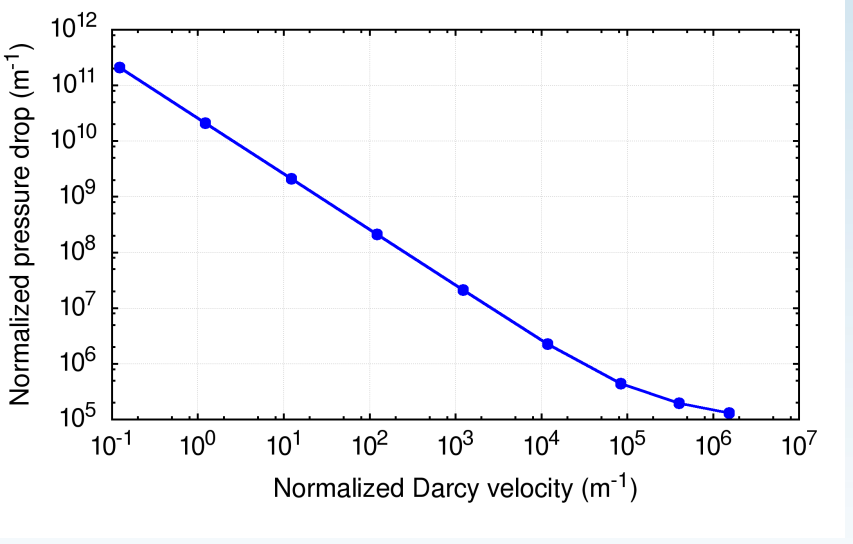
- OpenFOAM (SnappyHexMesh + SimpleFoam)
- ScalarTransportFoam + new solvers for steady perfect sink deposition and polydispersed particles
- $4 \cdot 10^7$ cells
- $R = 0$
- $\frac{\Delta P}{\Delta x} = 10^{-5} - 10^{2}$
- $Re = 10^{-5} - 10^{2}$
- $D = 10^{-9} - 10^{-12}$
- $Pe = 10^{-2} - 10^{6}$



3D results – Flow field

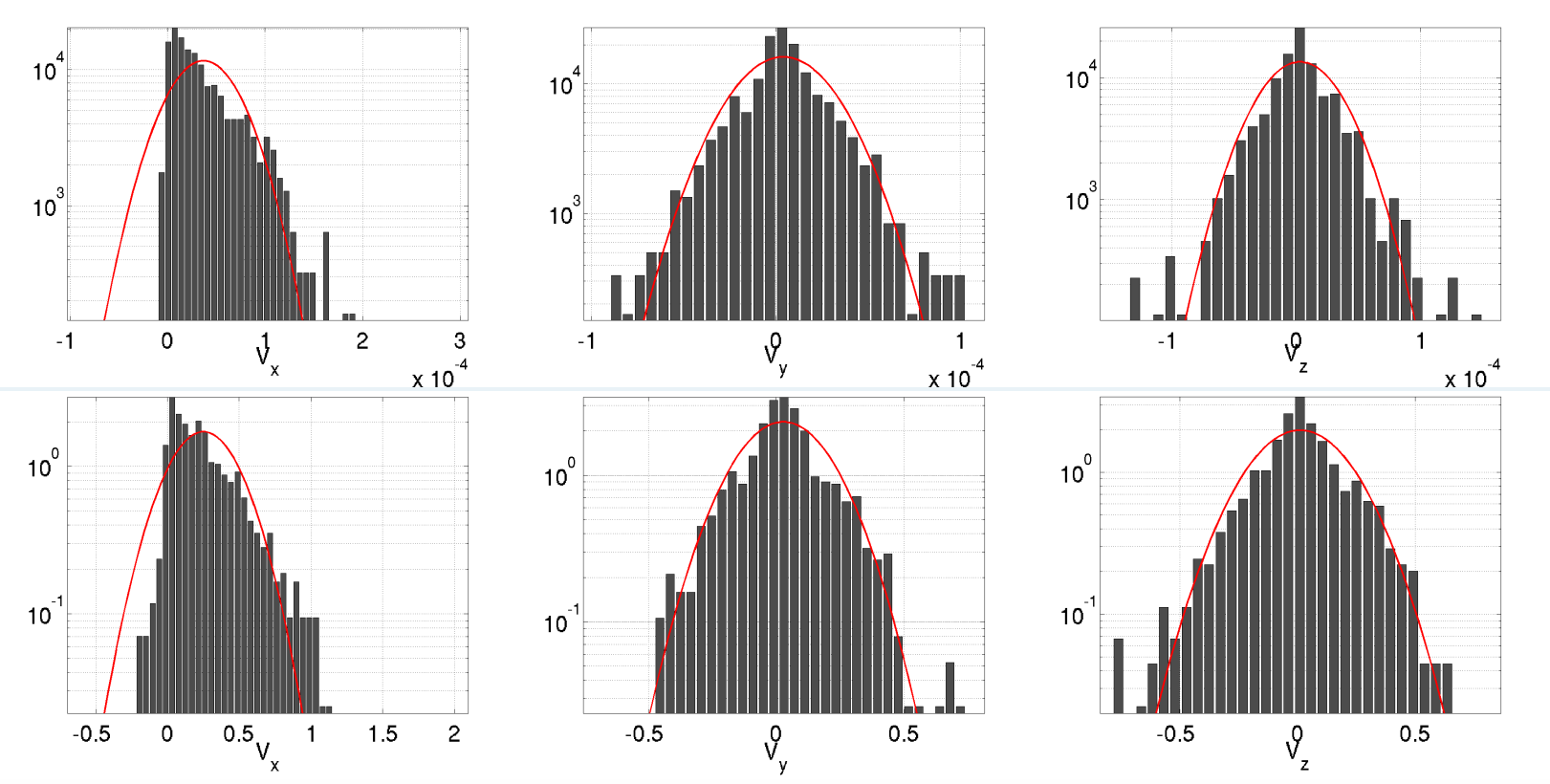




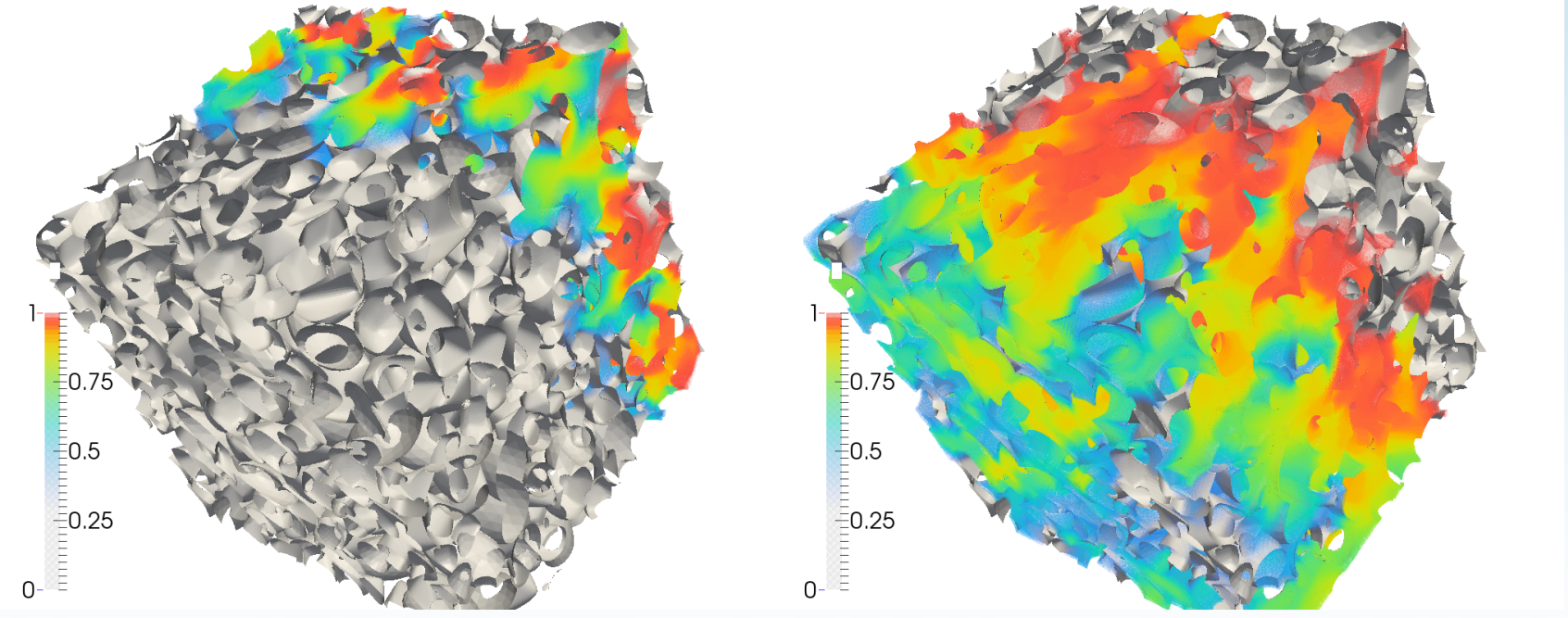
Tortuosity is estimated as $\frac{\int |U| dV}{\int U_x dV}$

Lagrangian tracers are also computed as post-processing

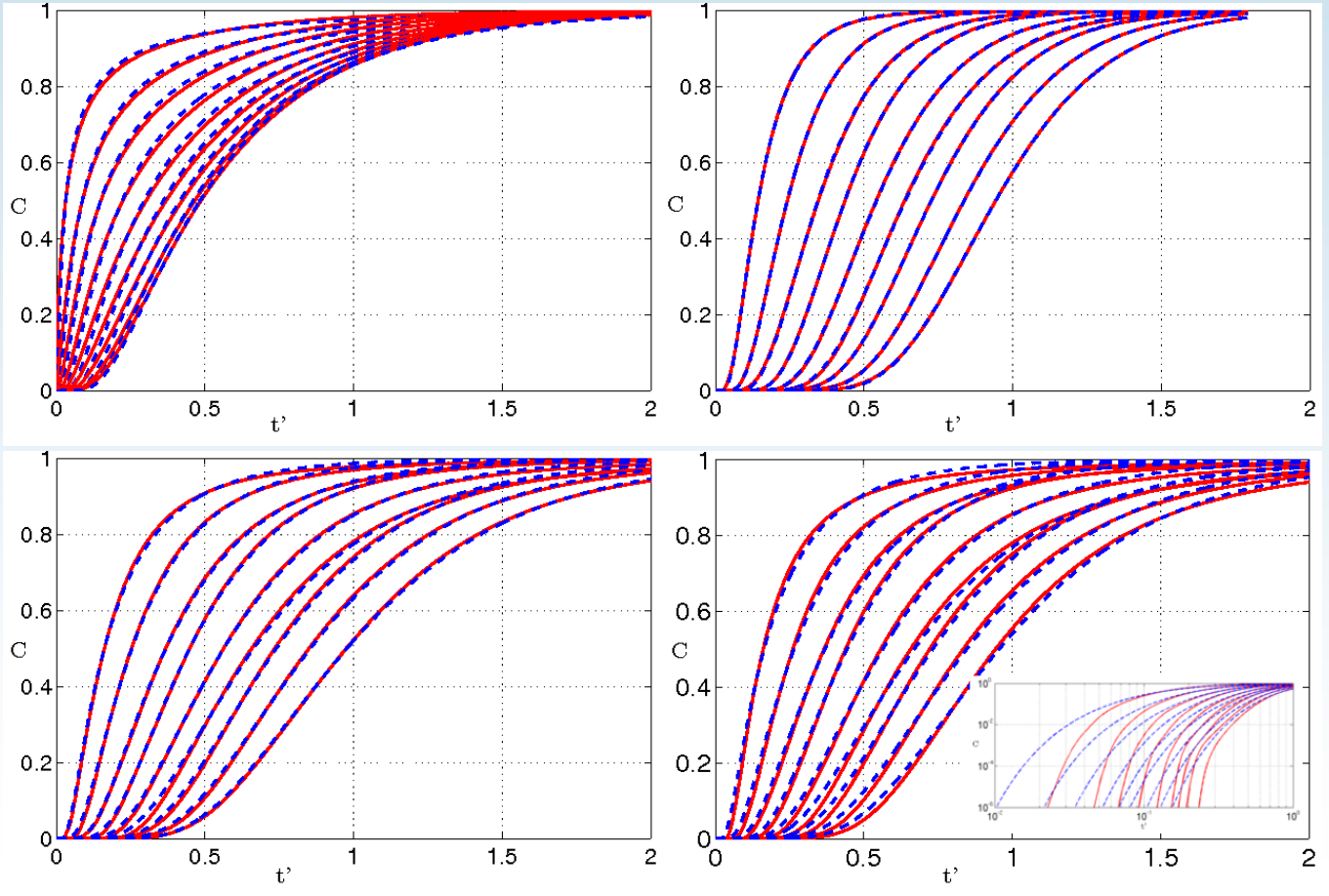
Velocity PDF



3D results – Scalar transport



Breakthrough curves and parameter estimation



Upscaled parameter estimation

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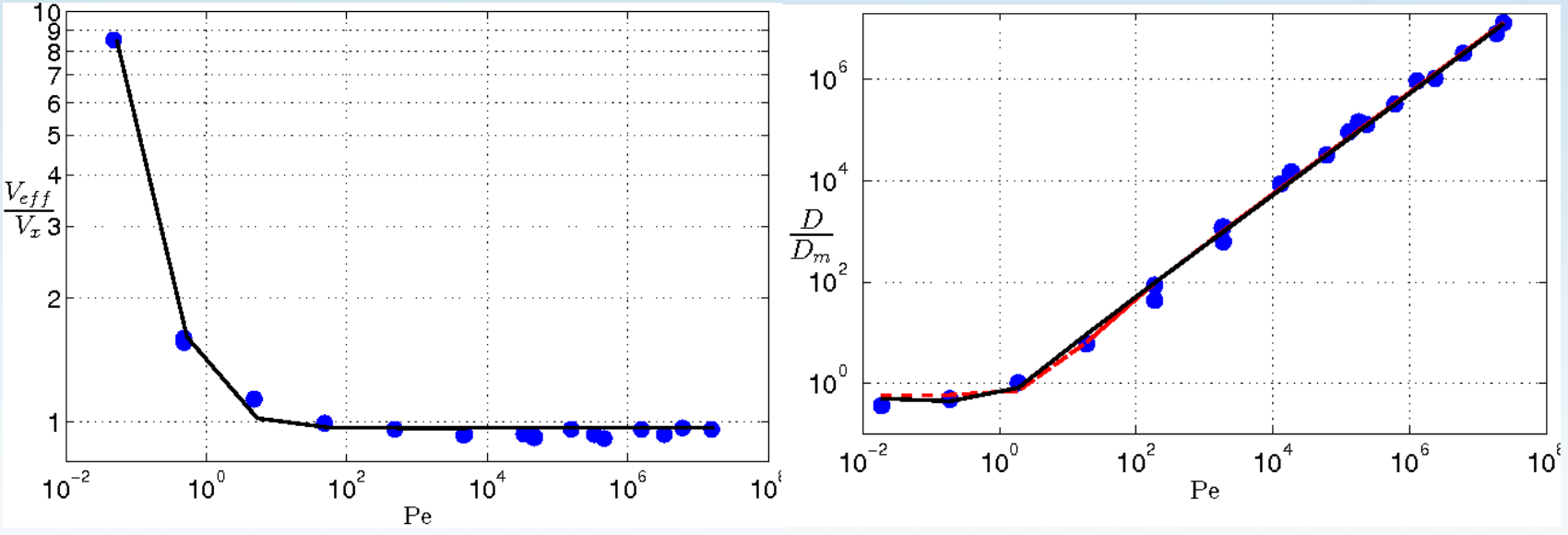
$$\frac{\partial C\phi}{\partial t} + \nabla \cdot (vC + D\phi \nabla C) = 0$$

- "brute-force" approach: non-linear least-square regression to find the best fitting
- for more complex models, Bayesian techniques can be used assuming a data misfit model
- in this work the upscaling can be computed in an explicit form using the method of moments

$$V_{eff} = \left(\frac{\epsilon L_x}{M_1}\right), \qquad D = \frac{M_2}{2L_x}\left(\frac{V}{\epsilon}\right)^3.$$

This is equivalent to the computation of the mean square displacement of Lagrangian tracers

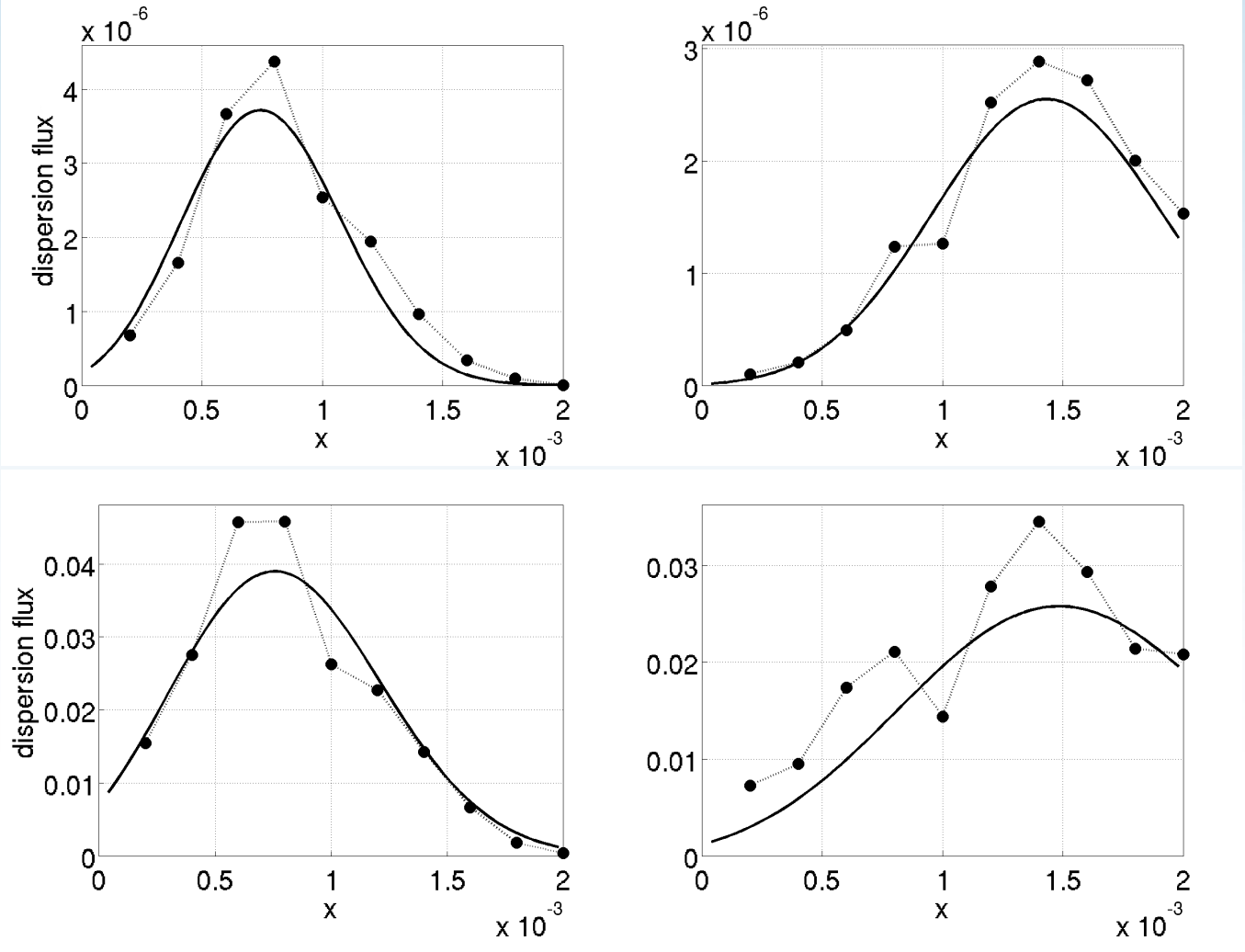
Hydrodynamical dispersion



Left: effective transport velocity.
Right: Hydrodynamical dispersion. Computational results vs. Van Milligen and Bons, and Bear correlations

Fickian dispersion

$$\langle v_x' c' \rangle \approx -D_L \frac{\partial C}{\partial x}.$$



Outline

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Kinetic and PDF equations

- Smoluchowski coagulation equation
- Population balance equation (PBE)
- Boltzmann equation (BE)
- Method of Moments
- Generalized population balance equation (GPBE)

Quadrature-based moment methods

- Numerical Methods and Closure problem
- Gaussian quadrature
- QMOM and DQMOM
- EQMOM
- Multivariate case
- Implementation in CFD codes / spatial inhomogeneity

Applications

- Poly-dispersed flows / coupling with turbulence and multiphase models
- Gas-liquid flows
- Non-equilibrium and granular flows / non-smooth kernels
- Turbulent reactive flows / PDF as modelling tool
- Porous media
- UQ and other applications

Quadrature-based Uncertainty Quantification

Passalacqua, Hu, Fox, 2013; Attar, Vedula, 2013

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The idea of QBMM is, in some sense, similar to the approach of arbitrary Polynomial Chaos Expansion (aPC, Oladyshkin and Nowak, 2012)

- Input random variables ξ_i known only by moments
- Moments induce orthogonal polynomials and quadrature rule
- Stochastic spectral and collocation approaches for computing the response

$$u(\xi) = \sum_{j=0}^{P} \alpha_j \psi_j(\xi), \qquad \langle u(\xi)^n \rangle = \sum_{j=0}^{M} w_j u_j^n$$

- Multidimensional correlated variables treated directly or decomposed with Karhunen-Loeve (or POD/PCA)
- in 1D, the n^{th}-moment of a random response $u \in \mathcal{P}^q$, for a k^{th}-order PCE, is exactly computed with

$$M = max(\frac{q+k+1}{2}, \frac{nq+1}{2}) \text{ collocation points (samples)}$$

- Forward propagation of uncertainty from moments of input to moments of response

Non-linear filtering with QBMM

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The main advantage in using only moments is the possibility of adaptively updating the quadrature rules, when the underlying PDF changes in time/space

Non-linear Fokker-Planck

- Attar and Vedula, 2008; Otten and Vedula, 2011
- Stochastic Differential equation

$$\dot{x}_i = h_i(x,t) + g_i(x,t)W_i, \qquad W_{ij} \text{ white noise}$$

- PDF discretized with DQMOM
- Applications in stochastic control and plasma physics

Non-linear filtering

- Xu and Vedula, 2009, 2010
- Propagation step through Fokker-Planck
- Bayesian update based on quadrature or on EnKF

Other applications of QBMM Bayesian update?

Conclusions

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+ QBMM are **easily implementable** in CFD codes
+ Handle complex physical systems, with moderate number of r.v., even if **correlation is not known**
+ the statistical accuracy is solely determined by the number of moments used (adaptivity) and the regularity of the kernels
+ specifically designed for evolving PDFs in time and space. It can be thought as a **dynamic optimal quadrature**
- High stochastic dimensions (it can become a + if an efficient inversion is found for brute-force approach)
- Moment realizability in advection problems
- Moments-to-quadrature (QMOM) or source-term (DQMOM) inversion can be ill-conditioned

Product-difference algorithm

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A smarter way is to employ the recursive relationship for the orthogonal polynomials:

$$\xi \begin{bmatrix} P_0(\xi) \\ P_1(\xi) \\ \vdots \\ P_{N-2}(\xi) \\ P_{N-1}(\xi) \end{bmatrix} = \begin{bmatrix} a_0 & 1 & & & \\ b_1 & a_1 & 1 & & \\ & & & \ddots & \\ & & & \ddots & 1 \\ & & & & a_{N-1} \end{bmatrix} \begin{bmatrix} P_0(\xi) \\ P_1(\xi) \\ \vdots \\ P_{N-2}(\xi) \\ P_{N-1}(\xi) \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ P_N(\xi) \end{bmatrix}. \tag{51}$$

The nodes of the quadrature approximation $\{\xi_\alpha\}$, are the eigenvalues of the tridiagonal matrix appearing in the equation.
This matrix is often re-written in terms of an equivalent tridiagonal symmetric matrix!

Product-difference algorithm

WARWICK

In fact the matrix can be made symmetric (preserving the eigenvalues) by a diagonal similarity transformation to give a Jacobi matrix:

$$J = \begin{bmatrix} a_0 & \sqrt{b_1} & & & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & & & \\ & \sqrt{b_2} & a_2 & \sqrt{b_3} & & & \\ & & \sqrt{b_3} & a_3 & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & \ddots & a_{N-2} & \sqrt{b_{N-1}} \\ & & & & & \sqrt{b_{N-1}} & a_{N-1} \end{bmatrix} \tag{52}$$

This procedure transforms the ill-conditioned problem of finding the roots of a polynomial into the well-conditioned problem of finding the eigenvalues and eigenvectors of a tridiagonal symmetric matrix.

The N weights can then be calculated as $w_\alpha = M_0 \varphi_{\alpha 1}^2$ where $\varphi_{\alpha 1}$ is the first component of the α^{th} eigenvector φ_α of the Jacobi matrix.

Product-difference algorithm

WARWICK

1. Construct the matrix P with components $P_{\alpha,\beta}$:

$$P_{\alpha,\beta} = P_{1,\beta-1}P_{\alpha+1,\beta-2} - P_{1,\beta-2}P_{\alpha+1,\beta-1}$$
$$\beta \in 3,\ldots,2N+1 \text{ and } \alpha \in 1,\ldots,2N+2-j. \quad (53)$$

2. where the first row of the matrix is:

$$P_{\alpha,1} = \delta_{\alpha 1} \quad \alpha \in 1,\ldots,2N+1, \quad (54)$$

3. where $\delta_{\alpha 1}$ is the Kronecker delta and where the components in the second column of P are

$$P_{\alpha,2} = (-1)^{\alpha-1}M_{\alpha-1} \quad \alpha \in 1,\ldots,2N. \quad (55)$$

4. Calculate the coefficients of the continued fraction $\{\zeta_\alpha\}$:

$$\zeta_\alpha = \frac{P_{1,\alpha+1}}{P_{1,\alpha}P_{1,\alpha-1}} \quad \alpha \in 2,\ldots,2N. \quad (56)$$

Product-difference algorithm

WARWICK

1. The coefficients of the symmetric tridiagonal Jacobi matrix are then obtained from sums and products of ζ_α:

$$a_\alpha = \zeta_{2\alpha} + \zeta_{2\alpha-1} \quad \alpha \in 1, \ldots, N \tag{57}$$

$$b_\alpha = -\sqrt{\zeta_{2\alpha+1}\zeta_{2\alpha}} \quad \alpha \in 1, \ldots, N-1. \tag{58}$$

2. For example for $N = 2$ the P matrix is

$$\begin{bmatrix} 1 & M_0 & M_1 & M_0M_2 - (M_1)^2 & M_0\left(M_3M_1 - (M_2)^2\right) \\ 0 & -M_1 & -M_2 & -(M_0M_3 - M_2M_1) & \\ 0 & M_2 & M_3 & & \\ 0 & -M_3 & & & \\ 0 & & & & \end{bmatrix}. \tag{59}$$

Spatial discretization and moment corruption

The convexity of the function $\square\square(M_k)$ with respect to k can be easily verified by building a difference table of $\square\square(M_k)$.
Example: VALID SET; moment of a Gaussian distribution ($M_0 = 1, M_1 = 5, M_2 = 26, M_3 = 140, M_4 = 778, M_5 = 4450, M_6 = 26140, M_7 = 157400$)

k	$d_0 = \square\square(M_k)$	d_1	d_2	d_3
0	0	1.609	0.039	-0.0043
1	1.609	1.648	0.034	-0.0033
2	3.258	1.683	0.031	-0.0027
3	4.941	1.715	0.028	-0.0022
4	6.656	1.743	0.026	-0.0019
5	8.400	1.770	0.024	0
6	10.171	1.795	0	0
7	11.966	0	0	0

Spatial discretization and moment corruption

The convexity of the function $\square\square(M_k)$ with respect to k can be easily verified by building a difference table of $\square\square(M_k)$.
Example: INVALID SET; moment of a Gaussian distribution ($M_0 = 1, M_1 = 5,$ $M_2 = 25, M_3 = 140, M_4 = 778, M_5 = 4450, M_6 = 26140,$ $M_7 = 157400$)

k	$d_0 = \square\square(M_k)$	d_1	d_2	d_3
0	0	1.609	0	0.113
1	1.609	1.609	0.113	-0.121
2	3.218	1.722	-0.007	0.036
3	4.941	1.715	0.028	-0.002
4	6.656	1.743	0.026	-0.001
5	8.400	1.770	0.024	0
6	10.171	1.795	0	0
7	11.966	0	0	0

Spatial discretization and moment corruption

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- When using first-order upwind spatial discretization schemes and first-order explicit time discretization schemes the validity of the moment set should be preserved
- In all the other cases it is very easy to CORRUPT the moment set and it is anyway safe to have algorithms that DETECT CORRUPTION AND CORRECT invalid moment set
- If we transform the moment set so that d_2 is positive, we are almost sure that the moment set is valid
- But how positive?
- The moments of a log-normal distribution have the smallest d_3

$$n(\xi) = \frac{N_T}{\sigma\sqrt{2\pi}\xi} \exp\left(\frac{-(\ln(\xi) - \mu)^2}{2\sigma^2}\right), \tag{60}$$

$$M_k = N_T \exp\left(k\mu + \frac{k^2\sigma^2}{2}\right), \tag{61}$$

- The log-normal distribution is the smoothest distribution!

Spatial discretization and moment corruption

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CORRECTION ALGORITHM BY MCGRAW

1. Build the difference table and check if d_2 is negative
2. Identify the moment order k that causes the biggest change in d_3
3. Change the moment (by multiplying it for a constant) in order to MINIMIZE d_3
4. Go back to point 1

CORRECTION ALGORITHM BY WRIGHT

1. Build the difference table and check if d_2 is negative
2. Replace the moments with those of a log-normal distribution with

$$\mu = \frac{j}{ij - i^2} \ln\left(\frac{M_i}{M_0}\right) + \frac{i}{ij - j^2} \ln\left(\frac{M_j}{M_0}\right) \tag{62}$$

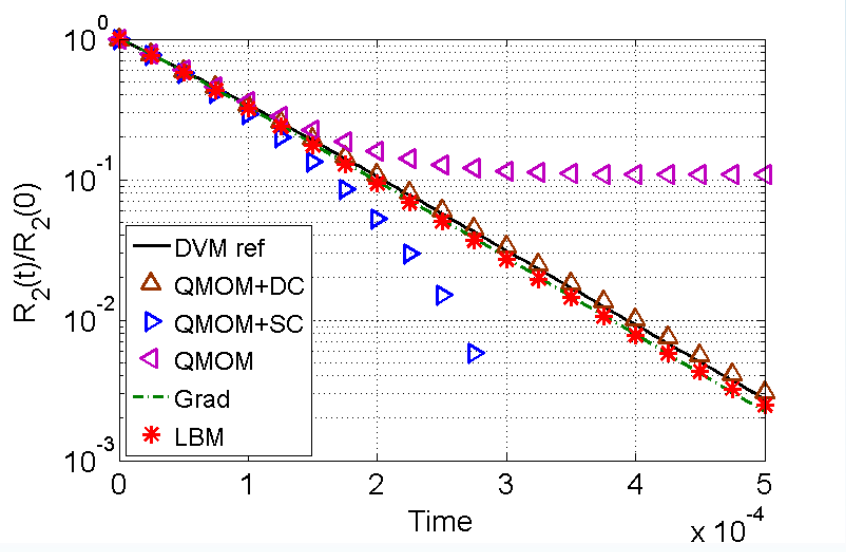
$$\sigma^2 = \frac{1}{1 - i/j}\left[\frac{2}{j^2} \ln\left(\frac{M_j}{M_0}\right) - \frac{2}{ij} \ln\left(\frac{M_i}{M_0}\right)\right] \tag{63}$$

QBMM approximation vs DVM, Grad, oLBM – 4

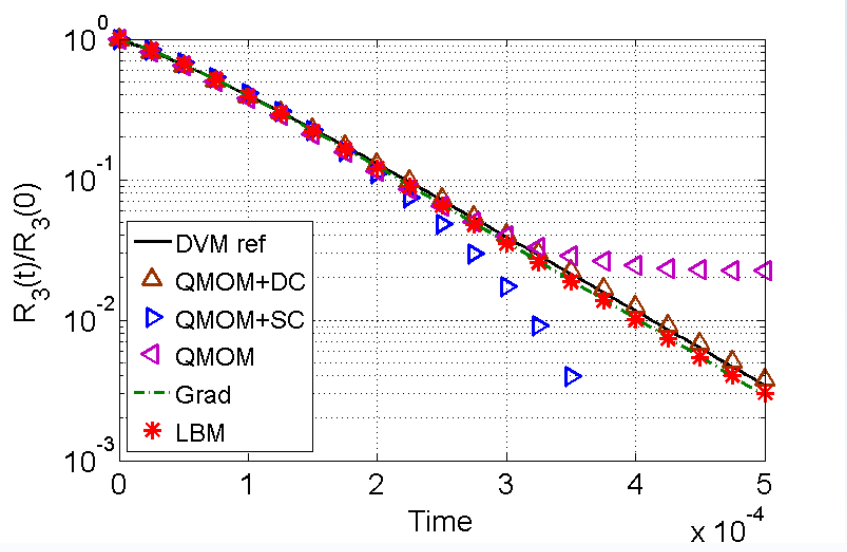
Homogeneous Isotropic Boltzmann Equation (HIBE)

$$M = 4$$

Normalized relaxation rate



2nd energy moment



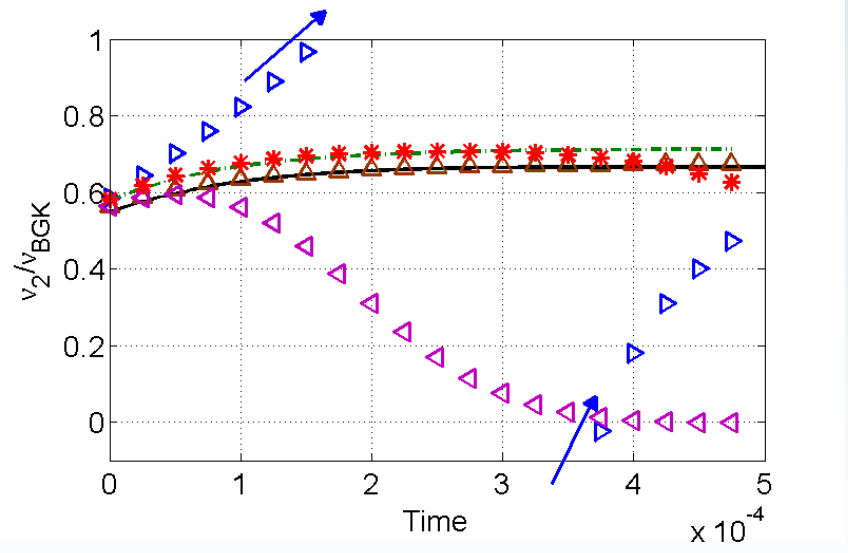
3rd energy moment

QMOM approximation vs DVM, Grad, oLBM – 5

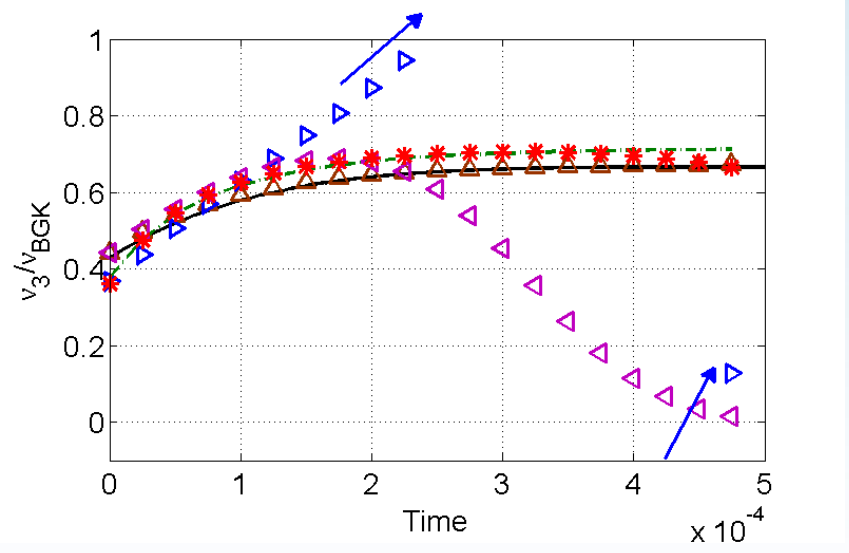
Homogeneous Isotropic Boltzmann Equation (HIBE)

$$M = 4$$

BGK-equivalent relaxation time $\nu_p(t) = \frac{d\Phi_p}{dt}\frac{1}{\Phi_p^{eq} - \Phi_p}$



2nd energy moment



3rd energy moment

Analytical equations for QBMM

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$$\frac{d\Phi_p}{dt} = \frac{\pi}{\sqrt{2}} \left(\sum_{i=1}^{M/2} \sum_{j=1}^{M/2} w_i w_j \Lambda^+_{ij,p} - \sum_{i=1}^{M/2} \sum_{j=1}^{M/2} w_i w_j \Lambda^-_{ij,p} \right)$$

$\delta_{ij} = \sqrt{E_j/E_i}$; $q_{ij} = q(x, y, E_i, E_j)$; $C^+_{ij,p} = C^+_p(x, y, E_i, E_j)$; $C^-_{i,p} = C^-_p(E_i)$; $\Lambda^+_{ij,p} = \int_{-1}^{+1} \int_{-1}^{+1} |q_{ij}| C^+_{ij,p} \, dx \, dy$; $\Lambda^-_{ij,p} = \int_{-1}^{+1} \int_{-1}^{+1} |q_{ij}| C^-_{i,p} \, dx \, dy$

$$\Lambda^+_{ij,p} = 2E_i^p \sqrt{E_+} \sum_{\alpha=0}^{p} \binom{p}{\alpha} \sum_{\beta=0}^{p-\alpha} \binom{p-\alpha}{\beta} (-1)^{\gamma_{ij}} E_i^{-\beta-\alpha} E_+^{\alpha} E_-^{\beta}$$

$$\left[\frac{2}{2\beta+1} \left(\frac{1 - r_{ij}^{2\alpha+2}}{2\alpha+2} + \frac{r_{ij}^{2\alpha+2}}{2\alpha+2\beta+3} \right) + \frac{1}{\beta+1} \left(\frac{r_{ij}^{2\alpha+2}}{2\alpha+1} - \frac{r_{ij}^{2\alpha+2}}{2\alpha+2\beta+3} \right) \right]$$

$$\Lambda^-_{ij,p} = 2E_i^p \sqrt{E_+} \left(1 + \frac{r_{ij}^2}{3} \right)$$

$$\gamma_{ij} = \begin{cases} \alpha & \text{if } E_i \geq E_j \\ \beta & \text{if } E_i < E_j \end{cases} \qquad E_+ = \square\square\square\left(E_i, E_j\right); \; E_- = \square\square\square\left(E_i, E_j\right); \; r_{ij} = \square\square\square\left(\sqrt{\frac{E_i}{E_j}}, \sqrt{\frac{E_j}{E_i}}\right)$$