On the implementation of moment transport equations in OpenFOAM to preserve conservation, boundedness and realizability

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Aim and motivation

- Description of industrial scale multiphase systems, in which at least one phase is dispersed
  - Elements of the dispersed phase are characterized by different velocities, size, temperature, composition ... (POLYDISPERSITY)
  - The evolution of polydisperse systems can be described through Population Balance Modeling (PBM)
  - PBM coupled with flow fields description given by Computational Fluid Dynamics (CFD) is able to provide a fully-predictive methodology
  - Quadrature Method of Moments (QMOM) or other Quadrature Based Moment Methods (QBMM) are efficient and robust approaches to solve the Population Balance Equation
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CFD & OpenFOAM

- CFD is a powerful tool used for the development and optimization of industrial equipments
- Method of Moments (MOM) implementation present in commercial codes does not consider the properties of the moments
- OpenFOAM is an open source CFD toolbox → a number of solvers is available to tackle different problems (e.g., chemical reactions, turbulence, multiphase flows)
- twoPhaseEulerFoam is a two-fluid Eulerian solver already present in the standard OpenFOAM distribution
- The implementation of new functionalities is extremely flexible, since the user has the freedom to customize every aspect of the solver
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Population balance model is based on the definition of a Number Density Function (NDF) → Particle Size Distribution, Bubble Size Distribution, Droplet Size Distribution ...

The evolution of the NDF can be predicted by solving a complex integro-differential equation called Population Balance Equation (PBE)

Among different numerical methods to solve the PBE, Methods of Moments (MOM) is a class of methods particularly suitable for solving problems characterized by significant spatial inhomogeneities

This method involves the solution of a small number of transport equation for the moments of the distribution

\[ M_k(x, t) = \int n(L; x, t) L^k \, dL \]
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Moments are mathematical objects that must satisfy the following properties:

- **realizability** → moments must represent a physical realization of the system → use of realizable discretization schemes. *

- **conservation** → in absence of source/sink terms, moments behave as conserved variables (passive scalar) → use of Finite Volume app.

- **boundedness** → moments are expression of physical quantities, bounded between physically reasonable values → use implementation proposed here.

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Transport equation for a generic order moment:

$$\frac{\partial M_k}{\partial t} + \nabla \cdot (U_d M_k) = S_k,$$  \hspace{1cm} (1)

where $U_d$ is not conservative ($\nabla \cdot U_d \neq 0$), boundedness of $M_k$ cannot be guaranteed.

It can be shown that in absence of mass transfer

$$\nabla \cdot (\alpha_d U_d + \alpha_c U_c) = \nabla \cdot \overline{U} = 0.$$  \hspace{1cm} (2)

Since $U_d = \overline{U} + \alpha_c U_{rel} = \overline{U} + (1 - \alpha_d) U_{rel}$ with $U_{rel} = U_d - U_c$ we can write:

$$\frac{\partial M_k}{\partial t} + \nabla \cdot (\overline{U} M_k) + \nabla \cdot ((1 - \alpha_d) M_k U_{rel}) = S_k$$  \hspace{1cm} (3)
Implementation details

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Test case description

- 2D geometry
- Incompressible two-fluid transient solver (twoPhaseEulerFoam)
- Gas-liquid bubble column (standard air-water)
- PBM implemented in OpenFOAM → QMOM with 3 nodes
- $k - \epsilon$ turbulence model for the liquid phase

It can be shown that

$$\alpha_d = \int k_V n(L) L^3 \, dL = k_V M_3$$

with $k_V = \pi/6$ for spherical bubbles
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Results
Not preserving boundedness implementation
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\[ M_3 = \frac{\alpha_1}{k_V} = \frac{6}{\pi} \approx 1.90986 \]
Results

Preserving boundedness implementation
Results
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\[ M_3 = \alpha_1 / k_V = 6 / \pi \approx 1.90986 \]
Preliminary results
Realizable higher order schemes
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First Order Upwind

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Preliminary results
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Realizable Second Order Upwind
The numerical implementation is crucial for preserving the properties of moment conservation, boundedness and realizability. Only if such properties are ensured the obtained solution is meaningful. Standard high order discretization schemes can not be used for moments because of moment corruption problem $\rightarrow$ realizable high order discretization schemes must be used.
Take-Home messages

- The numerical implementation is crucial for preserving the properties of moment conservation, boundedness and realizability.
- Only if such properties are ensured the obtained solution is meaningful.
- Standard high order discretization schemes can not be used for moments because of moment corruption problem $\rightarrow$ realizable high order discretization schemes must be used.
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THANKS FOR YOUR ATTENTION
Generic moment transport equation

\[ \frac{\partial M_{k,l}}{\partial t} + \frac{\partial}{\partial x} (U_b M_{k,l}) = S_{k,l} + \int_0^\infty k L^k G \text{d}L + \int_0^\infty l \dot{\phi}_b \phi_b \text{d}\phi_b, \]

\[ S_{k,l} = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N w_i w_j h_{i,j} \left[ (L_i^3 + L_j^3)^{k/3} (\phi_{b;i} + \phi_{b;j})^l \right. \]

\[ - L_i^k \phi_{b;i} - L_j^k \phi_{b;j} \] \left. + \sum_{i=1}^N w_i \beta_i [\dot{\bar{P}}^{(i)}_{k,l} - L_i^k \phi_{b;i}] \right. ,

\[ G_i = \frac{2kL M_w}{\rho_b} \left( \psi_c - \mathcal{H} \frac{\phi_{b;i}}{k V L_i^3} \right) , \]

\[ \dot{\phi}_{b;i} = \frac{6kL}{L_i} \left( \psi_c - \mathcal{H} \frac{\phi_{b;i}}{k V L_i^3} \right) . \]
CQMOM
Inversion algorithm details

1

\[ \begin{pmatrix} M_{0,0} \\ M_{1,0} \\ \vdots \\ M_{2N_1-2,0} \\ M_{2N_1-1,0} \end{pmatrix} \rightarrow \text{PD/Wheeler} \rightarrow \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_{N_1-1} \\ w_{N_1} \end{pmatrix} \]

2

\[ \begin{pmatrix} 1 & \cdots & 1 \\ L_1 & \cdots & L_{N_1} \\ \vdots & \vdots & \vdots \\ L_{N_1-1} & \cdots & L_{N_1} \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_{N_1} \end{pmatrix} = \begin{pmatrix} C_1(L_1) \\ C_1(L_2) \\ \vdots \\ C_1(L_{N_1-1}) \\ C_1(L_{N_1}) \end{pmatrix} \]

3

\[ \begin{pmatrix} 1 \\ C_1(L_i) \\ \vdots \\ C_{2N_2-2}(L_i) \\ C_{2N_2-1}(L_i) \end{pmatrix} \rightarrow \text{PD/Wheeler} \rightarrow \begin{pmatrix} w_{i,1} \\ w_{i,2} \\ \vdots \\ w_{i,N_2-1} \\ w_{i,N_2} \end{pmatrix} \begin{pmatrix} \phi_{b;i,1} \\ \phi_{b;i,2} \\ \vdots \\ \phi_{b;i,N_2-1} \\ \phi_{b;i,N_2} \end{pmatrix} \]
Schematic representation of a single time step of the segregated OpenFOAM solver, coupled with QMOM