OpenQBMM - A Next-Generation Open-Source Computational Fluid Dynamic Code for Polydisperse Multiphase Flows in Science and Engineering

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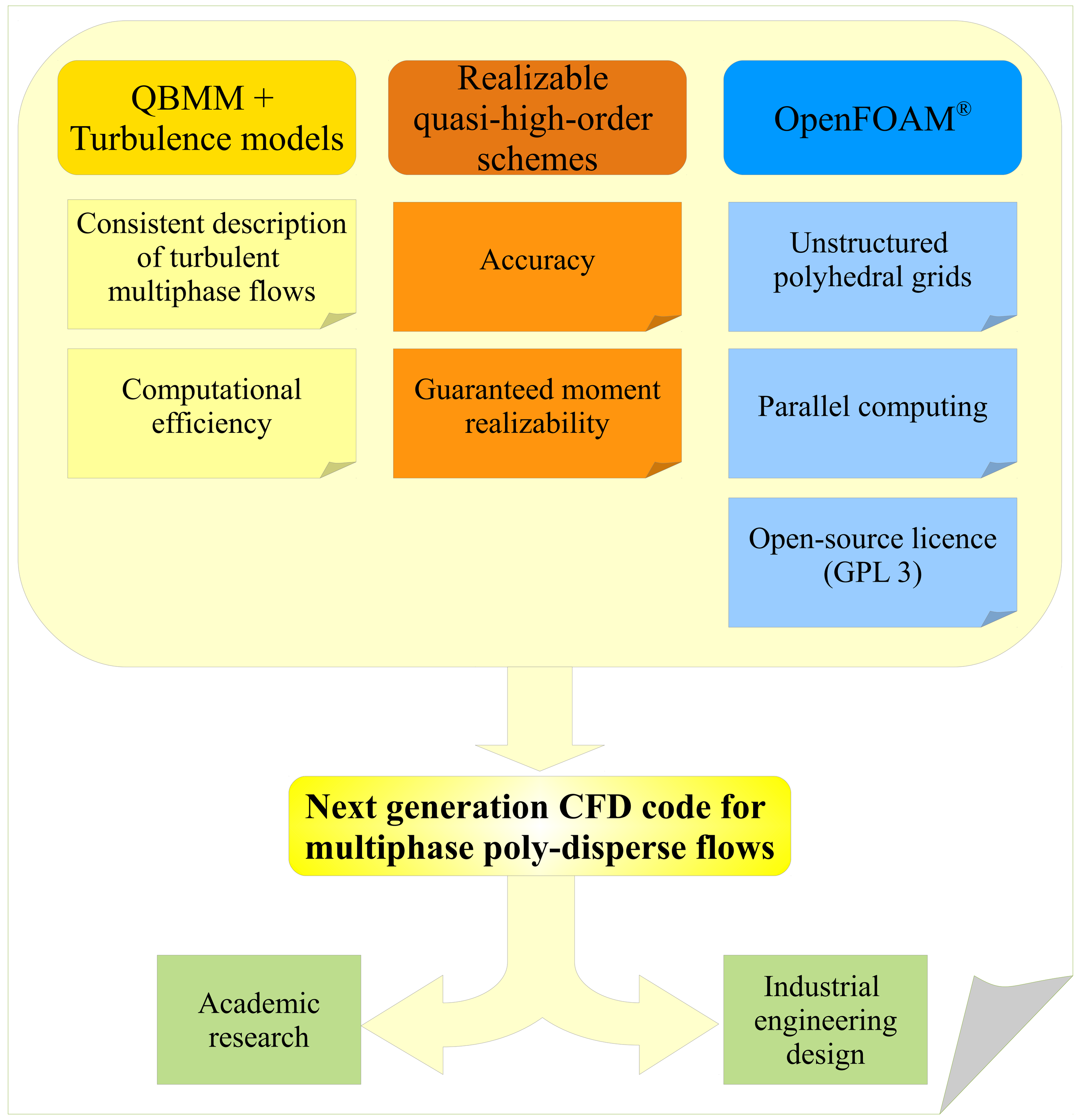
Contribution

OpenQBMM is an open-source suite of codes, based on OpenFOAM® for multiphase reacting flows. Target applications are:

- Turbulent reacting flows
- Gas-liquid flows
- Gas-solid flows

The computational framework

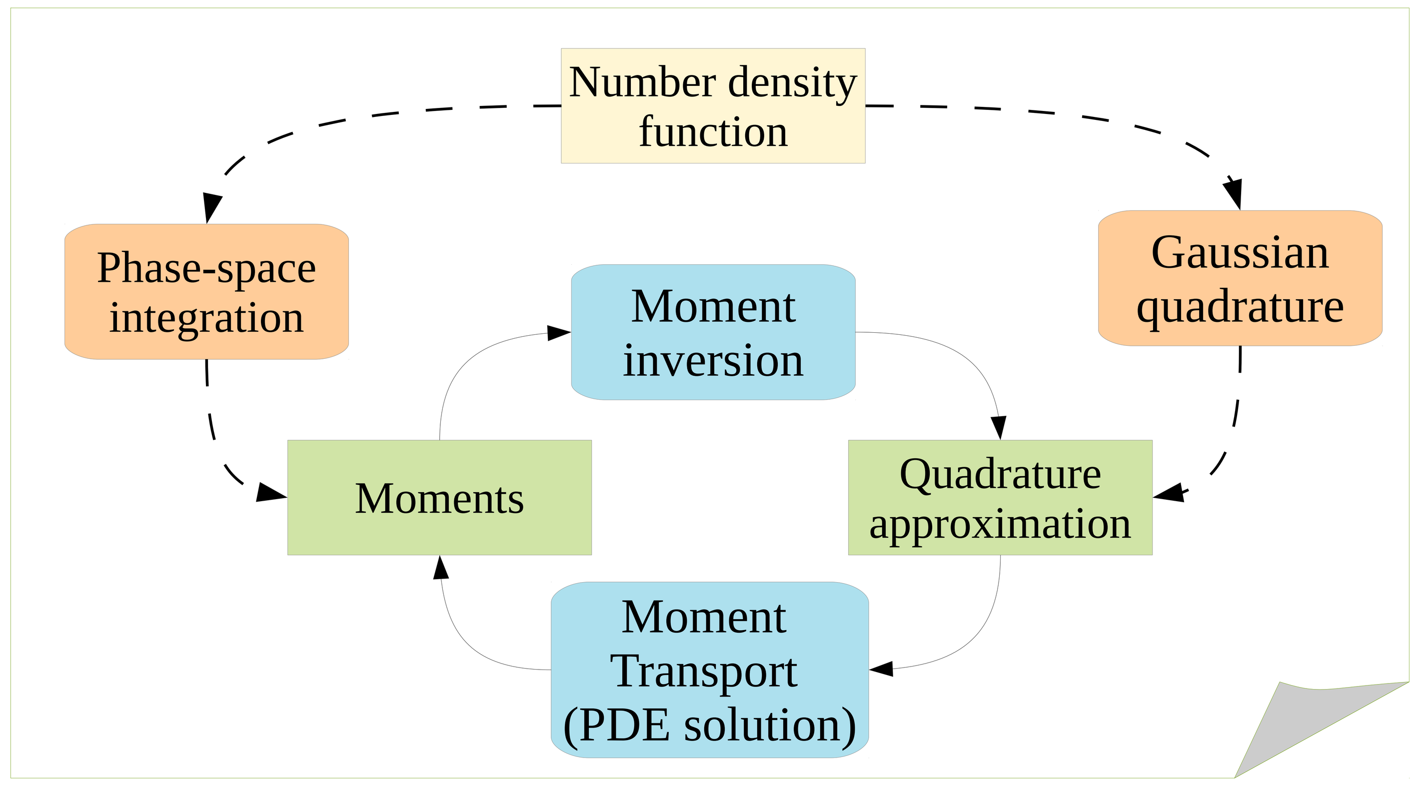
The computational framework that will be implemented relies on quadrature-based moment methods (QBMM) and high-order realizable numerical schemes to guarantee the moment realizability accuracy of the results.



The implementation will leverage the infrastructure offered by OpenFOAM, allowing complex geometries to be represented through unstructured grids. Parallel computation is automatically enabled via MPI, and will be extended to GPU's for key components. This will give origin to a set of tools to perform both academic research and industrial engineering design.

Quadrature-based moment methods

Multiphase reacting flows can be described by solving a generalized population balance equation, whose unknown is the number density function (NDF). To reduce the computational cost, transport equations are obtained for the moments of the NDF. These equations are closed using Gaussian quadrature formulae, which allow the calculation of the source terms in the moment transport equations.



QBMM allow the NDF to be reconstructed either with a weighted sum of Dirac delta functions or of non-negative kernel density functions, in case a continuous form of the approximate NDF is desired for accuracy.

The solver suite

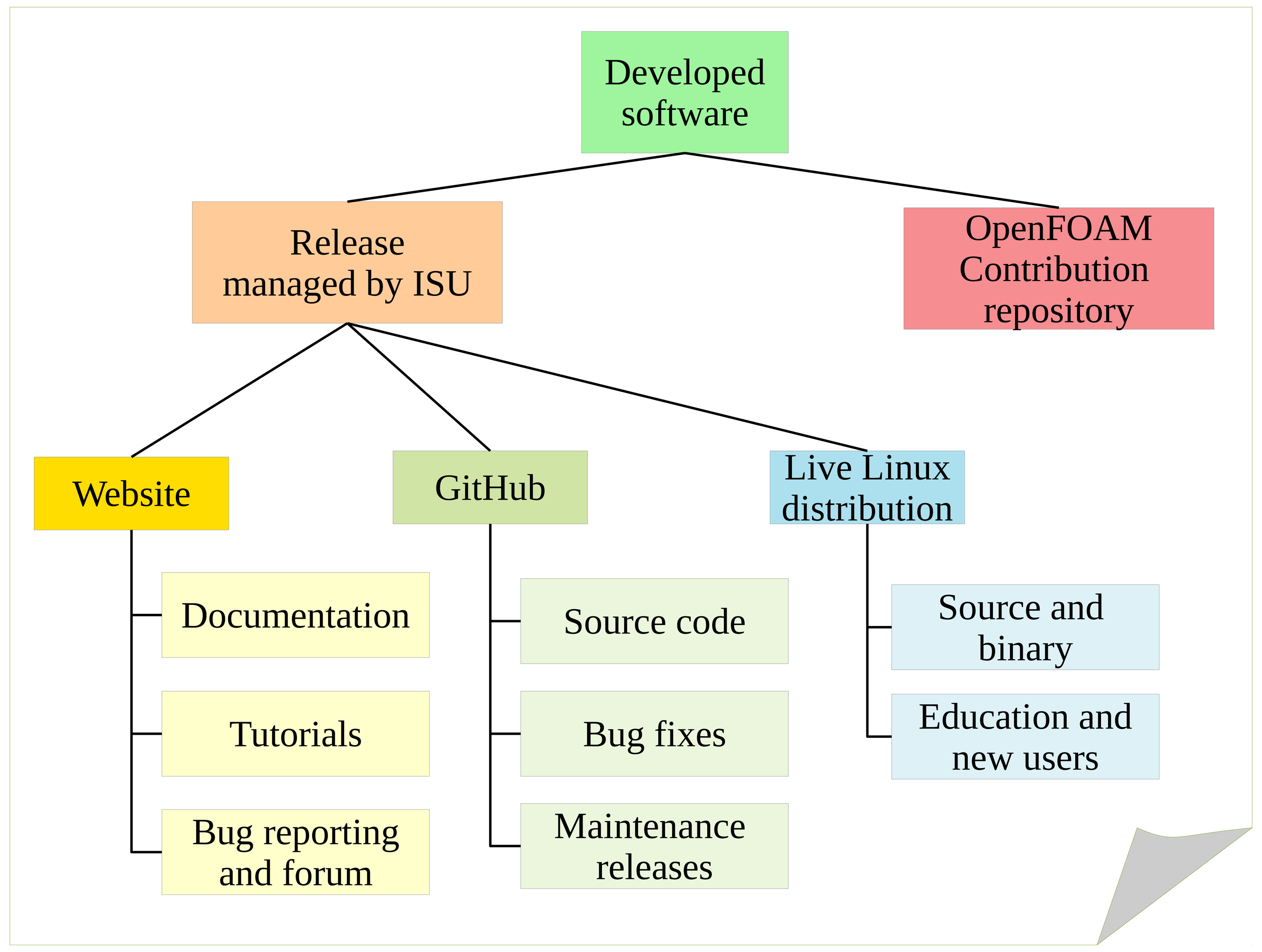
Three solvers will be developed as example applications of the QBMM framework:

- A PBE with advection and size-dependent diffusion, in the limit of small Stokes number, which is suitable to simulate flows at low particle concentration, with particles of small size, incapable of significantly affecting the fluid motion. A typical example application is the formation of nano-particles and aerosols for pharmaceutical uses
- A GPBE with size-dependent advection velocity with small, but finite, Stokes number, typical of bubble column reactors, widely used in the energy industry
- A GPBE with moderate to large Stokes number, capable of simulating turbulent gas-particle flows in risers of circulating fluidized beds

Each solver will be accompanied by a set of example applications and validation results.

Software distribution and community

The developed software package will be distributed under the GNU GPL 3 license, with documentation, tutorials, a bug-reporting system and a discussion forum.



The code will be freely available on GitHub, and external contributions will be accepted in a separate repository, and eventually merged into the main code. A live Linux distribution will be provided for distribution and educational purposes.

Contacts

OpenQBMM can be found here:

- Website: `www.openqbmm.org` – E-mail: openqbmm@outlook.com
- GitHub: `https://github.com/OpenQBMM`
- Follow us on Twitter: @OpenQBMM

References

[1] D. L. Marchisio and R. O. Fox, *Computational Models for Polydisperse Particulate and Multiphase Systems*, Cambridge Series in Chemical Engineering, Cambridge University Press, 2013.

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