Super droplets in OpenFOAM

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OpenFOAM - overview

OpenFOAM

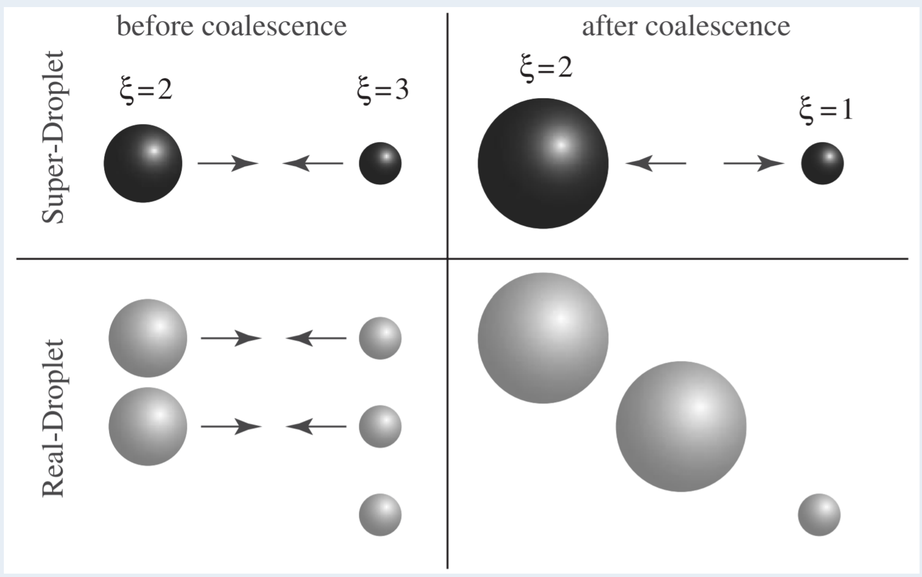
- Computational Fluid Dynamics Toolbox
- Built up from C++ modules (code reuse across applications)
- Object-oriented code design
- Parallelism (MPI) at the core of the design
- Free and open source
- Established community

Short history:

- 1993 - started as FOAM (Imperial College, London)
- 2004 - became open source as OpenFOAM 1.0
- 2018 - release latest version: OpenFOAM 6
- Nowadays - used both in academia and industry

Super Droplet Method (Shima et al. 2009)

- Particle-based collision-coalescence model
- Introduced in the context of cloud modelling
- Stochastic approach (as opposed to Smoluchowski eq.)
- Notion of super droplet (SD): a multiplicity of simulated particles of equal attributes (size, composition, location, ...)
- O(n) computational cost where n is the number of super-droplets



Schematic view of the coalescence of super-droplets (Fig. 1 from Shima et al. 2009)

$$P_{ij} = max(\xi_i, \xi_j) \cdot \underbrace{\pi (r_i + r_j)^2 \cdot |v_i - v_j|}_{\text{coalescence kernel}} \cdot \frac{\Delta t}{\Delta V} \cdot \frac{n \cdot (n-1)}{2} / \left[\frac{n}{2}\right]$$

P_{ij} - probability of collision of SDs i, j in ΔV and in $(t, t + \Delta t)$
ξ_i, ξ_j - multiplicities of SDs i, j (number of droplets represented by a SD)
r_i, r_j - radii of super droplets i, j
v_i, v_j - velocities of super droplets i, j
n - total number of super droplets in the cell

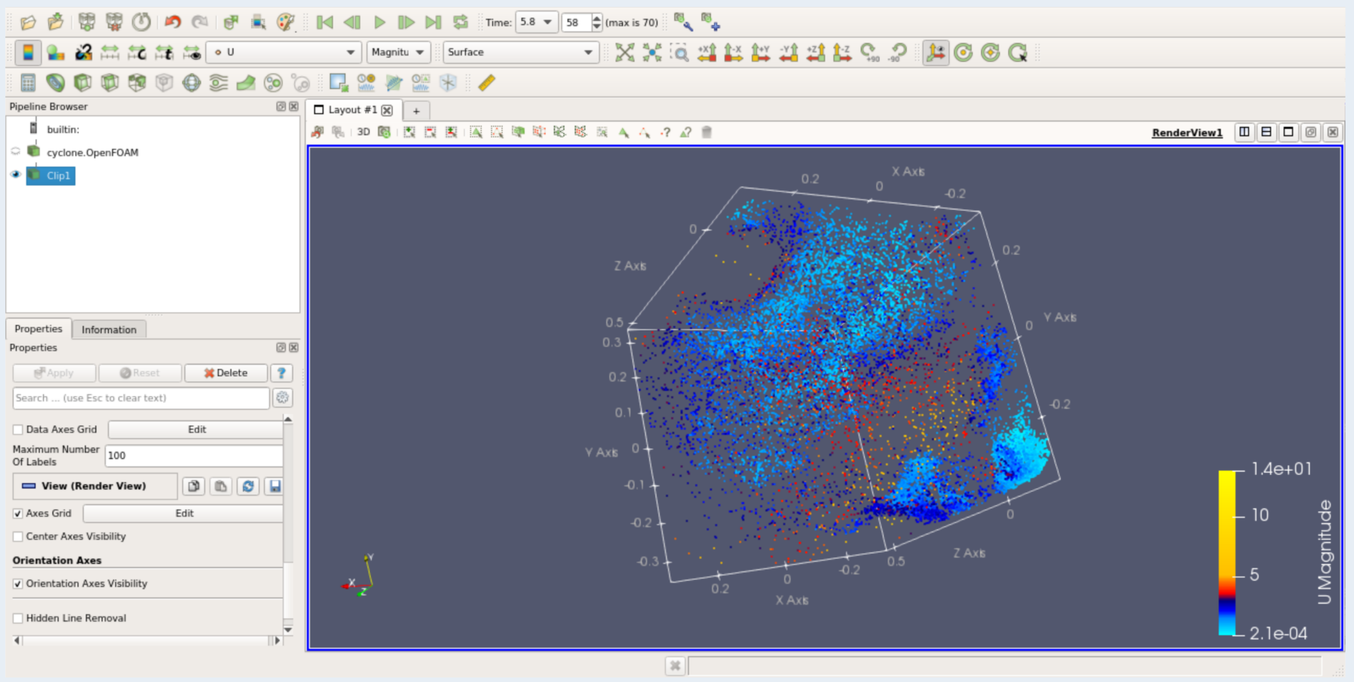
Open questions

1. Suitable test cases (from cloud physics and other domains)?
2. Test automation mechanisms?
3. Is it feasible to develop OpenFOAM-based Lagrangian Cloud Model?

OpenFOAM - selected components relevant to cloud modelling

- Large Eddy Simulation (LES) dynamics
- Multi-Phase Particle-in-Cell (MPPIC) Eulerian-Lagrangian coupling
- Particle collision representation using the O'Rourke method
- Radiative transfer models

ParaFOAM (ParaView)



ParaView-based tool bundled with OpenFOAM - useful for visualisation of the input/ouput of the simulations. Above: sample output visualisation from a simulation with Lagrangian super-particles.

Project goals (MSc thesis concept)

1. Implement Super Droplet Method in OpenFOAM (as an alternative to existing O'Rourke method)
2. Document scaleability characteristics in multi-core and multi-node setups
3. Explore possibilities for representation of particle breakup process

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