Advection-diffusion with sharp interfaces, coupled with a fluid

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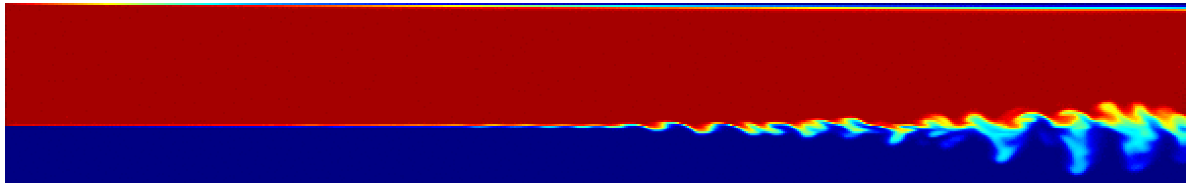
Introduction

- Lattice Boltzmann Method (+ HPC): significant achievements in CFD → modelling complex flows (multiphase fluids, thermal and buoyancy effects…)

- Advection-diffusion (AD) = common problem to simulate transport of quantities such as temperature, concentration of species…

Rayleigh-Bénard instability
N=100; Ra=1E+08; Pr=1



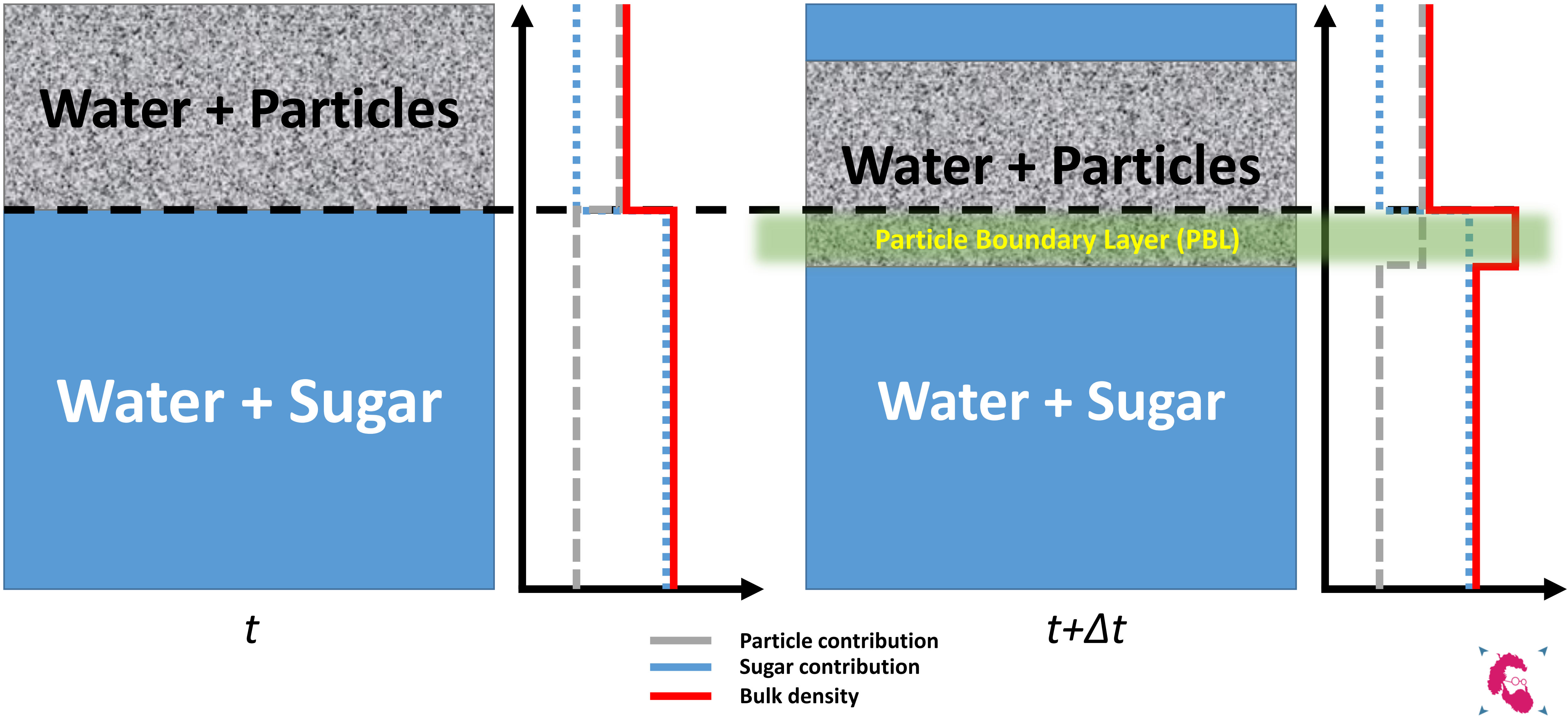
Lateral transport of volcanic ash in air

Introduction

- Advection-dominated problems = challenge for mesh-based schemes
- An example : transport of particles (modelled by a continuum field under some assumptions) with very low diffusivity.
- Interesting in order to avoid simulating individually very large number of particles
- If we add on top some sharp interfaces ➔ problems related to numerical diffusion, dispersion…

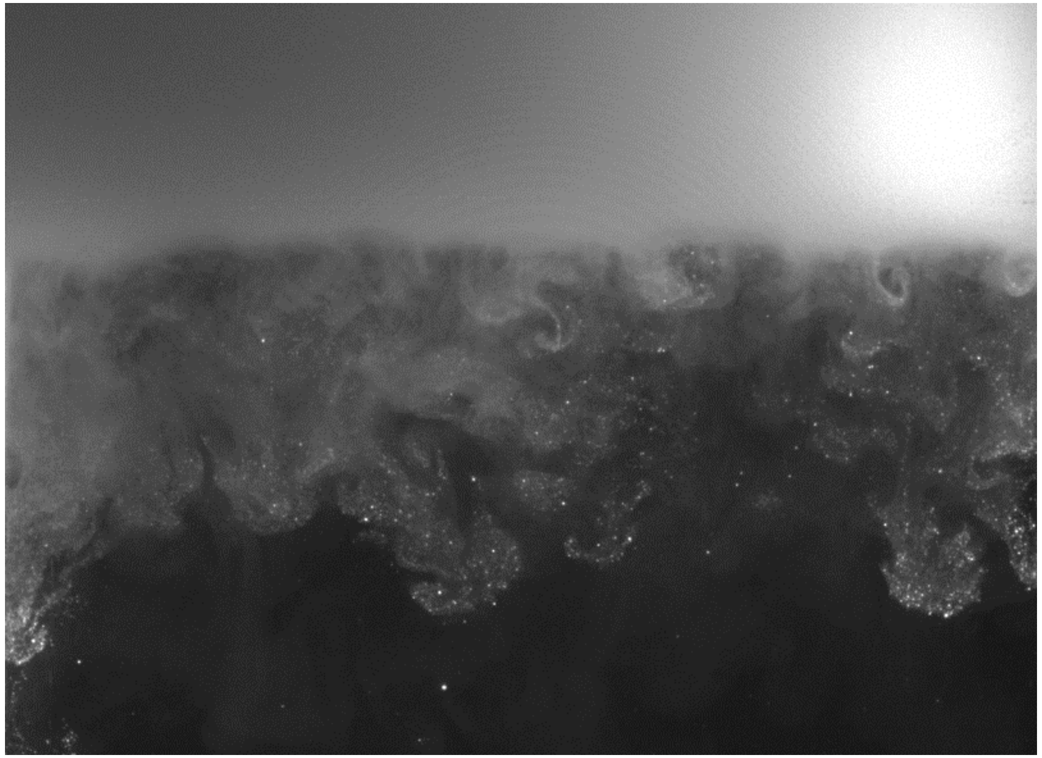
Coupled system

- <u>Case study</u>: A settling-driven Rayleigh-Taylor problem



Coupled system

- Unstable PBL collapses → downward moving fingers



Laboratory experiments on settling-driven
Raleigh-Taylor (Credits: Allan FRIES)

Coupled system - Governing equations

- How to model this ?

➔Three-way coupling between fluid, sugar and particles.

  - Fluid (momentum): $\frac{\partial \vec{u}_f}{\partial t} + (\vec{u}_f.\vec{\nabla})\vec{u}_f = -\frac{1}{\rho_0}\vec{\nabla}p + \nu\nabla^2\vec{u}_f + \left[\left(\frac{\rho_p-\rho_0}{\rho_0}\right)\emptyset + \left(\frac{\rho(S)}{\rho_0} - 1\right)(1-\emptyset)\right]\vec{g}$

  - Particles : $\frac{\partial \emptyset}{\partial t} + \vec{\nabla}.\left[\emptyset\left(\vec{u}_f - V_s(S)\vec{e_z}\right)\right] = D_c\nabla^2\emptyset$

  - Sugar : $\frac{\partial \rho}{\partial t} + \vec{u}_f.\overrightarrow{\nabla\rho} = D_S\nabla^2\rho$ *(assuming $\rho = \rho_0(1+\alpha S)$)*

- Assumptions to model particles as a continuum:
  - Small particles and large number
  - Drag force in equilibrium with gravitational force (Boussinesq)

- Particles have very small diffusivity ➔ Convection-dominated problem !

Coupled system - Governing equations

How to solve the advection-diffusion equations ?

Numerical schemes for Advection-Diffusion

1. <u>LBM for the Advection-Diffusion</u>

- Similar to Navier-Stokes equations (which can be seen as the AD of the momentum density vector $\rho\vec{u}$)

- For instance the BGK model, the relaxation time in the LB equation is given by:

$$\tau = \frac{D}{c_s^2} + \frac{\delta t}{2}$$

- All dynamics related to AD using LBM are in `palabos\src\complexDynamics\advectionDiffusionDynamics.h`

Numerical schemes for Advection-Diffusion

2. Upwind Finite-Difference 1st order:

- Adaptive scheme which takes in account the velocity direction in order to discretize (by a Taylor expansion) the convective term

$$u\frac{\partial a}{\partial x}$$

  - If $u > 0$ we use the backward difference

$$\left(\frac{\partial a}{\partial x}\right)_B \approx \frac{a_i^n - a_{i-1}^n}{\delta x}$$

  - If $u < 0$ we use the forward difference

$$\left(\frac{\partial a}{\partial x}\right)_F \approx \frac{a_{i+1}^n - a_i^n}{\delta x}$$

Numerical schemes for Advection-Diffusion

3. <u>Upwind Finite-Difference 2nd order:</u>

- If $u > 0$ we use the backward difference

$$\left(\frac{\partial a}{\partial x}\right)_B \approx \frac{3a_i^n - 4a_{i-1}^n + a_{i-2}^n}{2\delta x}$$

- If $u < 0$ we use the forward difference

$$\left(\frac{\partial a}{\partial x}\right)_F \approx \frac{-a_{i+2}^n + 4a_{i+1}^n - 3a_i^n}{2\delta x}$$

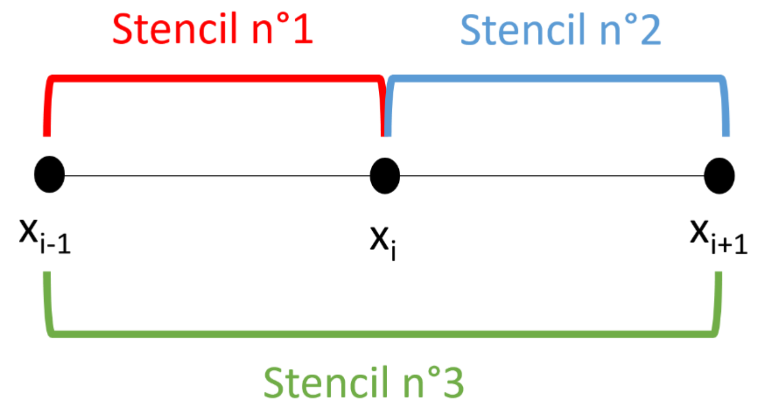
- Note that here we need 2 neighbours, which is important when initializing the scalar field associated (envelope)

Numerical schemes for Advection-Diffusion

4. WENO 3rd order

- Allows to solve hyperbolic partial differential equations of the form $\frac{\partial \emptyset}{\partial t} + \frac{\partial h}{\partial x} = 0$ where, in our case, the flux $h(\emptyset) = u\emptyset$ (Jiang and Shu, 1996; Liu et al. 1994)
- Ensures the suppression of spurious oscillations around discontinuities. Third order accurate in smooth regions and second order near discontinuities.
- Principle: build a convex combination of interpolants for the flux at given points of the domain, using two adjacent stencils of two points each
- Discretisation of the convective term:

$$\frac{\partial h}{\partial x} = \frac{h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}}}{\delta x}$$



- $h_{i+\frac{1}{2}}$ is the flux at the half node location $x_{i+\frac{1}{2}}$.
- 3 ways to approximate $h_{i+\frac{1}{2}}$:
  - $h^{(1)}_{i+\frac{1}{2}}$: interpolation with polynomials of degree 1 in Stencil 1 (second order accurate)
  - $h^{(2)}_{i+\frac{1}{2}}$: interpolation with polynomials of degree 1 in Stencil 2 (second order accurate)
  - $h^{(3)}_{i+\frac{1}{2}}$: interpolation with polynomials of degree 2 in Stencil 3 (third order accurate)

4. WENO 3rd order

- If h is smooth in the Stencil 3, we can write $h^{(3)}_{i+\frac{1}{2}}$ as a linear combination of the two second order approximations:

$$h^{(3)}_{i+\frac{1}{2}} = \gamma_1 h^{(1)}_{i+\frac{1}{2}} + \gamma_2 h^{(2)}_{i+\frac{1}{2}}$$

where $\gamma_1 = 3/4$ and $\gamma_2 = 1/4$

- What if there is a discontinuity in one of the stencils ?

The linear coefficients are replaced by « smoothness indicators » and we have:

$$h_{i+\frac{1}{2}} = \omega_1 h^{(1)}_{i+\frac{1}{2}} + \omega_2 h^{(2)}_{i+\frac{1}{2}}$$

If h is smooth in all the stencils, $\omega_i \to \gamma_i$ and ensures a third-order accuracy. Conversely, the presence of any discontinuity in the *i-th* stencil means $\omega_i \to 0$, decreasing the accuracy to second-order.

Numerical schemes for Advection-Diffusion

What about the time discretization ?

- For the 1st (and higher) order finite difference, we use the Euler explicit discretization for the time.

- For the WENO scheme (3rd order), to ensure a Total Variation Diminishing (TVD) property, we perform a 3rd order Runge-Kutta procedure for the time discretization.

Coupling in Palabos

- Let’s model the fluid motion using the LBM. Examples of dynamics taking in account a force term available in Palabos:
  - `NaiveExternalForceBGKdynamics`, `GuoExternalForceBGKdynamics`, `GuoExternalForceConsistentSmagorinskyCompleteRegularizedBGKdynamics`…

- Two “levels” of coupling:
  - Introduce the fluid velocity field in the convective term of the advection-diffusion
  - Implement the buoyant force term (which depends on the particle volume fraction and the sugar concentration)

Coupling in Palabos (Velocity)

```cpp
template< typename T, template<typename U1> class FluidDescriptor, template<typename U2> class VolfracDescriptor>
void VelocityCouplingProcessor2D<T,FluidDescriptor,VolfracDescriptor>::process (
        Box2D domain,
        BlockLattice2D<T,FluidDescriptor>& fluid,
        BlockLattice2D<T,VolfracDescriptor>& VolFrac )
{
    enum {velOffset   = VolfracDescriptor<T>::ExternalField::velocityBeginsAt,};
    Dot2D offset = computeRelativeDisplacement(fluid, VolFrac);
    for (plint iX=domain.x0; iX<=domain.x1; ++iX){
        for (plint iY=domain.y0; iY<=domain.y1; ++iY){
            T *u = VolFrac.get(iX+offset.x,iY+offset.y).getExternal(velOffset);
            Array<T,FluidDescriptor<T>::d> vel, vel_tot;
            fluid.get(iX,iY).computeVelocity(vel);
            vel_tot = vel + vsed;
            vel_tot.to_cArray(u);
        }
    }
}
```

Coupling in Palabos (Force term)

```
template< typename T, template<typename U> class FluidDescriptor >
void ForceTermProcessor2D<T,FluidDescriptor>::processGenericBlocks (
        Box2D domain, std::vector<AtomicBlock2D*> fields )
{
    typedef FluidDescriptor<T> D;
    enum {
        forceOffset = FluidDescriptor<T>::ExternalField::forceBeginsAt
    };
    PLB_PRECONDITION(fields.size()==3);
    BlockLattice2D<T, FluidDescriptor>* fluid = dynamic_cast<BlockLattice2D<T, FluidDescriptor>*>(fields[0]);
    ScalarField2D<T>* volfracfield = dynamic_cast<ScalarField2D<T>*>(fields[1]);
    ScalarField2D<T>* densityfield = dynamic_cast<ScalarField2D<T>*>(fields[2]);
    Dot2D offset1 = computeRelativeDisplacement(*fluid, *volfracfield);
    Dot2D offset2 = computeRelativeDisplacement(*fluid, *densityfield);

    for (plint iX=domain.x0; iX<=domain.x1; ++iX)
    {
        for (plint iY=domain.y0; iY<=domain.y1; ++iY)
        {
            T *force = fluid->get(iX,iY).getExternal(forceOffset);
            for (pluint iD = 0; iD < D::d; ++iD)
            {
                force[iD] = /* Implement the force term here */;
            }
        }
    }
}
```

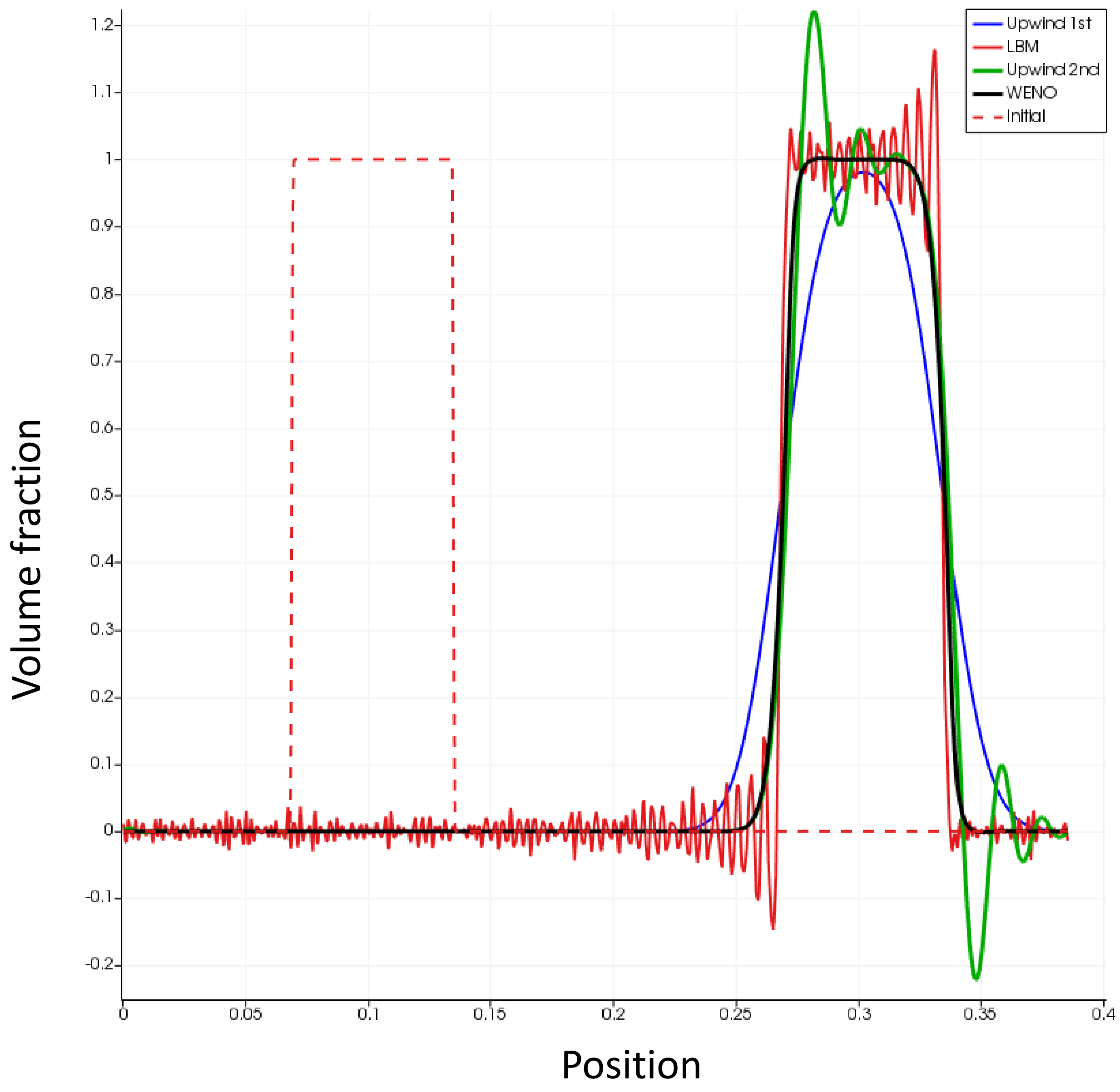
Application to problems with sharp interfaces

- Reminder for the LBM-BGK: $\tau = \frac{D}{c_s^2} + \frac{\delta t}{2}$

For very low diffusivity D, the scheme tends toward the stability limit and some spurious oscillations appear in the domain.

- Godunov theorem: *"Linear numerical schemes for solving partial differential equations (PDE's), having the property of not generating new extrema (monotone scheme), can be at most first-order accurate"*
- The upwind 1st order = stable but significant numerical diffusion (cf. Taylor expansion, the error term is $\sim u \frac{\delta x}{2} \frac{\partial^2}{\partial x^2}$)
- The second order: less numerical diffusion but introduces dispersion around interfaces (Godunov theorem !).
- <u>The 3rd order WENO is stable, and provides reduced numerical diffusion</u> (second-order accurate next to discontinuities). Possible to get higher order (e.g. WENO 5th order) but also higher computational cost.

Application to problems with sharp interfaces

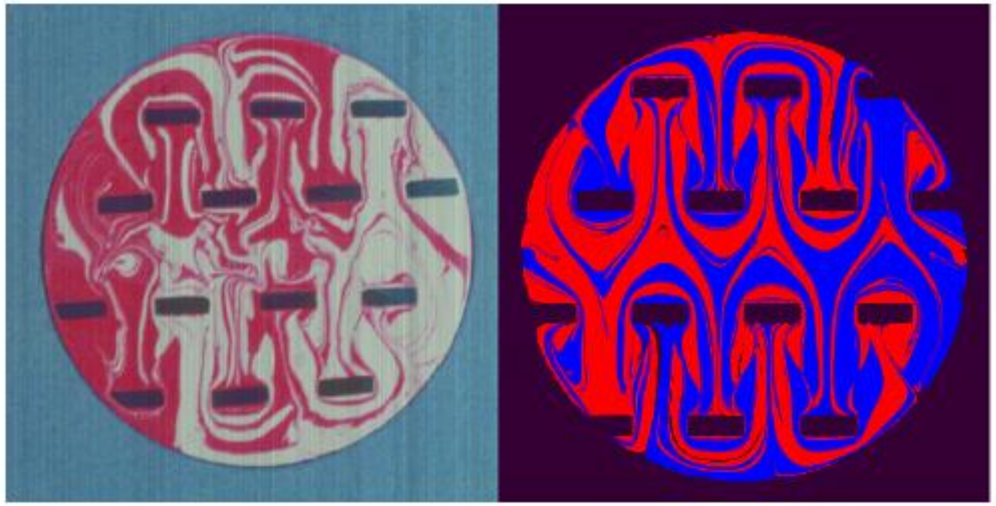


Conclusions

- Advection-diffusion possible using a full LBM scheme
- Capability to get hybrid models by coupling the LBM with finite-difference schemes ➔ more stable (at least when D<<1)
- The upwind schemes provide a stables model and are accurate for non convection-dominated problems and without sharp interfaces.
- The WENO procedure is interesting in order to model those problems, keeping the ease of implementation on uniform meshes.

Conclusions

- Particle-based approach: we don't solve any advection-diffusion equation.
- Injection of particle tracers in very large number in order to accurately follow the interface between different inviscid phases



J. Latt, D. Kontaxakis, L. Chatagny, F. Muggli, and B. Chopard, **Hybrid Lattice Boltzmann Method for the Simulation of Blending Process in Static Mixers**, *International Journal of Modern Physics C*, vol. 24, no. 12, p. 1340009, 2013

Exercises

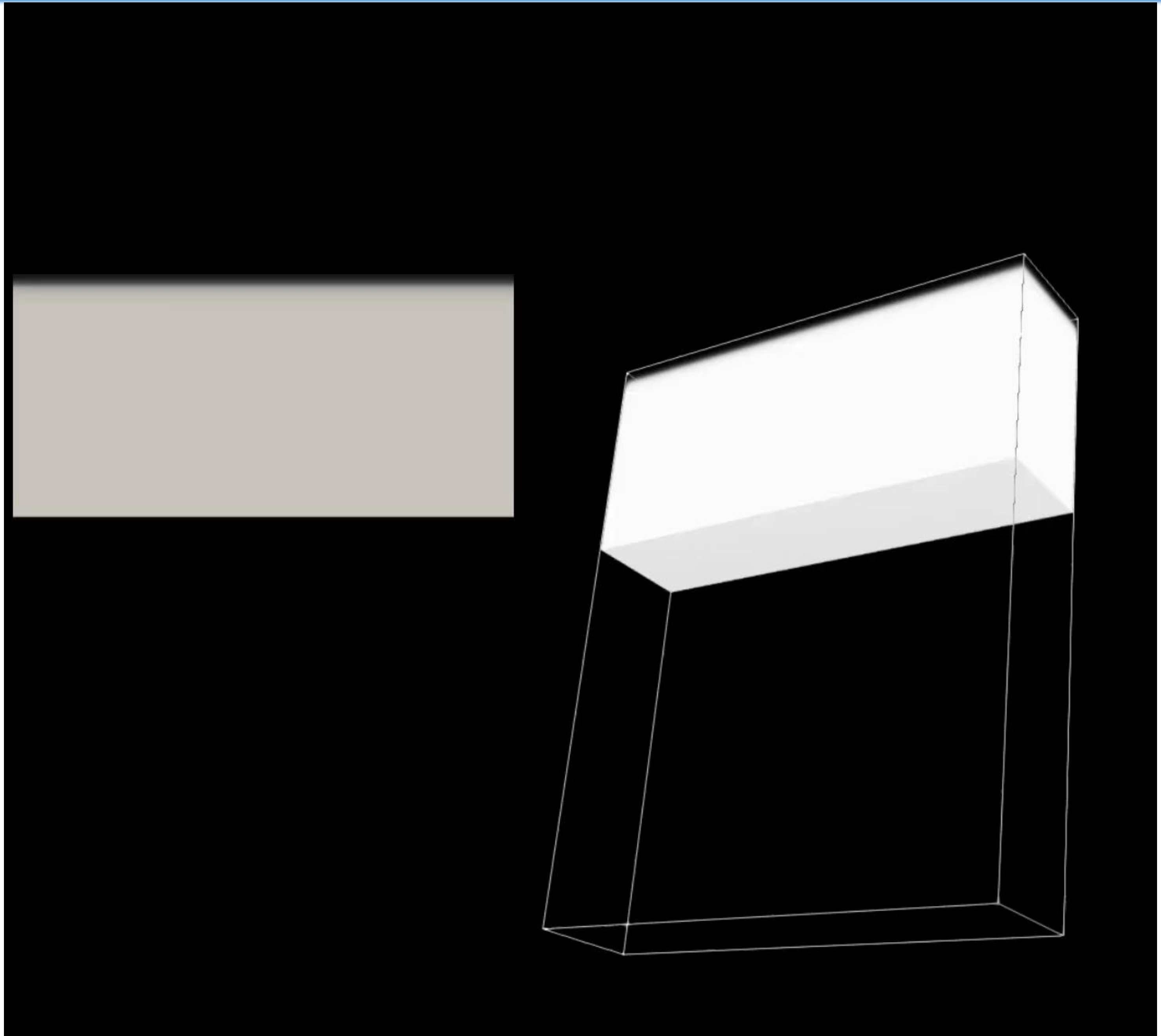
- Exercise 1:
  - Familiarize with the different Finite-difference schemes and see how they can be implemented in *Palabos.*
  - Compare them in order to highlights the main differences.
  - Check how the velocity coupling is implemented.

- Exercise 2:
  - More complex problem simulating our case study in 2D
  - Check the force term coupling and try to implement it:

$$\vec{F} = \left[\left(\frac{\rho_p - \rho_0}{\rho_0}\right)\emptyset + \left(\frac{\rho}{\rho_0} - 1\right)(1 - \emptyset)\right]\vec{g}$$

  - Run the simulation in order to observe the growing instability at the interface

Application to problems with sharp interfaces



THANK YOU !
QUESTIONS ?