Supporting Information

Description of confined nanoflow transport considering the effects of capillary condensation and heat transfer by means of a two-phase lattice Boltzmann model

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I. INVESTIGATION OF ANISOTROPY IN RADIALLY SYMMETRIC FLOW FILED

To address the imperfections observed in the velocity field of the droplet evaporation as the validation case, see section III B and Fig. 4, we (i) increased the size of the computational domain to move the boundary conditions away from the droplet and (ii) have introduced a new discretization scheme for the first order space derivative and Laplacian known as the isotropic central scheme with second-order accuracy for the discretization of energy equation.

A. Anisotropy investigation in a larger simulation box

The computational domain was made three times larger in the linear dimension, a box of 450×450 instead of 150×150 was used. Fig. 1 displays the anisotropy observed in simulations using a larger box while keeping the droplet size the same. This figure clearly shows that the anisotropy is especially noticeable around the droplet during evaporation.

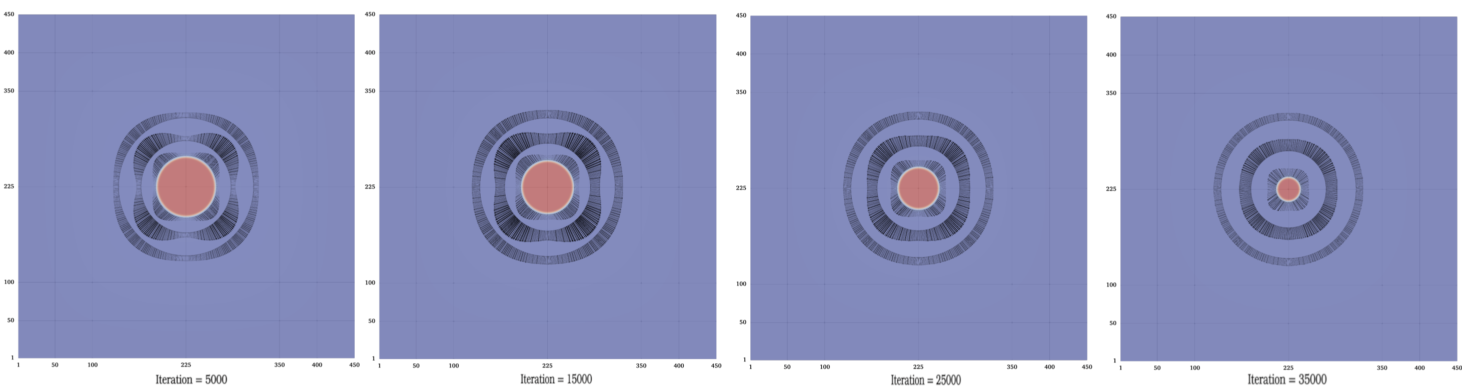

FIG. 1: Visualization of a droplet evaporating at constant pressure across different iterations. Velocity vectors are shown along circles centered on the droplet.

B. Isotropic scheme discretization to improved isotropy

A new discretization scheme for the space derivatives and Laplacian in the energy equation was implemented. The new scheme employs an isotropic central difference method with second-order accuracy. Below are the formulas used for 2D Simulation [1]:

First-order Space Derivatives:

$$\frac{\partial \phi}{\partial x} \approx \frac{1}{3}[\phi(i+1,j) - \phi(i-1,j)] + \frac{1}{12}[\phi(i+1,j+1) - \phi(i-1,j+1) + \phi(i+1,j-1) - \phi(i-1,j-1)] \qquad (1)$$

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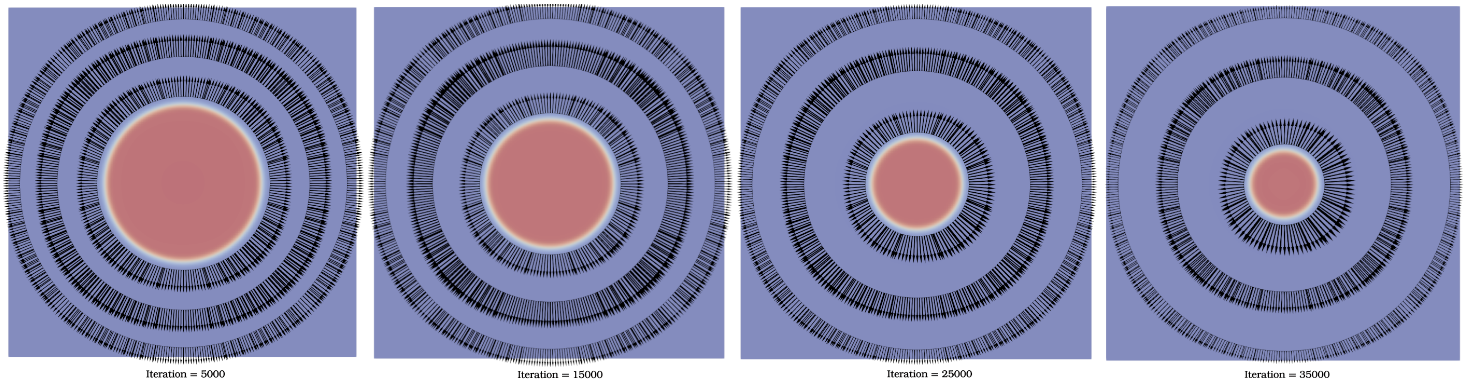

FIG. 2: Visualization of a droplet evaporating at constant pressure for different iterations. Velocity vectors are shown along circles centered on the droplet.

$$\frac{\partial \phi}{\partial y} \approx \frac{1}{3}[\phi(i,j+1) - \phi(i,j-1)] + \frac{1}{12}[\phi(i+1,j+1) - \phi(i+1,j-1) + \phi(i-1,j+1) - \phi(i-1,j-1)] \tag{2}$$

Laplacian:

$$\nabla^2 \phi \approx \frac{2}{3}[\phi(i+1,j)+\phi(i,j+1)+\phi(i-1,j)+\phi(i,j-1)]+\frac{1}{6}[\phi(i+1,j+1)+\phi(i+1,j-1)+\phi(i-1,j+1)+\phi(i-1,j-1)]-\frac{10}{3}\phi(i,j) \tag{3}$$

Fig. 2 illustrates the results of simulations using the new discretization method for the energy equation with the original box size. The figure demonstrates a considerable improvement in isotropy compared to the previous method.

[1] F. Qin, *Hybrid Lattice Boltzmann Modeling of Drying of Colloidal Suspensions in Micro-porous Structures*, Ph.D. thesis, ETH Zürich (2020).