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A Parallel Non-Dimensional Lattice Boltzmann Method for fluid flow and heat transfer with solid–liquid phase change

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ABSTRACT

A new mesoscopic scale Parallel Non-Dimensional Lattice Boltzmann Method (P-NDLBM) is developed to dramatically speed up the computation of transient fluid flow and heat transfer problems. The P-NDLBM code using message passing interface (MPI) was compiled in Fortran. The model is presented in dimensionless form to simplify application to a broad range of problems. The effective domain decomposition, data transfer between CPUs, and various boundary conditions based on the P-NDLBM are presented. The code is validated by comparison to prior experimental and single CPU computational studies of cavity flow and the Rayleigh–Bénard problem. The time costs of simulations with equal mesh size are compared for CPU numbers from 1 to 64 to show the effectiveness of the approach. To illustrate the utility of the code, simulations of the transient temperature and fluid velocity during charging and discharging of an integral collector storage solar system are presented. The modeled system has encapsulated phase change embedded in the water-filled enclosure. The results illustrate the capability of the code to capture the phase transition within the encapsulated phase change material as well as the details of the overall flow structure and temperature field.

1. Introduction

The lattice Boltzmann numerical method (LBM) provides the benefit of faster computational speed for prediction of fluid flow and heat transfer in numerous situations where finite difference, finite element, and control volume methods are slow [1–7]. One such example is for transient problems involving phase change. The early LBM models of phase change had two limitations. The moving interface between solid and liquid was treated as an infinitely thin boundary [8–10], which does not capture the true nature of a mixture of solid and liquid phases at the melt interface. Also the early models assumed the major heat flux direction required to calculate the transient boundary positions, which are not exactly on the nodes, was known apriori. To eliminate these limitations, Su and Davidson developed a single CPU based non-dimensional lattice Boltzmann method (NDLBM) for melting and solidification heat transfer and introduced the concept of porosity to describe the transient fluid component ratio in each mesoscopic element [11]. The porosity in the mixture zone varies from 1 to 0 to represent the changing character of the mixture of fluid and solid in the phase change material (PCM) [11]. With this approach the solid–liquid interface is treated as a dynamic zone instead of an ideal infinite thin layer, and it is possible to simulate natural convection with macroscopic Rayleigh numbers up to 10^{11} in reasonable computational time [11,12].

However, for many complex problems, larger grid numbers are required to accurately capture the flow and temperature fields in large multiscale domains. An example of such a domain is shown in Fig. 1. The system depicted is a combined solar collector and storage tank, referred to as an integral collector storage (ICS). The inclined ICS is filled with fluid in which tubes filled with PCM are immersed. Heating/charging of the ICS is via natural convection as solar radiation strikes the front surface. Cooling/discharging of the stored solar energy is via forced convection as cooler fluid introduced at the bottom of the enclosure flows over the PCM-filled tubes and pushes warmer fluid out the top to the user.

Pioneering studies on parallel computation with LBM or LBM combined with other methods such as finite element method show that LBM has inherent advantages for parallel computations [13–17]. Previous parallel LBM simulations were based on physical dimensional units and the papers describing these models did not provide details of the data transfer between CPUs. In the present study, an effective numerical scheme for Parallel Non-Dimensional Lattice Boltzmann Method (P-NDLBM) is developed

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Nomenclature

c_p	specific heat capacity, J/kg-K
c_s	lattice speed of sound, m/s
c	mesoscopic velocity scale, m/s
$\mathbf{c}$	mesoscopic velocity vector, m/s
$\mathbf{e}_g$	the unit vector in the gravity direction
$\mathbf{e}_\mathbf{v}$	the unit vector in the velocity direction
f	density distribution function, kg/m^3
F	force term, N/m^3
g	temperature distribution function, K
g	gravity acceleration, m/s^2
k	thermal conductivity, W/mK
L	macrosocpic length scale, m
L_f	latent heat per unit mass, J/kg
H	height of the enclosure, m
Ma	Mach number
Nu	Nusselt number
p	pressure, N/m^2
Pe	Peclet number
Pr	Prandtl number
Q	heat source, W/m^3
Ra	Rayleigh number
Re	Reynolds number
Ri	Richardson number
Ste	Stefan number
t	time, s
T	temperature, K
$\mathbf{v}$	velocity vector, m/s
U	macroscopic velocity scale, m/s
w	weighting factor
x, y	coordinates

Greek symbols

ΔT	temperature scale, K
Δt	time scale, s
$\Delta x, \Delta y$	lattice size in x, y direction, m
α	thermal diffusivity, m^2/s
β	thermal expansion coefficient
ζ	dimensionless equilibrium function
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3
τ	relaxation time, s
ϕ	porosity
Ω_p	subdomain index
ℓ	mesoscopic length scale, m

Subscripts

eq	equilibrium state
f	fluid
in	inlet
high	higher value
k	the index of the 9 directions
m	mixture of solid and liquid
od	opposite direction
ℓ	mesoscopic length scale
low	lower value
L	macroscopic length scale
PCM	phase change material
ref	reference
s	solid
w	wall
0	initial time value

Superscripts

–	space averaged value
$*$	dimensionless variables

in dimensionless form which facilitates application to a broad range of problems. The effective domain decomposition, data transfer between CPUs, and various boundary conditions based on the P-NDLBM are presented. The model is validated by comparison to well documented cases of cavity flow [18] and the Rayleigh–Bénard natural convection problem in a square enclosure [19]. To illustrate the P-NDLBM code, a case study of the transient temperature and velocity fluid during charging and discharging of the ICS of Fig. 1 is presented.

2. Numerical method

The P-NDLBM builds on the theoretical base of the NDLBM [11], described in Sections 2.1 and 2.2 with sufficient detail to understand the parallel scheme described in Section 2.3.

2.1. Dimensionless mesoscospic equations and governing parameters

The domain is treated as a porous medium where at each location and the time, porosity ϕ is defined as the fraction of the volume of the fluid phase,

$$\phi = \frac{V_f}{V_s + V_f}. \tag{1}$$

Because of the small range of temperature differences in the mixture of solid and fluid during phase change, the local thermal equilibrium assumption for porous medium is justified at the mesh size level. We use the mesoscopic length scale, $\ell = \Delta x = \Delta y$, mesoscopic velocity scale $c = c_s/c_s^*$ (c_s is the mesoscopic sound speed, and c_s^* is the dimensionless mesoscopic sound speed), and mesoscopic time scale $\Delta t = \ell/c$. With these scales the mesoscopic dimensionless momentum and energy equations are,

$$\frac{\partial^* \mathbf{v}^*}{\partial^* t^*} + \nabla^* \cdot (\mathbf{v}^* \mathbf{v}^*) = -\nabla^* p_f^* + \frac{1}{Re_{c,\ell}} \nabla^{*2} \mathbf{v}^* + F_{c,\ell}^*, \tag{2}$$

and

$$\frac{\partial^* T^*}{\partial^* t^*} + \nabla^* \cdot (\phi \mathbf{v}^* T^*) = \frac{1}{Pe_{c,\ell}} \nabla^{*2} T^* + Q_{c,\ell}^*. \tag{3}$$

The mesoscopic dimensionless governing parameters based on the mesoscopic velocity scale c and the mesoscopic length scale ℓ, are

$$Re_{c,\ell} = \frac{c\,\ell}{\nu_f} = \frac{Re_{U,\ell}}{c_s^* Ma_\ell}, \tag{4}$$

$$Pe_{c,\ell} = \frac{Pe_{U,\ell}}{c_s^* Ma_\ell} = \frac{Re_{U,\ell}}{c_s^* Ma_\ell} Pr_m, \tag{5}$$

where Ma_ℓ is the mesoscopic Mach number defined as,

$$Ma_\ell = \frac{U}{c_s} = \frac{U}{c_s^* c}, \tag{6}$$

and

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