A reaction-flow lattice Boltzmann model

LETTER TO THE EDITOR

A reaction-flow lattice Boltzmann model

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Abstract. We describe a development of a lattice Boltzmann fluid flow model enabling the simulation of the reaction and flow of low-concentration species in two dimensions. In principle any number of species and reactions can be implemented in this model. In making this development we derive an expression for the solution of the diffusion equation using the lattice Boltzmann approach.

A previous paper [1] describes a lattice Boltzmann (LB) model capable of simulating single-species Navier–Stokes flow in two dimensions. In this letter we describe a development of this model capable of simulating the reaction and flow of species in low concentration. In principle any number of species and reactions can be implemented in this model. In constructing this model we make the following assumptions (none of which are fundamental to the LB approach itself):

(a) Flow is modelled in two dimensions.

(b) The reactants are in sufficiently low concentration that they do not influence the flow.

(c) The reactants are in sufficiently low concentration that there are no interface effects (e.g. surface tension).

(d) There are no heat effects (e.g. exothermicity).

(e) There are no mass effects (e.g. buoyancy).

The main problem to be considered is the inclusion of the effect of the diffusion of species with respect to the flow. First we derive an expression which allows the direct prescription of a diffusion coefficient while maintaining full Galilean invariance and isotropy. It is then relatively straightforward to include reaction.

Assumptions (b) and (c) above mean that one can simulate pure advection (where by 'pure advection' we mean the transport of species by means of fluid flow alone) simply by modelling a single-species flow and on each timestep partitioning a nodal species concentration $g(r, t)$ between the lattice vectors in proportion to the flow density. If we denote a species concentration and the flow density in direction c_i ($i = 0$ (stationary particles), $1, 2, \ldots, 6$) at node r on the two-dimensional hexagonal grid at time t as $g_i(r, t)$ and $f_i(r, t)$ respectively, pure advection requires

$$g_i(r, t) = g(r, t) \frac{f_i(r, t)}{\rho(r, t)} \tag{1}$$

where the nodal flow density is given by

$$\rho(r, t) = \sum_i f_i(r, t). \tag{2}$$

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The advection step is completed by moving the concentrations $g_i(r, t)$ in directions c_i and summing at each node to obtain the new nodal concentrations:

$$g_i(r, t) = g_i(r - c_i, t - 1)$$
$$g(r, t) = \sum_i g_i(r, t). \tag{3}$$

In the following we will extend this model by including expressions for molecular diffusion with respect to the flow. The analysis is similar to that used to derive the LB flow model [1]; we use primes when referring to equation numbers in that paper.

The aim of this analysis is to be able to mimic the diffusion equation:

$$\frac{Dg}{Dt} = D\nabla^2 g \tag{4}$$

where D/Dt is the substantive derivative and D is the diffusion coefficient. We proceed by writing the lattice Bolzmann equation for species concentration (1′)

$$g_i(r, t+1) = g_i(r - c_i, t) + \Delta_i \tag{5}$$

where Δ_i is the flow collision function. Taking the Taylor expansion to first order, we obtain (5′)

$$\frac{Dg_i}{Dt} = (u - c_i)\nabla g_i + \Delta_i \tag{6}$$

where u is the flow velocity (3′)

$$u = \frac{\sum_i c_i f_i}{\rho}. \tag{7}$$

Noting that (6′)

$$\sum_i \Delta_i = 0 \tag{8}$$

we sum equation (6) over i to obtain

$$\frac{Dg}{Dt} = \sum_i (u - c_i)\nabla g_i. \tag{9}$$

As before, we write (13′)

$$g_i = \bar{g}_i + \delta g_i \tag{10}$$

where $\bar{g}_i$ is the pure advective term (equation (1)),

$$\bar{g}_i = \frac{g f_i}{\rho} \tag{11}$$

and δg_i is the diffusion term which equilibrates variation in concentration. In order to mimic the diffusion equation (4), we require δg_i to have the form

$$\delta g_i = \lambda c_i^\alpha \nabla^\alpha g \tag{12}$$

where λ needs to be determined.

The right-hand-side of equation (9) can be written

$$\sum_i (u - c_i)\nabla g_i = \sum_i \nabla(u - c_i)g_i - \sum_i g_i\nabla(u - c_i). \tag{13}$$

Since the derivatives of c_i are zero, and assuming incompressibility (7'), the final term in (13) is zero. Using equation (10) to substitute g_i from the remaining term on the right-hand-side, and using equations (11) and (7), we obtain

$$\sum_i \nabla(u - c_i) g_i = \sum_i \nabla(u - c_i)(\bar{g}_i + \delta g_i)$$

$$= \sum_i \nabla(u - c_i) \frac{g f_i}{\rho} + \sum_i \nabla(u - c_i) \delta g_i$$

$$= \sum_i \nabla(u - c_i) \delta g_i. \tag{14}$$

Substituting δg_i using equation (12),

$$\sum_i \nabla(u - c_i) g_i = \lambda \sum_i \nabla^\beta u^\beta c_i^\alpha \nabla^\alpha g - \lambda \sum_i \nabla^\beta c_i^\beta c_i^\alpha \nabla^\alpha g. \tag{15}$$

Over the summation, expressions in odd powers of c_i will be zero, while (22')

$$\sum_i c_i^\alpha c_i^\beta = 3\delta^{\alpha\beta}. \tag{16}$$

Therefore

$$\sum_i \nabla(u - c_i) g_i = -3\lambda \nabla^2 g. \tag{17}$$

We can now substitute the right-hand-side of equation (9), giving

$$\frac{\mathrm{D}g}{\mathrm{D}t} = -3\lambda \nabla^2 g \tag{18}$$

and the diffusion equation (4) is satisfied by putting

$$D = -3\lambda. \tag{19}$$

The steps in the computation are therefore:

(a) Calculate nodal concentrations using data from the previous timestep (equation (3)).

(b) Calculate the gradients (cf (43')):

$$\frac{\partial g}{\partial x}(r, t) = \tfrac{1}{3} \sum_i c_{i,x} g(r + c_i, t)$$

$$\frac{\partial g}{\partial y}(r, t) = \tfrac{1}{3} \sum_i c_{i,y} g(r + c_i, t). \tag{20}$$

(c) Finally, calculate the change in concentration distribution due to advection and diffusion (equations (10), (11), (12), (19)):

$$g_i(r, t+1) = \frac{g(r, t) f_i(r, t)}{\rho(r, t)} - \frac{D}{3} \left(c_{i,x} \frac{\partial g}{\partial x}(r, t) + c_{i,y} \frac{\partial g}{\partial y}(r, t) \right). \tag{21}$$

In principle, any number of species can be simulated using the model described above. We now consider the reaction of multiple species, taking as an example the reaction $A + B \rightarrow C$, where A, B and C represent chemical species. Using square brackets [ ] to denote the concentration of species, the reaction rate for each species is given by

$$-\frac{\mathrm{d}[A]}{\mathrm{d}t} = -\frac{\mathrm{d}[B]}{\mathrm{d}t} = \frac{\mathrm{d}[C]}{\mathrm{d}t} = k[A][B] \tag{22}$$

where k is the rate constant. Recalling the definition of a derivative,

$$\frac{dy}{dx} = \lim_{\delta x \to 0} \left(\frac{y(x + \delta x) - y(x)}{\delta x} \right) \tag{23}$$

it can be seen that for small timestep δt one can express the evolution of each species concentration in the above example as follows:

$$[A](t + \delta t) = [A](t) - k[A](t)[B](t)\delta t$$
$$[B](t + \delta t) = [B](t) - k[A](t)[B](t)\delta t \tag{24}$$
$$[C](t + \delta t) = [C](t) + k[A](t)[B](t)\delta t.$$

In the LB model δt is the unit timestep, and therefore the change in species concentration at each lattice node on each timestep is given by

$$[A](r, t + 1) = [A](r, t) - k[A](r, t)[B](r, t)$$
$$[B](r, t + 1) = [B](r, t) - k[A](r, t)[B](r, t) \tag{25}$$
$$[C](r, t + 1) = [C](r, t) + k[A](r, t)[B](r, t).$$

In principle, this approach can be generalized to any number of reactions, and each reaction can be of any order. In practice one would need to ensure that the computed reaction rate is independent of timestep size. One is free to specify the LB timestep size, which is related to physical timescales through the rate constant k.

We have derived expressions which enable the inclusion in a lattice Boltzmann flow model of the reaction and flow of species in low concentration. In doing so we have obtained an expression for the solution of the diffusion equation using the lattice Boltzmann approach.

References

[1] Kingdon R D, Schofield P and White L 1992 *J. Phys. A: Math. Gen.* **25** 3559–66