1 Initialisation schemes

There is more than one way to skin a cat, and there is more than one way to initialise a lattice Boltzmann model! Given an initial velocity field $\mathbf{u}_0$, which must be solenoidal (i.e. $\nabla \cdot \mathbf{u}_0 = 0$), we seek to find an initial set of distribution functions f_i.

The simplest option (codename "CEQ") is to specify an initial solenoidal velocity field $\mathbf{u}_0$ and set the initial distribution functions to $f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \bar{\rho})$, where $\bar{\rho} = 1$ is a uniform density everywhere. This guarantees the correct initial velocity field, but introduces error into the pressure and deviatoric stress. This leads to unphysical transients. For steady flow problems, these will eventually decay such that the model converges on a valid solution. However, for time–dependent problems, errors in the initialisation may corrupt to whole solution.

The next initialisation scheme (codename "FEQ") reduces some of this error by including information about the initial pressure field, $p_0(\mathbf{x})$. Suppose we have a method to calculate p_0 (for instance, by solving Poisson's equation, or having an analytical solution). Then we can calculate the corresponding lattice Boltzmann density field, $\rho_0(\mathbf{x})$, using

$$\rho_0(\mathbf{x}) = \bar{\rho} + \frac{p_0(\mathbf{x}) - \bar{p}}{c_s^2}, \tag{1}$$

where $\bar{p}$ is a constant reference pressure. The distributions are then set to $f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \rho_0(\mathbf{x}))$. This FEQ scheme sets the correct initial pressure and velocity fields, so improves greatly upon the CEQ scheme. However, since the initial distributions are set to equilibrium, all components of the stress tensor are zero. Thus, small errors are still introduced, which may corrupt complex time–dependent flows.

The NEQ scheme introduces first order non-equilibrium corrections to the FEQ scheme. The initial distributions are set to $f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \rho_0(\mathbf{x})) + f_i^{(1)}$, with first order correction

$$f_i^{(1)} = -w_i \frac{\tau \rho}{c_s^2} Q_{i\alpha\beta} \frac{\partial u_\beta}{\partial x_\alpha} - \frac{w_i \Delta t}{2 c_s^2} \left(c_{i\alpha} F_\alpha + \frac{Q_{i\alpha\beta}}{2 c_s^2} (u_\alpha F_\beta + F_\alpha u_\beta) \right), \tag{2}$$

where summation is performed over α and β. Here, $\rho \equiv \rho_0(\mathbf{x})$, $\mathbf{u} \equiv \mathbf{u}_0(\mathbf{x})$, and $Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}$. The velocity field gradients are calculated using a finite difference scheme.

Finally, we introduce Mei's consistent initialisation scheme (codename "MEI"). This scheme only requires an initial solenoidal velocity field $\mathbf{u}_o(\mathbf{x})$, and recreates the correct pressure and stress fields using an iterative scheme. The distributions are first initialised using any of the above schemes, CEQ, FEQ, or NEQ, and then modified lattice

Init. scheme	Value of initial distributions
CEQ	$f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \bar{\rho})$
FEQ	$f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \rho_0(\mathbf{x}))$
NEQ	$f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \rho_0(\mathbf{x})) + f_i^{(1)}$
MEI	Iterate $f_i(\mathbf{x} + \mathbf{e}_i) = \Omega(f_i, f_i^{\mathrm{eq}}(\mathbf{u}_0, \sum_i f_i))$ until converged

Table 1: **Initialisation schemes.** A summary of the different lattice Boltzmann distribution initialisation schemes tested in this work.

Boltzmann timesteps are performed until the distribution functions converge to within a specified tolerance. In the modified timesteps, density ρ is calculated from the sum of f_i at each point, as usual, but $\mathbf{u}$ is specified as the initial field $\mathbf{u}_0$, such that the collision step uses $f_i^{\mathrm{eq}}(\mathbf{u}_0(\mathbf{x}), \Sigma f_i(\mathbf{x}))$ for the equilibrium distribution functions. The streaming step is performed as usual. Once the distributions f_i have converged, the initial state obtained will have the correct pressure and stress fields. This method is more expensive than the NEQ scheme, often requiring thousands of iterations, especially if the CEQ scheme is used for the first step, but it has the advantage of not requiring an explicit calculation of the initial pressure field. This makes the method suitable for problem in complex geometries and with non–uniform physical fluid densities.

2 Benchmark: Taylor–Green Vortex

The Taylor–Green vortex is an analytic solution to the incompressible Navier Stokes equations in a two–dimensional periodic $l_x \times l_y$ domain. It consists of adjacent vortices, whose vorticity decays exponentially with time.

$$u_x = -u_0 \sqrt{k_y/k_x} \cos(k_x x) \sin(k_y y) e^{-t/td}, \tag{3}$$

$$u_y = u_0 \sqrt{k_x/k_y} \sin(k_x x) \cos(k_y y) e^{-t/td}, \tag{4}$$

$$p = p_0 - \frac{\rho u_0^2}{4} \left[\frac{k_x}{k_y} \cos(2k_x x) + \frac{k_x}{k_y} \cos(2k_y y) \right] e^{-2t/td}, \tag{5}$$

where ρ is the constant fluid density, u_0 is the reference velocity scale, p_0 is the reference pressure, $k_{x,y} = 2\pi/l_{x,y}$ are components of a wavevector $\mathbf{k}$ of the vortices, and $t_d = [\nu(k_x^2 + k_y^2)]^{-1}$ is the vortex decay timescale.

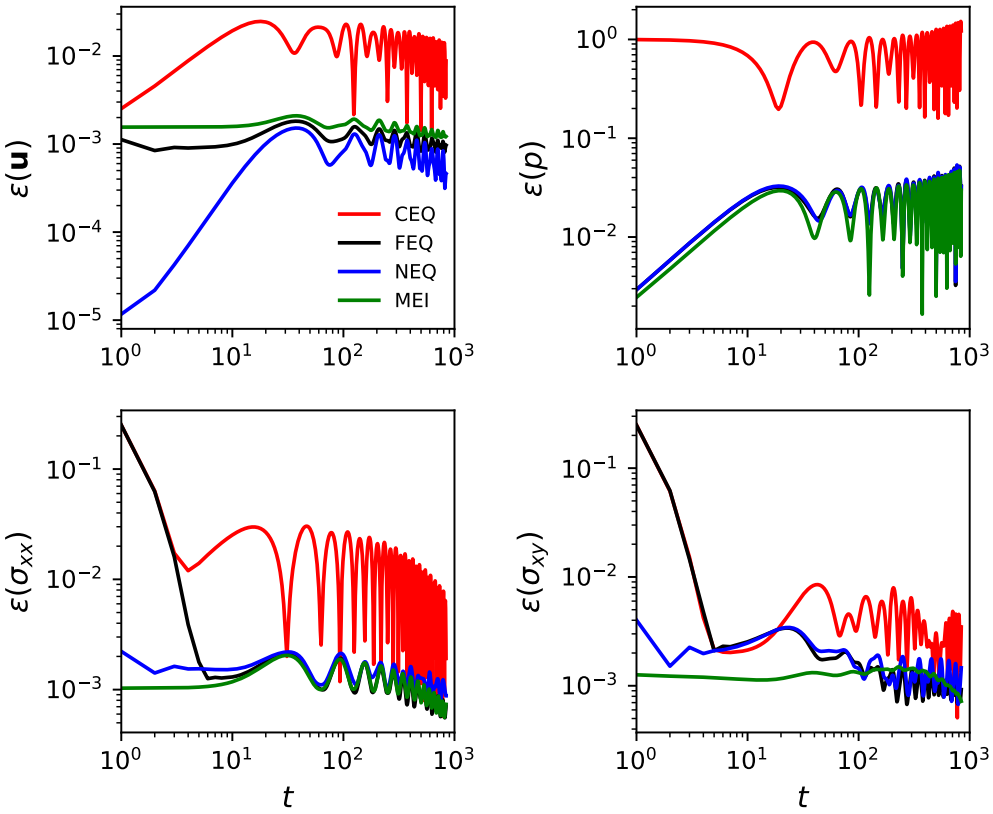

Figure 1: **Initialisation scheme error comparison.** The L2 error norm for velocity $\mathbf{u}$, density ρ, and deviatoric stress tensor components σ_{xx} and σ_{yy} are plotted at each time step for one decay timescale of a Taylor–Green vortex flow.

The components of the deviatoric stress tensor for this flow are

$$\sigma_{xx} = 2\rho\nu u_0 \sqrt{k_x k_y}\sin(k_x x)\sin(k_y y)e^{-t/t_d} \tag{6}$$

$$\sigma_{xy} = \rho\nu u_0 \left(\sqrt{k_x^3/k_y} - \sqrt{k_y^3/k_x}\right)\cos(k_x x)\cos(k_y y)e^{-t/t_d}, \tag{7}$$

$$\sigma_{yx} = \sigma_{xy}, \tag{8}$$

$$\sigma_{yy} = -\sigma_{xx}. \tag{9}$$

I initialised a Taylor–Green vortex in a 72×96 periodic domain with parameter values $u_0^\star = 0.03$, $\rho_0^\star = 1.0$, $p_0^\star = 0.0$, and $\nu^\star = 0.1$. The lattice model used was the D2Q9 lattice, and the collision operator was the SRT operator with $\tau^\star = 0.8$. The simulations were run for one complete vortex decay timescale, and the L2 error norms for $\mathbf{u}$, p, σ_{xx} and σ_{xy} were calculated at each timestep. This was repeated for the different initialisation schemes in Table 1. The results are shown in Fig. 1.

The CEQ initialisation generated the largest error at all times. Notably, the error in p remains $O(1)$ for the whole simulation. This incorrect pressure initialisation has corrupted

the accuracy of the whole solution. We conclude that the CEQ scheme should not be used to initialise lattice Boltzmann fluid models.

The other schemes all do better, tending to converge to small errors in all the variables at late times. The FEQ scheme incorrectly represents the stress tensor components at early times, but because this scheme sets the correct initial pressure, the errors in σ_{xx} and σ_{xy} diminish after a small number of time steps. The NEQ scheme obtains a correct velocity, pressure, and stress initialisation by introducing a first order non-equilibrium correction to the FEQ scheme. The MEI scheme, here seeded by the CEQ scheme, produces small errors comparable to FEQ and NEQ without requiring explicit calculation of the initial pressure distribution, so is well–suited for complex problems.