# A Three-Dimensional, Multi-component, Lattice-Boltzmann Model with Component Interaction

TECHNICAL REPORT
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We provide a detailed derivation of both the Euler equation and the Navier-Stokes equation for the case of a three-dimensional, multi-component, lattice-Boltzmann model, wherein the components may have non-trivial interaction. The model is derived from the multi-component, lattice-Boltzmann model due to Shan and Doolen (J. Stat. Physics, 81(1/2), 1995, and Phys. Rev. E 54(4), 1996) and Shan's simulation of Rayleigh-Bénard convection (Phys. Rev. E 55(3), 1997).

## 1. Definitions.

The key quantity of interest will be the per-component *directional density*, $f_{\sigma,i}(\vec{r},t)$, which is the density of component $\sigma$ arriving at lattice site $\vec{r} \in \Re^3$ at time $t$ in direction $\vec{c_i}$. The directions $\vec{c_i}$, $i$ = 0,1,...,18, are all the non-corner lattice points of a cube of unit radius, $\{-1,0,1\}^3$. We take $\vec{c_0} = (0,0,0)$, and $\vec{c_1}$ - $\vec{c_6}$ to be the axis directions. Note that these directions are really projections from 4D space of 24 lattice points that are equidistant from the 4D origin,

$$\begin{array}{cc} (\pm 1,0,0,\pm 1) & (0,\pm 1,\pm 1,0) \\ (0,\pm 1,0,\pm 1) & (\pm 1,0,\pm 1,0) \\ (0,0,\pm 1,\pm 1) & (\pm 1,\pm 1,0,0) \end{array}$$

where the projection is truncation of the fourth component. Thus the flow will be isotropic, but the axial directions will carry double weight in the discussions below.

Some additional definitions:

- $f_\sigma = (f_{\sigma,0}, f_{\sigma,1}, ..., f_{\sigma,18})$
- $\lambda$ is the lattice spacing
- $\tau$ is the time step
- $v = \lambda/\tau$
- $\vec{v_i} = v\vec{c_i}$ $i = 0, 1, ...18$
- component density per site is $\rho_\sigma(\vec{r},t) = \sum_{i=0}^{18} f_{\sigma,i}(\vec{r},t)$
- total density per site is $\rho(\vec{r},t) = \sum_\sigma \rho_\sigma(\vec{r},t)$
- component velocity per site is $\vec{u_\sigma}(\vec{r},t) = (\sum_{i=0}^{18} f_{\sigma,i}(\vec{r},t)\vec{v_i})/\rho_\sigma(\vec{r},t)$

The entire lattice Boltzmann computation is then just an iterated, synchronous update of the directional densities according to:

$$f_{\sigma,i}(\vec{r}+\lambda\vec{c_i}, t+\tau) - f_{\sigma,i}(\vec{r},t) = [\Omega_\sigma(f_\sigma)]_i \tag{1}$$

where $\Omega_\sigma : \Re^{19} \rightarrow \Re^{19}$ is a collision operator. Many collision operators have been proposed. (See Rasche et al., Lattice-Boltzmann Lighting, Proc. Eurographics Rendering Symp., 2004, for an operator appropriate for photon scattering.) Any operator must satisfy two equations:

$$\sum_{i=0}^{18} [\Omega_\sigma(f_\sigma)]_i = 0 \qquad \text{conservation of mass} \tag{2}$$

and

$$\sum_\sigma \sum_{i=0}^{18} [\Omega_\sigma(f_\sigma)]_i \, \vec{v_i} = 0 \qquad \text{conservation of total momentum} \tag{3}$$

If external force $\vec{F_\sigma}(\vec{r}, t)$ is applied to component $\sigma$, then instead of (3) we must have:

$$\sum_\sigma \sum_{i=0}^{18} [\Omega_\sigma(f_\sigma)]_i \, \vec{v_i} = \tau \sum_\sigma \vec{F_\sigma}(\vec{r}, t) \tag{4}$$

Nevertheless, if there is no net momentum flux at the boundaries (e.g. for periodic boundaries), then momentum of the entire system is still conserved.

Many collision operators satisfy these constraints. When we need little direct control over individual collision events, a convenient operator is the LBGK operator (Lattice - Bhatnager, Gross, Krook) given by:

$$[\Omega_\sigma(f_\sigma)]_i = -\frac{1}{\xi_\sigma}\left[f_{\sigma,i}(\vec{r}, t) - f_{\sigma,i}^{(eq)}(\vec{r}, t)\right] \tag{5}$$

where $\xi_\sigma$ is the *relaxation time* of the $\sigma^{th}$ component (a parameter), and

$$f_{\sigma,i}^{(eq)}(\vec{r}, t) = \begin{cases} \rho_\sigma(d - [\vec{u_\sigma}^{(eq)}]^2/(2v^2)) & \text{i = 0} \\ 2\rho_\sigma\left(\frac{1-d}{24} + \frac{1}{12v^2}\vec{v_i}\cdot\vec{u_\sigma}^{eq} + \frac{1}{8v^4}\vec{v_i}\vec{v_i} : \vec{u_\sigma}^{(eq)}\vec{u_\sigma}^{(eq)} - \frac{1}{24v^2}[\vec{u_\sigma}^{(eq)}]^2\right) & \text{i = 1,...,6} \\ \rho_\sigma\left(\frac{1-d}{24} + \frac{1}{12v^2}\vec{v_i}\cdot\vec{u_\sigma}^{eq} + \frac{1}{8v^4}\vec{v_i}\vec{v_i} : \vec{u_\sigma}^{(eq)}\vec{u_\sigma}^{(eq)} - \frac{1}{24v^2}[\vec{u_\sigma}^{(eq)}]^2\right) & \text{i = 7,...,18} \end{cases} \tag{6}$$

Here $d \in [0, 1]$ is a parameter (fraction of density with zero speed at equilibrium) and $\vec{u_\sigma}^{(eq)}$ is defined so that (3) or (4) holds. Specifically, if we use these identities:

- $\sum_{i=1}^{6} 2v_{i\alpha} + \sum_{i=7}^{18} v_{i\alpha} = 0 \quad \alpha \in \{x, y, z\}$
- $\sum_{i=1}^{6} 2v_{i\alpha}^2 + \sum_{i=7}^{18} v_{i\alpha}^2 = 12v^2 \quad \alpha \in \{x, y, z\}$
- $\sum_{i=1}^{6} 2v_{i\alpha}v_{i\beta} + \sum_{i=7}^{18} v_{i\alpha}v_{i\beta} = 0 \quad \alpha, \beta \in \{x, y, z\}, \quad \alpha \neq \beta$
- $\sum_{i=1}^{6} 2v_{i\alpha}^2 v_{i\beta} + \sum_{i=7}^{18} v_{i\alpha}^2 v_{i\beta} = 0 \quad \alpha, \beta \in \{x, y, z\}$
- $\sum_{i=1}^{6} 2v_{i\alpha}^2 v_{i\beta}^2 + \sum_{i=7}^{18} v_{i\alpha}^2 v_{i\beta}^2 = 4v^4 \quad \alpha, \beta \in \{x, y, z\}, \quad \alpha \neq \beta$
- $\sum_{i=1}^{6} 2v_{i\alpha}^4 + \sum_{i=7}^{18} v_{i\alpha}^4 = 12v^4 \quad \alpha \in \{x, y, z\}$

then it is easy to verify that

$$\sum_i f_{\sigma,i}^{(eq)} = \rho_\sigma \tag{7}$$

and

$$\sum_i \vec{v_i} f_{\sigma,i}^{(eq)} = \rho_\sigma \vec{u_\sigma}^{(eq)} \tag{8}$$

regardless of the definition of $\vec{u_\sigma}^{(eq)}$. To enforce constraint (3) we would then need

$$\begin{aligned}
0 &= \sum_\sigma \sum_i \left[\Omega_\sigma(f_\sigma)\right]_i \vec{v_i} \\
&= \sum_\sigma \sum_i -\frac{\vec{v_i}}{\xi_\sigma}\left[f_{\sigma,i} - f^{(eq)}_{\sigma,i}\right] \\
&= -\sum_\sigma \frac{\rho_\sigma \vec{u_\sigma}}{\xi_\sigma} + \sum_\sigma \frac{\rho_\sigma \vec{u_\sigma}^{(eq)}}{\xi_\sigma}
\end{aligned}$$

In the absence of external forces, we choose to make all $\vec{u_\sigma}^{(eq)}$s equal, i.e., independent of $\sigma$. Thus we are led to the definition:

$$\vec{u_\sigma}^{(eq)} = \vec{u}^{(eq)} = \left(\sum_\sigma \frac{\rho_\sigma \vec{u_\sigma}}{\xi_\sigma}\right) / \left(\sum_\sigma \frac{\rho_\sigma}{\xi_\sigma}\right) \tag{9}$$

In the presence of (possibly unequal) external forces, we instead define

$$\vec{u_\sigma}^{(eq)} = \vec{u}^{(eq)} + \frac{\xi_\sigma \tau}{\rho_\sigma}\vec{F_\sigma} \tag{10}$$

which guarantees that constraint (4) holds.

The principal reasons for the choice (5) are that it is computationally fast, and it will lead to the Navier-Stokes equations at the macroscopic ($\rho$, $\vec{u}$) level.

We have yet to define an overall, component-independent, fluid velocity, $\vec{u}$. This is again a matter of choice (within reason), since there is no apriori-correct weighting for the components. We observe that total momentum at a site before a collision is $\sum_\sigma \rho_\sigma \vec{u_\sigma}$ and total momentum after the collision is $\sum_\sigma \rho_\sigma \vec{u_\sigma} + \tau \sum_\sigma \vec{F_\sigma}$. If we want $\rho\vec{u}$ to match the cross-collisional average, we must have

$$\vec{u} = \left(\sum_\sigma \rho_\sigma \vec{u_\sigma} + \frac{\tau}{2}\sum_\sigma \vec{F_\sigma}\right)/\rho \tag{11}$$

All that remains is to derive the macroscopic behavior.

## 2. The Continuity Equation.

We will use the so-called *Chapman-Enskog expansion*, standard in lattice-Boltzmann modeling. (See, e.g., Chopard and Droz, Cellular Automata Modeling of Physical Systems, Cambridge Univ. Press, 1998.) We assume that $f_{\sigma,i}$ can be written as a small perturbation about some local equilibrium, $f^{(0)}_{\sigma,i}$:

$$f_{\sigma,i} = f^{(0)}_{\sigma,i} + \epsilon f^{(1)}_{\sigma,i} \tag{12}$$

where $\epsilon$ is the *Knudsen number*, which represents the mean free path between successive collisions.

The choice of $f^{(0)}$ is not necessarily unique. The constraints are that it carries the density and the momentum, specifically:

$$\sum_i f^{(0)}_{\sigma,i} = \rho_\sigma \tag{13}$$

and

$$\sum_i \vec{v_i} f^{(0)}_{\sigma,i} = \rho_\sigma \vec{u} \tag{14}$$

From (7) and (8), it is easy to find a suitable choice for $f^{(0)}_{\sigma,i}$: use (6), and replace every instance of $\vec{u_\sigma}^{(eq)}$ with $\vec{u}$.

We want to consider system behavior at multiple time scales as both lattice spacing and time step approach 0. We partition the time scale as

$$t = K\frac{t_0}{\epsilon} + (1-K)\frac{t_1}{\epsilon^2} \tag{15}$$

where $t_0 = o(\epsilon)$, $t_1 = o(\epsilon^2)$, and $K \in [0,1]$. Similarly, we write distance

$$\vec{r} = \frac{\vec{r_0}}{\epsilon} \tag{16}$$

where $\vec{r_0} = o(\epsilon)$. A variety of different behaviors in the limit ($\epsilon \to 0$) can then be achieved. If $K = 0$, we would obtain the diffusion equation of Rasche et al., but we do not make that assumption here.

Note that the relationship among the partials is given by:

$$\begin{aligned} \frac{\partial}{\partial t} &= \epsilon\frac{\partial}{\partial t_0} + \epsilon^2\frac{\partial}{\partial t_1} \\ \frac{\partial}{\partial r_\alpha} &= \epsilon\frac{\partial}{\partial r_{0\alpha}} \qquad \text{for} \quad \alpha \in \{x,y,z\} \end{aligned} \tag{17}$$

Now let

$$\begin{aligned} \nabla^A &= (\partial/\partial t, \nabla) \\ &= (\epsilon\partial/\partial t_0 + \epsilon^2\partial/\partial t_1, \epsilon\nabla_0) \\ &= (\epsilon\partial/\partial t_0 + \epsilon^2\partial/\partial t_1, \epsilon\partial/\partial r_{0x}, \epsilon\partial/\partial r_{0y}, \epsilon\partial/\partial r_{0z}) \end{aligned}$$

and expand the left side of (1) in a Taylor series:

$$[(\tau, \lambda\vec{c_i}) \cdot \nabla^A] f_{\sigma,i}(\vec{r},t) + \frac{[(\tau,\lambda\vec{c_i}) \cdot \nabla^A]^2}{2!} f_{\sigma,i}(\vec{r},t) + ... = [\Omega_\sigma(f_\sigma(\vec{r},t))]_i \tag{18}$$

If we sum over $i$, the right side vanishes due to conservation of mass (2). If we then divide by $\tau$, substitute (12) and (17), and equate coefficients of $\epsilon^1$, we obtain

$$\sum_i \frac{\partial f^{(0)}_{\sigma,i}}{\partial t_0} + \sum_i \vec{v_i} \cdot \nabla_0 f^{(0)}_{\sigma,i} = 0 \tag{19}$$

that is

$$\frac{\partial \rho_\sigma}{\partial t_0} + \nabla_0 \cdot (\rho_\sigma \vec{u}) = 0 \tag{20}$$

the *continuity equation* at time scale $t_0$.

## 3. The Euler Equation.

The continuity equation arises from the conservation of mass (2). Next we want to use the conservation of total momentum (4), so we will multiply both sides of (18) by $\vec{v_i}$, sum over $i$, sum over $\sigma$, divide by $\tau$, and then equate coefficients of $\epsilon^1$. The external forces lend a bit of a wrinkle here. After multiplying (18) by $\vec{v_i}$, summing over $i$ and $\sigma$, and dividing by $\tau$, we obtain an equation whose right-hand side is $\sum_\sigma \vec{F_\sigma}$, and we need to identify the coefficient of $\epsilon^1$ therein. Fortunately, this is straightforward. From (11) we have:

$$\begin{aligned} \sum_\sigma \vec{F_\sigma} &= (2/\tau)(\rho\vec{u} - \sum_\sigma \rho_\sigma \vec{u_\sigma}) \\ &= (2/\tau)(\sum_\sigma\sum_i f^{(0)}_{\sigma,i}\vec{v_i} - \sum_\sigma\sum_i f_{\sigma,i}\vec{v_i}) \\ &= (2/\tau)(-\sum_\sigma\sum_i \epsilon f^{(1)}_{\sigma,i}\vec{v_i}) \end{aligned} \tag{21}$$

If we let $\vec{H} = (2/\tau)(-\sum_\sigma \sum_i f^{(1)}_{\sigma,i}\vec{v_i})$ then we have $\epsilon\vec{H} = \sum_\sigma \vec{F_\sigma}$, and our result is:

$$\sum_\sigma \sum_i \vec{v_i}\partial f^{(0)}_{\sigma,i}/\partial t_0 + \sum_\sigma \sum_i \left[\vec{v_i} \cdot \nabla_0 f^{(0)}_{\sigma,i}\right]\vec{v_i} = \vec{H} \tag{22}$$

which can be simplified to:

$$\frac{\partial(\rho\vec{u})}{\partial t_0} + \sum_\sigma \nabla_0 \cdot \Pi^{(0)}_\sigma = \vec{H} \tag{23}$$

where $\Pi^{(0)}_\sigma$ denotes the *momentum tensor* based on $f^{(0)}_\sigma$, i.e.,

$$\Pi^{(0)}_\sigma = \begin{bmatrix} \sum_i f^{(0)}_{\sigma,i} v_{ix}^2 & \sum_i f^{(0)}_{\sigma,i} v_{ix}v_{iy} & \sum_i f^{(0)}_{\sigma,i} v_{ix}v_{iz} \\ \sum_i f^{(0)}_{\sigma,i} v_{ix}v_{iy} & \sum_i f^{(0)}_{\sigma,i} v_{iy}^2 & \sum_i f^{(0)}_{\sigma,i} v_{iy}v_{iz} \\ \sum_i f^{(0)}_{\sigma,i} v_{ix}v_{iz} & \sum_i f^{(0)}_{\sigma,i} v_{iy}v_{iz} & \sum_i f^{(0)}_{\sigma,i} v_{iz}^2 \end{bmatrix} \tag{24}$$

We can use the identities on the $v_i$s to write this as:

$$\Pi^{(0)}_\sigma = \begin{bmatrix} v^2\left(\frac{1-d}{2}\right)\rho_\sigma + \rho_\sigma u_x^2 & \rho_\sigma u_x u_y & \rho_\sigma u_x u_z \\ \rho_\sigma u_x u_y & v^2\left(\frac{1-d}{2}\right)\rho_\sigma + \rho_\sigma u_y^2 & \rho_\sigma u_y u_z \\ \rho_\sigma u_x u_z & \rho_\sigma u_y u_z & v^2\left(\frac{1-d}{2}\right)\rho_\sigma + \rho_\sigma u_z^2 \end{bmatrix} \tag{25}$$

and then substitute into (23) to obtain:

$$\frac{\partial(\rho\vec{u})}{\partial t_0} + \nabla_0 \cdot \left[v^2\left(\frac{1-d}{2}\right)\rho I + \rho\vec{u}\vec{u}\right] = \vec{H} \tag{26}$$

All that remains is to give an appropriate definition of *pressure* for this system. Assume that, for those external forces, $\vec{F_\sigma}$, that contribute to pressure (typically, all component interactions but not gravity), we can find a *potential*, i.e., a function $V$ with the property that $\nabla V = -\sum_\sigma \vec{F_\sigma}$. We then define pressure as

$$p = v^2\left(\frac{1-d}{2}\right)\rho + V \tag{27}$$

so that

$$\nabla p = v^2\left(\frac{1-d}{2}\right)\nabla\rho - \sum_\sigma \vec{F_\sigma} \tag{28}$$

and, in particular,

$$\nabla_0 p = v^2\left(\frac{1-d}{2}\right)\nabla_0\rho - \vec{H} \tag{29}$$

We can then write (26) in the form

$$\frac{\partial(\rho\vec{u})}{\partial t_0} + \nabla_0 \cdot [\rho\vec{u}\vec{u}] = -\nabla_0 p \tag{30}$$

It turns out that we can now factor $\rho$ from the left hand side. If we proceed with the differentiation:

$$\frac{\partial\rho}{\partial t_0}\vec{u} + \rho\frac{\partial\vec{u}}{\partial t_0} + (\nabla_0 \cdot \rho\vec{u})\,\vec{u} + (\rho\vec{u}) \cdot \nabla_0\vec{u} = -\nabla_0 p \tag{31}$$

and apply the continuity equation at timescale $t_0$ (20), we see the first and third summands on the left cancel, and we have:

$$\frac{\partial\vec{u}}{\partial t_0} + \vec{u} \cdot \nabla_0\vec{u} = -\left(1/\rho\right)\nabla_0 p \tag{32}$$

This is the *Euler equation of hydrodynamics* (at scale $t_0$), which is just the Navier-Stokes equation without the dissipative effects of viscosity.

## 4. Timescale $t_1$.

Now we need to repeat the procedures above for the $\epsilon^2$ terms. If we sum both sides of (18) over $i$, divide by $\tau$, and equate coefficients of $\epsilon^2$, we get

$$\frac{\partial}{\partial t_0}\sum_i f_{\sigma,i}^{(1)}+\sum_i \vec{v_i}\cdot\nabla_0 f_{\sigma,i}^{(1)}+\frac{\partial}{\partial t_1}\sum_i f_{\sigma,i}^{(0)}+(\tau/2)\nabla_0\cdot\left[\nabla_0\cdot\Pi_\sigma^{(0)}\right]+\tau\frac{\partial}{\partial t_0}\sum_i \vec{v_i}\cdot\nabla_0 f_{\sigma,i}^{(0)}+(\tau/2)\frac{\partial^2}{\partial t_0^2}\sum_i f_{\sigma,i}^{(0)}=0 \tag{33}$$

Using (13), (14), and the (related) fact that $\sum_i f_{\sigma,i}^{(1)}=0$, we can simplify this to

$$\sum_i \vec{v_i}\cdot\nabla_0 f_{\sigma,i}^{(1)}+\frac{\partial\rho_\sigma}{\partial t_1}+(\tau/2)\nabla_0\cdot\left[\nabla_0\cdot\Pi_\sigma^{(0)}\right]+\tau\frac{\partial}{\partial t_0}\left(\nabla_0\cdot(\rho_\sigma\vec{u})\right)+(\tau/2)\frac{\partial}{\partial t_0}\left[\frac{\partial\rho_\sigma}{\partial t_0}\right]=0 \tag{34}$$

Now the fourth and fifth terms on the left can be combined by the continuity equation at timescale $t_0$. The result can then be combined with the third term:

$$\sum_i \vec{v_i}\cdot\nabla_0 f_{\sigma,i}^{(1)}+\frac{\partial\rho_\sigma}{\partial t_1}+(\tau/2)\nabla_0\cdot\left[\frac{\partial}{\partial t_0}\left(\rho_\sigma\vec{u}\right)+\nabla_0\cdot\Pi_\sigma^{(0)}\right]=0 \tag{35}$$

The term in square brackets can be rewritten in terms of $\rho$, $\rho_\sigma$, and $p$. If we multiply both sides of (32) by $\rho_\sigma$ and reverse the steps of (30) - (32) we obtain

$$\frac{\partial(\rho_\sigma\vec{u})}{\partial t_0}+\nabla_0\cdot\left[\rho_\sigma\vec{u}\vec{u}\right]=-(\rho_\sigma/\rho)\nabla_0 p \tag{36}$$

Thus, from (25) we have

$$\begin{aligned}\left[\frac{\partial}{\partial t_0}\left(\rho_\sigma\vec{u}\right)+\nabla_0\cdot\Pi_\sigma^{(0)}\right] &= \frac{\partial(\rho_\sigma\vec{u})}{\partial t_0}+\nabla_0\cdot\left[v^2\left(\frac{1-d}{2}\right)\rho_\sigma I+\rho_\sigma\vec{u}\vec{u}\right]\\ &= -(\rho_\sigma/\rho)\nabla_0 p+v^2\left(\frac{1-d}{2}\right)\nabla_0\rho_\sigma \end{aligned}\tag{37}$$

We still need to relate the $f^{(1)}$ term of (35) to $\rho$, $\rho_\sigma$, $p$, and $\vec{u}$, and this is trickier. We return to (18), multiply by $\vec{v_i}$, divide by $\tau$, and sum over $i$. This yields

$$\frac{\partial}{\partial t_0}\left(\rho_\sigma\vec{u}\right)+\nabla_0\cdot\Pi_\sigma^{(0)}=\sum_i\frac{\vec{v_i}}{\tau}\left[\Omega_\sigma(f_\sigma)\right]_i \tag{38}$$

If we were also to sum over $\sigma$, we would be repeating the derivation of the Euler equation. We cannot use conservation of momentum here, since that does not apply on a per-component basis, but we can use the explicit form of the collision operator (5) to obtain

$$\sum_i\frac{\vec{v_i}}{\tau}\left[\Omega_\sigma(f_\sigma)\right]_i=-\sum_i\frac{\vec{v_i}}{\tau\xi_\sigma}\left[f_{\sigma,i}-f_{\sigma,i}^{(eq)}\right] \tag{39}$$

Thus from (37), (38), and (39) we have

$$\begin{aligned}-(\rho_\sigma/\rho)\nabla_0 p+v^2\left(\frac{1-d}{2}\right)\nabla_0\rho_\sigma &= -\sum_i\frac{\vec{v_i}}{\epsilon\tau\xi_\sigma}\left[f_{\sigma,i}-f_{\sigma,i}^{(eq)}\right]\\ &= -\sum_i\frac{\vec{v_i}}{\epsilon\tau\xi_\sigma}\left[f_{\sigma,i}^{(0)}+\epsilon f_{\sigma,i}^{(1)}-f_{\sigma,i}^{(eq)}\right]\\ &= -\frac{1}{\epsilon\tau\xi_\sigma}\left[\rho_\sigma(\vec{u}-\vec{u}^{(eq)})+\epsilon\sum_i\vec{v_i}f_{\sigma,i}^{(1)}-\xi_\sigma\tau\vec{F_\sigma}\right]\end{aligned}$$

where the last equality uses (8) and (10).

Now we solve for the $f^{(1)}$ term:

$$\sum_i \vec{v}_i f^{(1)}_{\sigma,i} = -\frac{\rho_\sigma(\vec{u}-\vec{u}^{(eq)})}{\epsilon} + \frac{\xi_\sigma \tau \vec{F_\sigma}}{\epsilon} - \tau\xi_\sigma\left[-(\rho_\sigma/\rho)\nabla_0 p + v^2\left(\frac{1-d}{2}\right)\nabla_0\rho_\sigma\right] \tag{40}$$

We still need to eliminate the $\vec{u}^{(eq)}$, but here we can just use (21) and sum (40) over $\sigma$ to obtain

$$-\frac{\tau}{2\epsilon}\sum_\sigma \vec{F_\sigma} = -\frac{\rho(\vec{u}-\vec{u}^{(eq)})}{\epsilon} + \frac{\tau}{\epsilon}\sum_\sigma \xi_\sigma \vec{F_\sigma} + \frac{\tau\nabla_0 p}{\rho}\sum_\sigma \xi_\sigma\rho_\sigma - v^2\left(\frac{1-d}{2}\right)\tau\sum_\sigma \xi_\sigma\nabla_0\rho_\sigma \tag{41}$$

So

$$\frac{\rho_\sigma(\vec{u}-\vec{u}^{(eq)})}{\epsilon} = (\rho_\sigma/\rho)\left[\frac{\tau}{2\epsilon}\sum_\sigma \vec{F_\sigma} + \frac{\tau}{\epsilon}\sum_\sigma \xi_\sigma \vec{F_\sigma} + \frac{\tau\nabla_0 p}{\rho}\sum_\sigma \xi_\sigma\rho_\sigma - v^2\left(\frac{1-d}{2}\right)\tau\sum_\sigma \xi_\sigma\nabla_0\rho_\sigma\right] \tag{42}$$

and

$$\begin{aligned}\sum_i \vec{v}_i f^{(1)}_{\sigma,i} &= \frac{\xi_\sigma \tau \vec{F_\sigma}}{\epsilon} - \tau\xi_\sigma\left[-(\rho_\sigma/\rho)\nabla_0 p + v^2\left(\frac{1-d}{2}\right)\nabla_0\rho_\sigma\right] \\ &- (\rho_\sigma/\rho)\left[\frac{\tau}{2\epsilon}\sum_\sigma \vec{F_\sigma} + \frac{\tau}{\epsilon}\sum_\sigma \xi_\sigma \vec{F_\sigma} + \frac{\tau\nabla_0 p}{\rho}\sum_\sigma \xi_\sigma\rho_\sigma - v^2\left(\frac{1-d}{2}\right)\tau\sum_\sigma \xi_\sigma\nabla_0\rho_\sigma\right] \end{aligned} \tag{43}$$

If we now return to (35) and substitute expressions obtained in (37) and (43), we get

$$\begin{aligned}\frac{\partial\rho_\sigma}{\partial t_1} &= -\frac{\xi_\sigma\tau}{\epsilon}\nabla_0\cdot\vec{F_\sigma} + (\tau\xi_\sigma - \tau/2)\nabla_0\cdot\left[-(\rho_\sigma/\rho)\nabla_0 p + v^2\left(\frac{1-d}{2}\right)\nabla_0\rho_\sigma\right] \\ &+ \nabla_0\cdot\frac{\rho_\sigma}{\rho}\left[\frac{\tau}{2\epsilon}\sum_\sigma \vec{F_\sigma} + \frac{\tau}{\epsilon}\sum_\sigma \xi_\sigma \vec{F_\sigma} + \frac{\tau\nabla_0 p}{\rho}\sum_\sigma \xi_\sigma\rho_\sigma - v^2\left(\frac{1-d}{2}\right)\tau\sum_\sigma \xi_\sigma\nabla_0\rho_\sigma\right]\end{aligned} \tag{44}$$

**5. Timescale $t$.** We can now recover behavior at timescale $t$. Add $\epsilon\times$(20) + $\epsilon^2\times$(44). We get

$$\begin{aligned}\frac{\partial\rho_\sigma}{\partial t} + \nabla\cdot(\rho_\sigma\vec{u}) &= -\xi_\sigma\tau\nabla\cdot\vec{F_\sigma} + (\tau\xi_\sigma - \tau/2)\nabla\cdot\left[-(\rho_\sigma/\rho)\nabla p + v^2\left(\frac{1-d}{2}\right)\nabla\rho_\sigma\right] \\ &+ \tau\nabla\cdot\frac{\rho_\sigma}{\rho}\left[\frac{1}{2}\sum_\sigma \vec{F_\sigma} + \sum_\sigma \xi_\sigma \vec{F_\sigma} + \frac{\nabla p}{\rho}\sum_\sigma \xi_\sigma\rho_\sigma - v^2\left(\frac{1-d}{2}\right)\sum_\sigma \xi_\sigma\nabla\rho_\sigma\right]\end{aligned} \tag{45}$$

It is worth noting that if we sum (45) over $\sigma$, we obtain

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0 \tag{46}$$

the ordinary continuity equation at timescale $t$. Thus the interesting, per-component behavior is contained in (45).

## 6. Forces.

We assume the interaction potential, $V$, is of the form:

$$V = (1/2)\sum_{\sigma_1}\sum_{\sigma_2} G_{\sigma_1,\sigma_2}\Psi_{\sigma_1}(\rho_{\sigma_1})\Psi_{\sigma_2}(\rho_{\sigma_2}) \tag{47}$$

where $G_{\sigma_1,\sigma_2} = G_{\sigma_2,\sigma_1}$ is a symmetric *strength of interaction* and $\Psi_{\sigma_i}$ is an *effective density*. Since

$$\nabla V = \sum_{\sigma_1}\sum_{\sigma_2} G_{\sigma_1,\sigma_2}\Psi_{\sigma_1}(\rho_{\sigma_1})\Psi'_{\sigma_2}(\rho_{\sigma_2})\nabla\rho_{\sigma_2} \tag{48}$$

we can take

$$\vec{F_{\sigma_1}} = -\Psi_{\sigma_1}(\rho_{\sigma_1}) \sum_{\sigma_2} G_{\sigma_1,\sigma_2} \Psi'_{\sigma_2}(\rho_{\sigma_2}) \nabla \rho_{\sigma_2} \tag{49}$$

so that $\nabla V = -\sum_\sigma \vec{F_\sigma}$, as required.

To include external forces that are not interactions, e.g., gravity and buoyancy, we write instead

$$\vec{F_{\sigma_i}} = -\Psi_{\sigma_i}(\rho_{\sigma_i}) \sum_{\sigma_j} G_{\sigma_i,\sigma_j} \Psi'_{\sigma_j}(\rho_{\sigma_j}) \nabla \rho_{\sigma_j} + \rho_{\sigma_i} \vec{g_{\sigma_i}} \tag{50}$$

where $\vec{g_{\sigma_i}}$ carries the non-interactive external force on component $\sigma_i$. Now $\nabla V = -\sum_\sigma \vec{F_\sigma} + \sum_\sigma \rho_\sigma \vec{g_\sigma}$, and so we need to correct (28) and all subsequent expressions involving $\nabla p$, in particular, (32) and (45), by replacing $\nabla p$ with $\nabla p - \sum_\sigma \rho_\sigma \vec{g_\sigma}$ wherever it occurs.

## 7. Thermal Energy.

In his simulation of Rayleigh-Bénard convection (Physical Review E 55(3), March 1997), Shan argues that when viscous and compressive heating effects can be neglected, temperature can be modeled as a separate component whose molecular mass is (relatively) 0. Assume we have only two components where the second is thermal energy. To simplify notation, assume $\xi_1 = \xi_2 = \xi$. Then from (45) and (28) we have

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \vec{u}) = \tau \nabla \cdot \left[ (\xi - 1/2) v^2 \left( \frac{1-d}{2} \right) \left[ \frac{\rho_1}{\rho} \nabla \rho_2 - \frac{\rho_2}{\rho} \nabla \rho_1 \right] + \xi \left[ \frac{\rho_2}{\rho} \vec{F_1} - \frac{\rho_1}{\rho} \vec{F_2} \right] \right] \tag{51}$$

If we now use (49) and assume that $G_{i,j} = 0$ for $i \neq j$, we can collect coefficients of density gradients to obtain

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \vec{u}) = \tau \nabla \cdot \left[ \frac{\rho_1}{\rho} \left( (\xi - 1/2) v^2 \frac{1-d}{2} + \xi \Psi_2 G_{22} \Psi'_2 \right) \nabla \rho_2 - \frac{\rho_2}{\rho} \left( (\xi - 1/2) v^2 \frac{1-d}{2} + \xi \Psi_1 G_{11} \Psi'_1 \right) \nabla \rho_1 \right] \tag{52}$$

If the relative densities now approach limits, $\rho_1/\rho \to 1$ and $\rho_2/\rho \to 0$ we get

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \vec{u}) = \tau \nabla \cdot \left[ \left( (\xi - 1/2) v^2 \left( \frac{1-d}{2} \right) + \xi \Psi_2 G_{22} \Psi'_2 \right) \nabla \rho_2 \right] \tag{53}$$

If we also have $G_{22} = 0$, we get

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot (\rho_2 \vec{u}) = D \nabla^2 \rho_2 \tag{54}$$

where $D = \tau(\xi - 1/2) v^2 \left( \frac{1-d}{2} \right)$. Thus thermal energy is advected and diffused.

## 8. Phase Transition.

Again suppose we have two components where the second is thermal energy. Assume $G_{\sigma_1,\sigma_2} = 0$, except for $G_{11}$, so $V = G_{11} \Psi_1^2(\rho_1)$. From (27) we have

$$p = v^2 \left( \frac{1-d}{2} \right) (\rho_1 + \rho_2) + G_{11} \Psi_1^2(\rho_1) \tag{55}$$

If $G_{11}$ is negative and $\Psi_1$ is increasing and bounded, there can be a range (of $\rho_1$) over which $dp/d\rho_1$ is negative, which signals a phase transition.

## 9. The Navier-Stokes Equation.

The remaining step is to derive the Navier-Stokes equation. The procedure here is similar to what we have already done. In particular, we need to multiply both sides of (18) by $\vec{v}_i$, sum over $i$, sum over $\sigma$, divide by $\tau$, and then equate coefficients of $\epsilon^2$.

We obtain:

$$\frac{\partial(\rho\vec{u})}{\partial t_1} + \sum_\sigma \nabla_0 \cdot \Pi_\sigma^{(1)} + (\tau/2)\frac{\partial^2(\rho\vec{u})}{\partial t_0^2} + \tau\frac{\partial}{\partial t_0}\left(\sum_\sigma \nabla_0 \cdot \Pi_\sigma^{(0)}\right) + (\tau/2)\sum_\sigma \nabla_0 \cdot \left(\nabla_0 \cdot S_\sigma^{(0)}\right) = 0 \qquad (56)$$

where $\Pi_\sigma^{(1)}$ is the momentum tensor of (24) with $f^{(0)}$ replaced by $f^{(1)}$, and $S_\sigma^{(0)}$ is a third-order tensor:

$$S_\sigma^{(0)}(\vec{r},t)_{\alpha\beta\gamma} = \sum_i v_{i\alpha}v_{i\beta}v_{i\gamma}f_{\sigma,i}^{(0)}(\vec{r},t) \qquad \text{where } \alpha,\beta,\gamma \in \{\text{x,y,z}\} \qquad (57)$$

We can combine the third and fourth summands on the left of equation (56) by using the preliminary form of the Euler equation (23). This gives us:

$$\frac{\partial(\rho\vec{u})}{\partial t_1} + \sum_\sigma \nabla_0 \cdot \Pi_\sigma^{(1)} + (\tau/2)\frac{\partial}{\partial t_0}\left(\vec{H} + \sum_\sigma \nabla_0 \cdot \Pi_\sigma^{(0)}\right) + (\tau/2)\sum_\sigma \nabla_0 \cdot \left(\nabla_0 \cdot S_\sigma^{(0)}\right) = 0 \qquad (58)$$

We now obtain the preliminary form of the Navier-Stokes equation as $\epsilon\times$(23) + $\epsilon^2\times$(58):

$$\frac{\partial(\rho\vec{u})}{\partial t} + \sum_\sigma \nabla \cdot \Pi_\sigma + (\tau/2)\left[\epsilon\frac{\partial}{\partial t_0}\left(\sum_\sigma \vec{F}_\sigma + \sum_\sigma \nabla \cdot \Pi_\sigma^{(0)}\right) + \sum_\sigma \nabla \cdot \left(\nabla \cdot S_\sigma^{(0)}\right)\right] = \sum_\sigma \vec{F}_\sigma \qquad (59)$$

Reducing this equation to its conventional form will require considerable effort.

First, we can use (28) to replace the right side, and we can use the identities on the $v_i$s to reduce the third-order tensor,

$$\sum_\sigma \nabla \cdot \left(\nabla \cdot S_\sigma^{(0)}\right) = (2/3)v^2\left[\nabla\left(\nabla \cdot (\rho\vec{u})\right) + (1/2)\nabla^2(\rho\vec{u})\right] \qquad (60)$$

Making these substitutions, we have

$$\begin{aligned}\frac{\partial(\rho\vec{u})}{\partial t} + \sum_\sigma \nabla \cdot \Pi_\sigma \quad &+ \quad \frac{\tau}{2}\left[\frac{\epsilon\partial}{\partial t_0}\left(\sum_\sigma \vec{F}_\sigma + \sum_\sigma \nabla \cdot \Pi_\sigma^{(0)}\right) + \frac{2}{3}v^2\left[\nabla\left(\nabla \cdot (\rho\vec{u})\right) + \frac{1}{2}\nabla^2(\rho\vec{u})\right]\right] \\ &= \quad v^2\frac{1-d}{2}\nabla\rho - \nabla p + \sum_\sigma \rho_\sigma\vec{g}_\sigma \end{aligned} \qquad (61)$$

The term $\sum_\sigma \nabla \cdot \Pi_\sigma$ on the left-hand side of (61) contains $\sum_\sigma \nabla \cdot \Pi_\sigma^{(0)}$ as a summand. We have already seen (25) that we can write this summand as

$$\sum_\sigma \nabla \cdot \Pi_\sigma^{(0)} = v^2\frac{1-d}{2}\nabla\rho + \nabla \cdot (\rho\vec{u}\vec{u}) \qquad (62)$$

The first term of (62) will cancel the corresponding term on the right-hand side of (61). The second term of (62) can be combined with the first term on the left-hand side of (61), using the argument of (31), to factor $\rho$. We are left with

$$\begin{aligned}\rho\left(\frac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) \quad &+ \quad \epsilon\sum_\sigma \nabla \cdot \Pi_\sigma^{(1)} + \frac{\tau\epsilon}{2}\frac{\partial}{\partial t_0}\left(\sum_\sigma \vec{F}_\sigma + \sum_\sigma \nabla \cdot \Pi_\sigma^{(0)}\right) + \frac{\tau v^2}{3}\left[\nabla\left(\nabla \cdot (\rho\vec{u})\right) + \frac{1}{2}\nabla^2(\rho\vec{u})\right] \\ &= \quad -\nabla p + \sum_\sigma \rho_\sigma\vec{g}_\sigma \end{aligned} \qquad (63)$$

For differentiation with respect to $t_0$, we will use an order 1 approximation in $\rho$ and $\vec{u}$. Thus

$$\begin{aligned}
\frac{\tau\epsilon}{2}\frac{\partial}{\partial t_0}\left(\sum_\sigma \nabla\cdot\Pi_\sigma^{(0)}\right) &= \frac{\tau\epsilon}{2}\nabla\cdot\left(\frac{\partial}{\partial t_0}\sum_\sigma \Pi_\sigma^{(0)}\right) \\
&= \frac{\tau\epsilon}{2}\nabla\cdot\left(\frac{\partial}{\partial t_0}v^2\frac{1-d}{2}\rho I\right) \qquad \text{(order 1)} \\
&= -\frac{\tau v^2(1-d)}{4}\nabla\cdot(\nabla\cdot(\rho\vec{u})I) \qquad \text{(continuity equation)} \\
&= -\frac{\tau v^2(1-d)}{4}\nabla\left(\nabla\cdot(\rho\vec{u})\right) \qquad (64)
\end{aligned}$$

Making this substitution into (63), we have

$$\rho\left(\frac{\partial\vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u}\right)+\epsilon\sum_\sigma\nabla\cdot\Pi_\sigma^{(1)}+\frac{\tau\epsilon}{2}\frac{\partial}{\partial t_0}\sum_\sigma\vec{F}_\sigma+\tau v^2(\frac{1}{3}-\frac{1-d}{4})\nabla\left(\nabla\cdot(\rho\vec{u})\right)=-\nabla p+\sum_\sigma\rho_\sigma\vec{g}_\sigma-\frac{\tau v^2}{6}\nabla^2(\rho\vec{u}) \qquad (65)$$

All that remains is to reduce the second and third terms on the left-hand side of (65). For the second term, observe that

$$\left(\epsilon\Pi_\sigma^{(1)}\right)_{\alpha\beta}=\sum_i\epsilon f_{\sigma,i}^{(1)}v_{i\alpha}v_{i\beta} \qquad \text{for } \alpha,\beta\in\{\text{x,y,z}\} \qquad (66)$$

and so we need an expression for $\epsilon f_{\sigma,i}^{(1)}$ in terms of $\rho$ and $\vec{u}$. If we insert the definition of $\Omega_\sigma$ (5) into the Taylor expansion (18) and simply equate coefficients of $\epsilon^1$, we obtain

$$\frac{\partial}{\partial t_0}f_{\sigma,i}^{(0)}+\vec{v}_i\cdot\nabla_0 f_{\sigma,i}^{(0)}=-\frac{1}{\xi_\sigma\tau\epsilon}\left(f_{\sigma,i}^{(0)}+\epsilon f_{\sigma,i}^{(1)}-f_{\sigma,i}^{(eq)}\right) \qquad (67)$$

and so

$$\epsilon f_{\sigma,i}^{(1)}=-\epsilon\tau\xi_\sigma\left(\frac{\partial}{\partial t_0}f_{\sigma,i}^{(0)}+\vec{v}_i\cdot\nabla_0 f_{\sigma,i}^{(0)}\right)-\left(f_{\sigma,i}^{(0)}-f_{\sigma,i}^{(eq)}\right) \qquad (68)$$

and

$$\left(\epsilon\Pi_\sigma^{(1)}\right)_{\alpha\beta}=-\epsilon\tau\xi_\sigma\left(\sum_i\frac{\partial}{\partial t_0}f_{\sigma,i}^{(0)}v_{i\alpha}v_{i\beta}\right)-\epsilon\tau\xi_\sigma\left(\sum_i\vec{v}_i\cdot\nabla_0 f_{\sigma,i}^{(0)}v_{i\alpha}v_{i\beta}\right)-\sum_i\left(f_{\sigma,i}^{(0)}-f_{\sigma,i}^{(eq)}\right)v_{i\alpha}v_{i\beta} \qquad (69)$$

We will now reduce each of the three principal summands on the right-hand side of (69). We again resort to an order 1 approximation, i.e.,

$$f_{\sigma,i}^{(0)}(\vec{r},t)=\begin{cases}\rho_\sigma d & \text{i = 0}\\ 2\rho_\sigma\left(\frac{1-d}{24}+\frac{1}{12v^2}\vec{v}_i\cdot\vec{u}\right) & \text{i = 1,...,6}\\ \rho_\sigma\left(\frac{1-d}{24}+\frac{1}{12v^2}\vec{v}_i\cdot\vec{u}\right) & \text{i = 7,...,18}\end{cases} \qquad (70)$$

with a like expression for $f_{\sigma,i}^{(eq)}$, obtained by replacing $\vec{u}$ with $\vec{u}^{(eq)}$.

The rightmost term of (69) vanishes. The difference has $\vec{v}_i$ as a factor, and it is easy to verify that $\sum_i v_{i\alpha}v_{i\beta}v_{i\gamma}=0$ for any $\alpha,\beta,\gamma$.

To the leftmost term on the right-hand side of (69) we apply the chain rule:

$$\frac{\partial f_{\sigma,i}^{(0)}}{\partial t_0}=\frac{\partial f_{\sigma,i}^{(0)}}{\partial\rho_\sigma}\frac{\partial\rho_\sigma}{\partial t_0}+\sum_{\gamma\in\{\text{x,y,z}\}}\frac{\partial f_{\sigma,i}^{(0)}}{\partial(\rho_\sigma\vec{u})_\gamma}\frac{\partial(\rho_\sigma\vec{u})_\gamma}{\partial t_0} \qquad (71)$$

The first term on the right-hand side of (71) is now easily reduced. From the order 1 approximation we have:

$$\frac{\partial f_{\sigma,i}^{(0)}}{\partial\rho_\sigma}=\begin{cases}d & \text{i = 0}\\ \frac{1-d}{12} & \text{i = 1,...,6}\\ \frac{1-d}{24} & \text{i = 7,...,18}\end{cases} \qquad (72)$$

and by the continuity equation

$$\frac{\partial \rho_\sigma}{\partial t_0} = -\nabla_0 \cdot (\rho_\sigma \vec{u}) \tag{73}$$

The remaining terms on the right-hand side of (71) contribute nothing. To see this, observe that

$$\frac{\partial f^{(0)}_{\sigma,i}}{\partial(\rho_\sigma \vec{u})_\gamma} = \begin{cases} 0 & \text{i = 0} \\ \frac{v_{i\gamma}}{6v^2} & \text{i = 1,...,6} \\ \frac{v_{i\gamma}}{12v^2} & \text{i = 7,...,18} \end{cases} \tag{74}$$

and by (36)

$$\frac{\partial(\rho_\sigma \vec{u})}{\partial t_0} = -\nabla_0 \cdot [\rho_\sigma \vec{u}\vec{u}] - (\rho_\sigma/\rho)\nabla_0 p \tag{75}$$

and so each summand will have a single $v_{i\gamma}$ as a factor. Again we rely on the identity, $\sum_i v_{i\alpha} v_{i\beta} v_{i\gamma} = 0$. Thus the total contribution to (69) is

$$-\epsilon\tau\xi_\sigma \left( \sum_i \frac{\partial}{\partial t_0} f^{(0)}_{\sigma,i} v_{i\alpha} v_{i\beta} \right) = \tau\xi_\sigma \left[\nabla \cdot (\rho_\sigma \vec{u})\right] \left(\frac{1-d}{2}\right) v^2 \delta_{\alpha\beta} \tag{76}$$

where $\delta_{\alpha\beta}$ denotes Kronecker delta.

Finally, the middle term on the right-hand side of (69) can be handled similarly. We observe that, to order 1,

$$\vec{v}_i \cdot \nabla_0 f^{(0)}_{\sigma,i} = \begin{cases} d\vec{v}_i \cdot \nabla_0 \rho_\sigma & \text{i = 0} \\ 2\left(\frac{1-d}{24}\vec{v}_i \cdot \nabla_0 \rho_\sigma + \frac{1}{12v^2}\vec{v}_i \cdot \nabla_0(\rho_\sigma \vec{v}_i \cdot \vec{u})\right) & \text{i = 1,...,6} \\ \left(\frac{1-d}{24}\vec{v}_i \cdot \nabla_0 \rho_\sigma + \frac{1}{12v^2}\vec{v}_i \cdot \nabla_0(\rho_\sigma \vec{v}_i \cdot \vec{u})\right) & \text{i = 7,...,18} \end{cases} \tag{77}$$

Then again we can use the identity, $\sum_i v_{i\alpha} v_{i\beta} v_{i\gamma} = 0$, to obtain

$$\begin{aligned} -\epsilon\tau\xi_\sigma \left( \sum_i \vec{v}_i \cdot \nabla_0 f^{(0)}_{\sigma,i} v_{i\alpha} v_{i\beta} \right) &= -\frac{\tau\xi_\sigma}{12v^2} \sum_{\gamma,\delta\in\{\text{x,y,z}\}} \sum_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} \frac{\partial(\rho_\sigma u_\gamma)}{\partial \delta} \\ &= -\tau\xi_\sigma \frac{v^2}{3}\left[\left(\frac{\partial(\rho_\sigma u_\alpha)}{\partial\beta} + \frac{\partial(\rho_\sigma u_\beta)}{\partial\alpha}\right) + \delta_{\alpha\beta}\nabla\cdot(\rho_\sigma\vec{u})\right] \end{aligned} \tag{78}$$

Collecting (76) and (78), we have reduced the second term of (65):

$$\epsilon \sum_\sigma \nabla \cdot \Pi^{(1)}_\sigma = -\tau v^2 \sum_\sigma \xi_\sigma \left[\left(\frac{2}{3} - \frac{1-d}{2}\right)\nabla\left[\nabla\cdot(\rho_\sigma\vec{u})\right] + \frac{1}{3}\nabla^2(\rho_\sigma\vec{u})\right] \tag{79}$$

Thus (65) can be written

$$\begin{aligned} \rho\left(\frac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u}\right) + \frac{\tau\epsilon}{2}\frac{\partial}{\partial t_0}\sum_\sigma \vec{F}_\sigma &= -\tau v^2\left(\frac{1}{3} - \frac{1-d}{4}\right)\sum_\sigma(1-2\xi_\sigma)\nabla\left(\nabla\cdot(\rho_\sigma\vec{u})\right) \\ &- \nabla p + \sum_\sigma \rho_\sigma \vec{g}_\sigma - \frac{\tau v^2}{6}\sum_\sigma (1-2\xi_\sigma)\nabla^2(\rho_\sigma\vec{u}) \end{aligned} \tag{80}$$

The final term, $\frac{\tau\epsilon}{2}\frac{\partial}{\partial t_0}\sum_\sigma \vec{F}_\sigma$, would be troublesome in the general case, but here we can take advantage of its explicit form. In particular, if $\Psi_{\sigma_i}(\rho_{\sigma_i})$ is the effective density, then to order 1 we can assume it is the identity function. Thus we have

$$\epsilon\frac{\partial}{\partial t_0}\sum_\sigma \vec{F}_\sigma = \sum_\sigma\left[\rho_\sigma\left(\sum_{\sigma'} G_{\sigma\sigma'}\nabla\left[\nabla\cdot(\rho_{\sigma'}\vec{u})\right]\right) - \nabla\cdot(\rho_\sigma\vec{u})\left(\vec{g}_\sigma - \sum_{\sigma'} G_{\sigma\sigma'}\nabla\rho_{\sigma'}\right)\right] \tag{81}$$

If we insert (81) into (80) and move to the incompressible limit, $\nabla\cdot(\rho_\sigma\vec{u}) \to 0$, we recover the conventional Navier-Stokes equation:

$$\frac{\partial\vec{u}}{\partial t} + \vec{u}\cdot\nabla\vec{u} = -(1/\rho)\nabla p + \sum_\sigma(\rho_\sigma/\rho)\vec{g}_\sigma - \frac{\tau v^2}{6\rho}\sum_\sigma(1-2\xi_\sigma)\nabla^2(\rho_\sigma\vec{u}) \tag{82}$$