Mechanical properties of a Lattice Boltzmann solid body

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1 The model

A simple, two-dimensional solid model can be defined as an array of particles connected according to a square topology. Each particle $\vec{\ell} = (i, j)$ is characterized by its spatial location $\vec{r}_{\vec{\ell}}(t)$ at the discrete time t and the list of neighbors it is connected to. A bulk particle is typically connected to four other particles (at North, West, South and East) but the shape of the solid boundary can be arbitrary and border particles may have three, two or even one neighbor.

Figure 1 gives an example of the type of solid body our model can deal with. A square sheet of particle with a given initial velocity keep bouncing over surrounding rigid walls. When a particle at the boundary of the solid reaches a wall, it is stopped and the solid start deforming until the entire object has bounced back. When the solid and the wall do not interact, the center of mass of the solid follows a straight line, as it should for a body whose momentum is conserved.

The internal dynamics of an object such as that of Fig. 1 can be expressed in terms of the forces $\vec{f}_i$ acting on each particles labeled $\vec{\ell}$ and caused by the elastic interactions with the neighbor connected through link i. The links are labeled from 1 to 4, for a square topology and could be thought of as some idealized springs. Figure 2 illustrates the situation and Fig. 3 explain the symbols.

The dynamic we propose to describe the propagation of the forces and deformation in the solid is based on the LB wave equation (see [1, 2]). For this reason, we also introduce a "rest" force $\vec{f}_0(\vec{\ell}, t)$ which can be used to adjust some internal properties of the solid.

Assuming that an external force $\vec{F}$ may be acting on the system, the dynamics can be written as

$$\begin{aligned} \vec{f}_i(\vec{\ell} + \vec{c}_i, t + \tau) &= M_{\vec{\ell}}^{-1} \vec{\Psi}_{\vec{\ell}}(t) - \vec{f}_{i+2}(\vec{\ell}, t) + M_{\vec{\ell}}^{-1} \frac{\vec{F}_{\vec{\ell}}(t)}{2} \\ \vec{f}_0(\vec{\ell}, t + \tau) &= M_0(\vec{\ell}) M_{\vec{\ell}}^{-1} \vec{\Psi}_{\vec{\ell}}(t) - \vec{f}_0(\vec{\ell}, t) + M_0(\vec{\ell}) M_{\vec{\ell}}^{-1} \frac{\vec{F}_{\vec{\ell}}(t)}{2} \end{aligned} \tag{1}$$

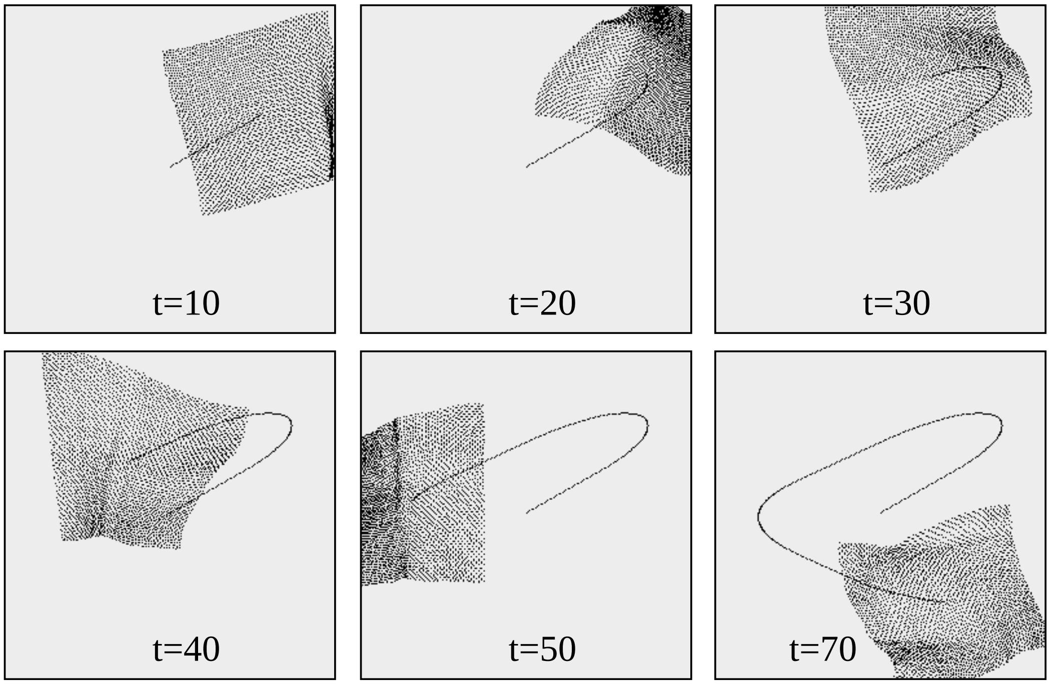

Figure 1: Simulation of a 2D LB solid object with an initial momentum and moving in a container with rigid walls.

where i runs over the links that connect the particle $\vec{\ell}$ to its neighbor. For bulk particle, i runs from 1 to 4, but at the boundary several links may be missing. The unit vectors $\vec{c}_i$ are typically $\vec{c}_1 = (1,0)$, $\vec{c}_2 = (0,1)$, $\vec{c}_3 = (-1,0)$ and $\vec{c}_4 = (0,-1)$ if the solid is aligned with the x- and y-axis.

Note that, according to our numering scheme, if the link $\vec{c}_{i+2}$ is present, then $\vec{f}_{i+2}(\vec{\ell},t)$ exists, as well as $\vec{f}_i(\vec{\ell}+\vec{c}_i, t+\tau)$. The first quantity is the incoming field and the second the outgoing one. They both travel across the bond connecting particles $\vec{\ell}$ and $\vec{\ell}+\vec{c}_i$.

In this equation $\vec{\Psi}$ is defined as

$$\vec{\Psi}_{\vec{\ell}}(t) = M_0(\vec{\ell})\vec{f}_0(\vec{\ell},t) + \sum_{i=1,4} \vec{f}_i(\vec{\ell},t) \tag{2}$$

and $M_{\vec{\ell}}$ is a mass which depends on the number of links the particle $\vec{\ell}$ is connected to and M_0 is a mass associated with the rest link. In this theory, it is posssible that M_0 be a 2×2 matrix (in 2D), coupling the x and y deformations. It may depends on the patricle $\vec{\ell}$

$$M_0(\vec{\ell}) = \begin{pmatrix} a_{\vec{\ell}} & b_{\vec{\ell}} \\ c_{\vec{\ell}} & d_{\vec{\ell}} \end{pmatrix} \tag{3}$$

The following remarks are important

- The rest field $\vec{f}_0 \neq 0$ and $M_0 \neq 0$ allows us to tune the speed of sound in the model. It is also a way to adjust the **elasticity contant** of the material.
- The idea of considering M_0 as a matrix allows us to couple the x and y deformations. Without it, a 2D solid will have only one elasticity constant.
- So far we have not much results when M_0 is a matrix. However, we keep it such in the following derivations in order to be general. Note that many of the proofs given below are algebraically much simple when M_0 is a scalar.

The appropriate choice for M is to consider a contribution of the rest mass M_0 plus 1/2 per link (see also [3]). Thus, if particle $\vec{\ell}$ has K neighbors, we define

$$M_{\vec{\ell}} = \frac{1}{2}\left(M_0^2(\vec{\ell}) + K\mathbf{1}\right) \tag{4}$$

where $\mathbf{1}$ is the identity matrix.

For the 2D case, the number of links is smaller than or equal to 4. But this model extends easily to 3D.

It is easy to show that Eq. (1), although it is a vector equation, has the same form as the BGK Eq. (5)

$$N_i(\vec{r}+\tau\vec{v}_i, t+\tau) = N_i(\vec{r},t) + \omega\left(N_i^{(0)}(\vec{r},t) - N_i(\vec{r},t)\right) \tag{5}$$

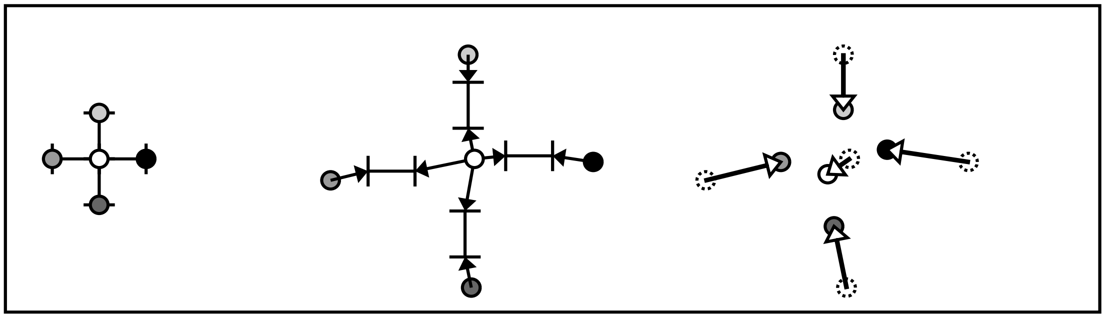

Figure 2: The internal dynamics of a LB solid. The $\vec{f}_k$'s are interpreted as the forces acting on a particle due to the local deformation of the structure. These forces result in the motion of the particle which, in turn give rise to a redistribution of the forces to the nearest neighbors. On the left, a fragment of five particles in a rest configuration is shown; in the middle, the fragment is under strain; on the right, the particle displacement caused by the forces is displayed.

with $\omega = 2$ (which ensures time reversal invariance) and

$$N_i^{(0)} = \frac{1}{2} M^{-1} \vec{\Psi} + \frac{1}{2} \vec{c}_i J$$

where the tensor J reads

$$J_{\alpha\beta} = \sum_{i>0} c_{i\alpha} f_{i\beta}$$

1.1 Link with the LB wave equation

The LB wave equation is expressed as

$$\begin{aligned} N_i^{\text{out}} &= \frac{1}{dn^2}\Psi - N_{i+2} \\ N_0^{\text{out}} &= 2\frac{n^2-1}{n^2}\Psi - N_0 \end{aligned} \tag{6}$$

where d is the dimension of the space and n the refraction index. Here, in addition Ψ is defined as $\Psi = N_0 + \sum_{i>0} N_i$

Therefore, the change of variable to connect with relation (1) is $f_0 = N_0/M_0$, $f_i = N_i$. By dividing the second equation of the above system by M_0 one obtains

$$\begin{aligned} f_i^{\text{out}} &= \frac{1}{dn^2}\Psi - f_{i+2} \\ f_0^{\text{out}} &= 2\frac{n^2-1}{n^2}\frac{1}{M_0}\Psi - f_0 \end{aligned} \tag{7}$$

with

$$\Psi = M_0 \frac{N_0}{M_0} + \sum_{i>0} N_i = M_0 f_0 + \sum_{i>0} f_i$$

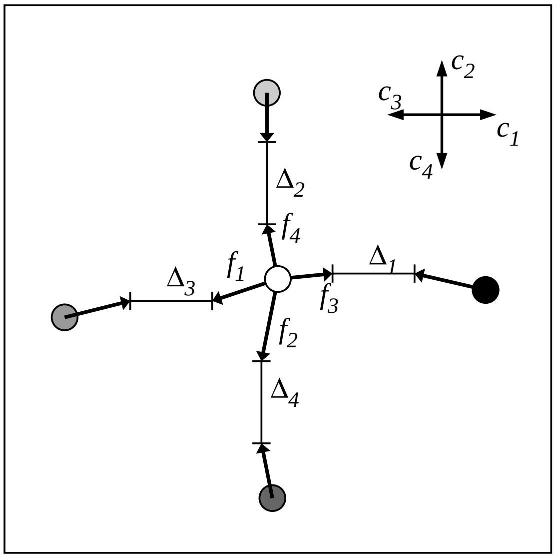

Figure 3: Labeling of the forces and directions. By definition, the forces are labeled according to the direction through which the interaction has propagated. For instance, $\vec{f}_3(\vec{\ell})$ comes from particle $\vec{\ell}+\vec{c}_1$ through link $\vec{c}_3$. Finally, the quantities $\vec{\Delta}_i$ designate the spring at rest connecting particle $\vec{\ell}$ to $\vec{\ell}+\vec{c}_i$.

By identification of the coefficient in (7) and (1) one then obtains

$$M = dn^2 \qquad \frac{M_0^2}{M} = 2\frac{n^2-1}{n^2}$$

With the fact that the number of links is twice the dimension, i.e. $K = 2d$, one recover the relation $M_0^2 + 2d = 2M$ and we can relate the refraction index through the relation

$$n^2 = 1 + \frac{M_0^2}{K}$$

2 Motion of the particles

Equation (1) describes how the forces evolve in the solid. These forces also cause the solid particles to move. Let $\vec{r}_{\vec{\ell}}(t)$ denote the location of particle $\vec{\ell}$. Usually, this location does not correspond to a lattice site. The rule of motion is

$$\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t) + M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) + M_{\vec{\ell}}^{-1}\frac{\vec{F}_{\vec{\ell}}(t)}{2} \tag{8}$$

A geometrical interpretation of this relation is given in [1] for a particular case. A more formal proof is given by the fact that $\vec{\Psi}$ is a locally conserved quantity which represents the momentum of each particle (see below). This equation can be seen as the integration over a time step unity of Newton's law $F = ma$.

3 Boundary conditions

In this model, there are boundary conditions for the $\vec{f}_i$ which, as explained perviously, are naturally implemented through the presence or absence of the links connecting a particle with its neighbor. For example, in a fracture process, some bond may break if the local stress is too large.

However, other boundary conditions are necessary if the solid body is not in an infinit free space. In cas of obstacles, Eq. 8 must be supplemented by some conditions expressing the fact that the new position $\vec{r}_{\vec{\ell}}(t+\tau)$ is constraint locally, as for instance the rigid wall in fig. 1.

The external force $\vec{F}$ is a way to impose such constaints. For instance, if a particle is forced to stay motionless, it is easy to compute the value $\vec{F}_{\vec{\ell}}(t)$ necessary to have $\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t)$

4 Conservation of momentum

The quantity $\vec{\Psi}_{\vec{\ell}}(t) = M_0(\vec{\ell})\vec{f}_0 + \sum_i \vec{f}_i(\vec{\ell}, t)$ can be interpreted as the momentum of the particle. We shall see that it is locally conserved for any shape of the object, as long as the external force is zero. Otherwise, the variation of $\vec{\Psi}_{\vec{\ell}}$ between two iteration is equal to the force, as expected in Newtionian mechanics.

It is convenient to define the post-collision forces

$$\vec{f}_i^{\text{out}}(\vec{\ell}) = \vec{f}_i(\vec{\ell} + \vec{c}_i, t+\tau)$$

that is the quantities that will propagate to the neighboring site.

From eqs. (1) and (2), we may compute the sum of the $\vec{f}_i^{\text{out}}$'s that we note $\vec{\Psi}_{\vec{\ell}}^{\text{out}}$

$$\begin{aligned} \vec{\Psi}^{\text{out}} &\equiv M_0\vec{f}_0^{\text{out}} + \sum_{i>0} \vec{f}_i^{\text{out}} \\ &= M_0^2 M^{-1}\vec{\Psi} - M_0\vec{f}_0 + M_0^2 M^{-1}\frac{\vec{F}}{2} \\ &\quad +KM^{-1}\vec{\Psi} - \vec{\Psi} + M_0\vec{f}_0 + KM^{-1}\frac{\vec{F}}{2} \end{aligned} \tag{9}$$

where we have used that $\sum_i \vec{\Psi} = K\vec{\Psi}$ since there are K links and $\sum_{i>0} \vec{f}_{i+2} = \vec{\Psi} - M_0\vec{f}_0$. Therefore, we obtain

$$\begin{aligned} \vec{\Psi}^{\text{out}} &= \left[\left(M_0^2 + K)M^{-1}\right)\vec{\Psi}\right] - \vec{\Psi} + \left(M_0^2 + K)M^{-1}\right)\vec{F} \\ &= \vec{\Psi} + \vec{F} \end{aligned} \tag{10}$$

since $M_0^2 + K = 2M$ (see eq. (4)). In other words, the variation of $\vec{\Psi}$ from time t to time $t+\tau$ is the the external force. This justifies our interpretation of $\vec{\Psi}_{\vec{\ell}}$ as the momentum of particle $\vec{\ell}$.

5 Conservation of Energy

A second conserved quantity that can be defined in this model is

$$E_{\vec{\ell}}(t) = \sum_{i \geq 0} \vec{f}_i^{\,2}(\vec{\ell}, t) \tag{11}$$

that we shall interpret as the energy of node $\vec{\ell}$. We now compute how this quantity changes after one iteration.

It is convenient to define

$$\vec{\Phi} = \vec{\Psi} + \frac{\vec{F}}{2} \tag{12}$$

so that the dynamics (1) simply reads

$$\begin{aligned} \vec{f}_i^{\text{out}} &= M^{-1}\vec{\Phi} - \vec{f}_{i+2} \\ \vec{f}_0^{\text{out}} &= M_0 M^{-1}\vec{\Phi} - \vec{f}_0 \end{aligned} \tag{13}$$

Therefore the energy change after the interaction can be expressed as

$$\begin{aligned} E^{\text{out}} = & \sum_{i \geq 0} \left(\vec{f}_i^{\text{out}}\right)^2 \\ = & \left(M_0 M^{-1}\vec{\Phi} - \vec{f}_0\right)^2 + \sum_{i>0} \left(M^{-1}\vec{\Phi}\vec{f}_{i+2}^{\,2}\right)^2 \\ = & (M_0 M^{-1}\vec{\Phi})^T (M_0 M^{-1}\vec{\Phi}) - 2(M_0 M^{-1}\vec{\Phi})^T \vec{f}_0 + \vec{f}_0^{\,2} \\ + & \sum_{i>0} \left[(M^{-1}\vec{\Phi})^T (M^{-1}\vec{\Phi}) - 2(M^{-1}\vec{\Phi})^T \vec{f}_{i+2} + f_{i+2}^2\right] \\ = & E^{\text{in}} + \vec{\Phi}^T (M^{-1})^T \left[M_0^T M_0 + K\right] M^{-1}\vec{\Phi} \\ - & 2\vec{\Phi}^T M_0^T (M^{-1})^T \vec{f}_0 - 2\vec{\Phi}^T (M^{-1})^T \sum_{i>0} \vec{f}_{i+2} \end{aligned} \tag{14}$$

where the subscript ^{T} designate the matrix transpose operation. Using that (see eq. 12))

$$\sum_{i>0} \vec{f}_{i+2} = \vec{\Phi} - \frac{\vec{F}}{2} - M_0 \vec{f}_0$$

and

$$M_0^T M_0 + K = 2M$$

which follows from (4) provided that M_0 is **symmetric**, one obtains

$$\begin{aligned} E^{\text{out}} = & E^{\text{in}} + 2\vec{\Phi}^T (M^{-1})^T \vec{\Phi} - 2\vec{\Phi}^T M_0^T (M^{-1})^T \vec{f}_0 \\ - & 2\vec{\Phi}^T (M^{-1})^T \vec{\Phi} + \vec{\Phi}^T (M^{-1})^T \vec{F} + 2\vec{\Phi}^T (M^{-1})^T M_0 \vec{f}_0 \\ = & E^{\text{in}} + \left(M^{-1}\Phi\right)^T \vec{F} \end{aligned} \tag{15}$$

From eq. (8), one has

$$M^{-1}\Phi = \vec{r}(t+\tau) - \vec{r}(t)$$

and the energy variation for particle $\vec{\ell}$ in then

$$E^{\rm out} = E^{\rm in} + (\vec{r}(t+\tau) - \vec{r}(t)) \cdot \vec{F} \qquad (16)$$

In conclusion,

- When the external force vanishes, the energy $E = \sum_{i\geq 0} \vec{f}_i^2$ is exaclty conserved for any shape of the object (i.e. our result does not depends on the number K of links).
- Otherwise, the variation of the energy is the work done by the external force.

This justifies our interpretation of E as the energy.

It turns out that the energy can be split into a kinetic plus an elastic contribution as can be seen in the next sections.

6 Case of a free particle

In this section we consider the case of a single particle, for which $K = 0$, i.e. it is not connected to any neighbors.

One has then $M = M_0^2/2$ (or $M^{-1} = 2M_0^{-2}$) and, since the $\vec{f}_i$'s do not exists for $i > 0$, there is only a dynamics for $\vec{f}_0$ which reduces to

$$\vec{f}_0^{\rm out} = M_0 M^{-1}\vec{\Psi} - \vec{f}_0 + M_0 M^{-1}\frac{\vec{F}}{2}$$

with

$$\vec{\Psi} = M_0 \vec{f}_0$$

Therefore,

$$\vec{f}_0^{\rm out} = 2M_0 M_0^{-2} M_0 \vec{f}_0 - \vec{f}_0 + M_0^{-1}\vec{F} = \vec{f}_0 + M_0^{-1}\vec{F}$$

This equation can be iterated n times to give

$$\vec{f}_0(n\tau) = \vec{f}_0(0) + nM_0^{-1}\vec{F} \quad \text{and} \quad \vec{\Psi}(n\tau) = \vec{\Psi}(0) + n\vec{F}$$

The motion of the particle is then given by

$$\begin{aligned}
\vec{r}(n\tau) = & \quad \vec{r}(n\tau-\tau) + M^{-1}\vec{\Psi}(n\tau-\tau) + M^{-1}\frac{\vec{F}}{2} \\
= & \quad \vec{r}(0) + \sum_{s=0}^{n-1} M^{-1}\vec{\Psi}(s\tau) + \frac{n}{2}M^{-1}\vec{F} \\
= & \quad \vec{r}(0) + nM^{-1}\vec{\Psi}(0) + M^{-1}\vec{F}\sum_{s=0}^{n-1} s + \frac{n}{2}M^{-1}\vec{F} \\
= & \quad \vec{r}(0) + nM^{-1}\vec{\Psi}(0) + \frac{n^2}{2}M^{-1}\vec{F} \qquad (17)
\end{aligned}$$

This is exactly the expression expected for a free particle of mass M submitted to a constant force $\vec{F}$ provided one interprets $M^{-1}\vec{\Psi}(0)$ as $\vec{v}(0)$, the speed of the particle at time $t=0$ and $M^{-1}\vec{F}$ as the acceleration.

It is also interesting to consider the energy defined in (11 for a free particle. In this case, E reduces to

$$E = \vec{f}_0^2$$

It is easy to show that this energy corresponds to the kinetic energy of the particle $E_{\text{cin}} = \vec{p}^2/2M$ where $\vec{p}$ is the momentum. In our case we have $\vec{p} = \vec{\Psi}/M$ and

$$E_{\text{cin}} = \frac{\vec{\Psi}^2}{2M} = \frac{(M_0\vec{f}_0)^2}{M_0^2} = E$$

These results give a kinetic justification of the interpretation we propose for the physical quantities involved in the model.

7 Dissipation and the stationary state

In the above formulation, our solid has no internal dissipation and if moved away from equilibrium, its atoms will keep oscillating for ever, possibly producing an overall motion of the object. In order to be able to reach a time-independent state when an external force is applied (i.e. to measure the static deformation resulting from an applied stress), it is convenient to add some dissipation in some *ad hoc* way.

We propose the following change in the dynamics

$$\begin{aligned} \vec{f}_i(\vec{\ell}+\vec{c}_i, t+\tau) &= \mu M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) - \vec{f}_{i+2}(\vec{\ell},t) + \frac{\mu}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t) &(18)\\ \vec{f}_0(\vec{\ell}, t+\tau) &= M_0(\vec{\ell})M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) - \vec{f}_0(\vec{\ell},t) + \frac{\mu}{2}M_0M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t) &(19)\end{aligned}$$

and

$$\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t) + \mu M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) + \frac{\mu}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t) \qquad (20)$$

where μ is a scalar in the range $0 < \mu \leq 1$. When $\mu = 1$, no dissipation take place, but as soon as $\mu < 1$, the momentum $\vec{\Psi}$ is no longer conserved and a damping of the motion occurs as if the entire solid would be subject to some external friction. This can be shown y defining

$$\vec{\Phi} = \mu\left(\vec{\Psi} + \frac{\vec{F}}{2}\right)$$

and repeating the derivation leading to (10).

$$\vec{\Psi}^{\text{out}} = M_0\vec{f}_0^{\text{out}} + \sum_{i>0}\vec{f}_i^{\text{out}}$$

$$\begin{aligned}
&= M_0^2 M^{-1}\vec{\Phi} - M_0\vec{f}_0 + KM^{-1}\vec{\Phi} \\
&\quad -\frac{1}{\mu}\vec{\Phi} + M_0\vec{f}_0 + \frac{\vec{F}}{2} \\
&= \left(2 - \frac{1}{\mu}\right)\vec{\Phi} + \frac{\vec{F}}{2} \\
&= (2\mu - 1)\vec{\Psi} + \mu\vec{F} \qquad (21)
\end{aligned}$$

When the sum of the external forces $\sum_{\vec{\ell}}\vec{F}_{\vec{\ell}}$ is zero, this relation implies that the total momentum relaxes to zero

$$\vec{\Psi}^{\rm tot}(t+\tau) = (2\mu - 1)\vec{\Psi}^{\rm tot}(t)$$

and the solid eventually reaches a state where all particles are at rest, in static equilibrium between the external and internal forces. We show that this final stage is independent of the value of μ.

For a situation at rest (no time dependence), one has $\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t)$, thus $\mu M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) + \frac{\mu}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t) = 0$ that is

$$\vec{\Psi}_{\vec{\ell}} + \frac{1}{2}\vec{F}_{\vec{\ell}} = 0 \qquad (22)$$

After substitution of this condition in (19), one obtains

$$\begin{aligned}
\vec{f}_i(\vec{\ell} + \vec{c}_i) &= -\vec{f}_{i+2}(\vec{\ell}) && (23) \\
\vec{f}_0(\vec{\ell}) &= -\vec{f}_0(\vec{\ell}) \quad thatis \quad \vec{f}_0(\vec{\ell}) = 0 && (24)
\end{aligned}$$

8 Relation between the fs and the deformation

From evolution rule (1)

$$\vec{f}_i(\vec{\ell} + \vec{c}_i, t+\tau) = M_{\vec{\ell}}^{-1}\vec{\Psi}_{\vec{\ell}}(t) - \vec{f}_{i+2}(\vec{\ell}, t) + \frac{1}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t)$$

one obtains, for $t \to t - \tau$

$$M_{\ell}^{-1}\vec{\Psi}_{\vec{\ell}}(t-\tau) = \vec{f}_i(\vec{\ell} + \vec{c}_i, t) + \vec{f}_{i+2}(\vec{\ell}, t-\tau) - \frac{1}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t-\tau) \qquad (25)$$

and, also, for $\vec{\ell} \to \vec{\ell} + \vec{c}_i$, $i \to i+2$, $t \to t - \tau$

$$M_{\vec{\ell}+\vec{c}_i}^{-1}\vec{\Psi}_{\vec{\ell}+\vec{c}_i}(t-\tau) = \vec{f}_{i+2}(\vec{\ell}, t) + \vec{f}_i(\vec{\ell} + \vec{c}_i, t-\tau) - \frac{1}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}+\vec{c}_i}(t-\tau) \qquad (26)$$

On the other hand, from definition (8) of the particle motion

$$\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t) + M_{\vec{\ell}}^{-1}\Psi_{\ell}(t) + \frac{1}{2}M_{\vec{\ell}}^{-1}\vec{F}_{\vec{\ell}}(t),$$

The separation between two adjacent particles $\vec{\ell}$ and $\vec{\ell}+\vec{c}_i$ is given by

$$\begin{aligned} \vec{r}_{\vec{\ell}+\vec{c}_i}(t)-\vec{r}_{\vec{\ell}}(t) &= \vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau)-\vec{r}_{\vec{\ell}}(t-\tau) \\ &\quad +M^{-1}_{\vec{\ell}+\vec{c}_i}\vec{\Psi}_{\vec{\ell}+\vec{c}_i}(t-\tau)+\frac{1}{2}M^{-1}_{\vec{\ell}}\vec{F}_{\vec{\ell}+\vec{c}_i}(t-\tau) \\ &\quad -M^{-1}_{\vec{\ell}}\vec{\Psi}_{\vec{\ell}}(t-\tau)-\frac{1}{2}M^{-1}_{\vec{\ell}}\vec{F}_{\vec{\ell}}(t-\tau) \end{aligned} \tag{27}$$

Using (25) and (26), we then obtain

$$\begin{aligned} \vec{r}_{\vec{\ell}+1}(t)-\vec{r}_{\vec{\ell}}(t) &= \vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau)-\vec{r}_{\vec{\ell}}(t-\tau) \\ &\quad +\vec{f}_{i+2}(\vec{\ell},t)+\vec{f}_i(\vec{\ell}+\vec{c}_i,t-\tau) \\ &\quad -\vec{f}_i(\vec{\ell}+\vec{c}_i,t)-\vec{f}_{i+2}(\vec{\ell},t-\tau) \end{aligned} \tag{28}$$

Rearranging the terms gives

$$\vec{r}_{\vec{\ell}+\vec{c}_i}(t)-\vec{r}_{\vec{\ell}}(t)+\vec{f}_i(\vec{\ell}+\vec{c}_i,t)-\vec{f}_{i+2}(\vec{\ell},t)=\vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau)-\vec{r}_{\vec{\ell}}(t-\tau)+\vec{f}_i(\vec{\ell}+\vec{c}_i,t-\tau)-\vec{f}_{i+2}(\vec{\ell},t-\tau) \tag{29}$$

In other words, the following quantity in a constant of the motion

$$\vec{r}_{\vec{\ell}+\vec{c}_i}(t)-\vec{r}_{\vec{\ell}}(t)+\vec{f}_i(\vec{\ell}+\vec{c}_i,t)-\vec{f}_{i+2}(\vec{\ell},t)=\Delta^0_i(\vec{\ell}) \tag{30}$$

which we interpret as the equilibrium separation between particles $\vec{\ell}$ and $\vec{\ell}+\vec{c}_i$ because that is what it should be when the $\vec{f}$'s are zero. Note that eq. (30) should be used to specify correctly the relation between the inital position of the particles and the f's at time $t=0$.

Thus, the local deformation of the solid along direction i is computed as

$$\begin{aligned} \Delta_i(\vec{\ell},t) &\equiv \vec{r}_{\vec{\ell}+\vec{c}_i}(t)-\vec{r}_{\vec{\ell}}(t)-\Delta^0_i(\vec{\ell}) \\ &= -\vec{f}_i(\vec{\ell}+\vec{c}_i,t)+\vec{f}_{i+2}(\vec{\ell},t) \end{aligned} \tag{31}$$

Note that this relation justifies picture given in fig. 3.

Also note that the above derivation works when dissipation is turned on by changing $\Psi\to\mu\Psi$ and $\vec{F}\to\mu\vec{F}$.

8.1 Case of $\vec{f}_0$

A relation similar to (31) can be derived for $\vec{f}_0$. From

$$\vec{f}_0(\vec{\ell},t+\tau)=M_0(\ell)M^{-1}_{\ell}\vec{\Psi}_{\vec{\ell}}(t)-\vec{f}_0(\vec{\ell},t)+M_0(\ell)M^{-1}_{\ell}\frac{\vec{F}_{\vec{\ell}}(t)}{2}$$

one obtains

$$\begin{aligned} M^{-1}_{\vec{\ell}}\vec{\Psi}_{\vec{\ell}}(t-\tau) &= M_0(\vec{\ell})^{-1}\left[\vec{f}_0(\vec{\ell},t)+\vec{f}_0(\vec{\ell},t-\tau)\right]-M^{-1}_{\vec{\ell}}\frac{\vec{F}_{\vec{\ell}}(t-\tau)}{2} \\ M^{-1}_{\vec{\ell}+\vec{c}_i}\vec{\Psi}_{\vec{\ell}+\vec{c}_i}(t-\tau) &= M_0(\vec{\ell}+\vec{c}_i)^{-1}\left[\vec{f}_0(\vec{\ell}+\vec{c}_i,t)+\vec{f}_0(\vec{\ell}+\vec{c}_i,t-\tau)\right]-M^{-1}_{\vec{\ell}+\vec{c}_i}\frac{\vec{F}_{\vec{\ell}+\vec{c}_i}(t-\tau)}{2} \end{aligned}$$

In addition, one has

$$\begin{aligned}
\vec{r}_{\vec{\ell}+\vec{c}_i}(t) - \vec{r}_{\vec{\ell}}(t) = & \quad \vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau) - \vec{r}_{\vec{\ell}}(t-\tau) \\
& + \; M^{-1}_{\vec{\ell}+\vec{c}_i}\vec{\Psi}_{\vec{\ell}+\vec{c}_i}(t-\tau) + M^{-1}_{\vec{\ell}+\vec{c}_i}\frac{\vec{F}_{\vec{\ell}+\vec{c}_i}(t-\tau)}{2} \\
& - \; M^{-1}_{\vec{\ell}}\vec{\Psi}_{\vec{\ell}}(t-\tau) - M^{-1}_{\vec{\ell}}\frac{\vec{F}_{\vec{\ell}}(t-\tau)}{2} \qquad (32)
\end{aligned}$$

From the previous equation one obtains

$$\begin{aligned}
\vec{r}_{\vec{\ell}+\vec{c}_i}(t) - \vec{r}_{\vec{\ell}}(t) = & \quad \vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau) - \vec{r}_{\vec{\ell}}(t-\tau) \\
& + \; M_0^{-1}(\vec{\ell}+\vec{c}_i)\left[\vec{f}_0(\vec{\ell}+\vec{c}_i,t) + \vec{f}_0(\vec{\ell}+\vec{c}_i,t-\tau)\right] \\
& - \; M_0^{-1}(\vec{\ell})\left[\vec{f}_0(\vec{\ell},t) + \vec{f}_0(\vec{\ell},t-\tau)\right] \qquad (33)
\end{aligned}$$

And, by rearranging the terms, we see that

$$\begin{aligned}
\vec{r}_{\vec{\ell}+\vec{c}_i}(t) - \vec{r}_{\vec{\ell}}(t) \; & + \; M_0^{-1}(\vec{\ell})\vec{f}_0(\vec{\ell},t) - M_0^{-1}(\vec{\ell}+\vec{c}_i)\vec{f}_0(\vec{\ell}+\vec{c}_i,t) \\
& = \; \vec{r}_{\vec{\ell}+\vec{c}_i}(t-\tau) - \vec{r}_{\vec{\ell}}(t-\tau) - M_0^{-1}(\vec{\ell})\vec{f}_0(\vec{\ell},t-\tau) \\
& \quad + M_0^{-1}(\vec{\ell}+\vec{c}_i)\vec{f}_0(\vec{\ell}+\vec{c}_i,t-\tau) \qquad (34)
\end{aligned}$$

This relation has the form $A(t)+B(t) = A(t-\tau) - B(t-\tau)$ and we can conclude that, in a stationary state $B=0$.

9 Static deformation under the action of a force

9.1 A 1D chain

Consider a chain of 2 particles A and B on which a force F is applied so that $F(A) = -F$ and $F(B) = F$.

Due to the geometry of the system we have $K=1$ and we assume that M_0 is a scalar, as well as $M = (M_0^2 + K)/2$. The only internal fields are $f_0(A)$, $f_3(A)$, $f_0(B)$ and $f_1(B)$, which we want to compute in a static situation.

From eqs. (23) and (24), one has

$$f_1(B) = -f_3(A) \qquad f_0(A) = f_0(B) = 0$$

Since in this particular problem one has $\Psi(A) = M_0 f_0(A) + f_3(A) = f_3(A)$ and $\Psi(B) = M_0 f_0(B) + f_1(B) = f_1(B)$, the conditions (22) $\Psi_{A,B} = -F_{A,B}/2$ give

$$f_3(A) = -\frac{F(A)}{2} = \frac{F}{2} \qquad f_1(B) = -\frac{F(B)}{2} = \frac{-F}{2}$$

Therefore the deformation is

$$r_B - r_A - \Delta^0 = f_3(A) - f_1(B) = F$$

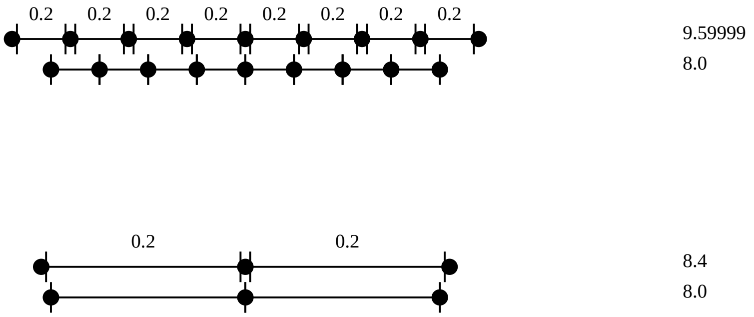

Figure 4: Deformation of a chain of particles subject to a streching force $F = 0.1$ applied at le left and right extremities. The upper case corresponds to a situation with 9 particles and a total deformation of 1.6. In the lower case, the chain is only made of three particles but has the same rest length of 8. With the same force, the deformation is now 0.4. In both cases we see that each link is subject to a deformation of 2 times the external force.

Consequently, the elasticity constant is for a system with 2 particles. It can be adjusted by having a chain of N particles with rest separation $\Delta^0/(N-1)$ which then produces an object if the same length.

Indeed, with N particles and an external force applied on particle 1 and N, the above solution generalizes easily

$$f_3(\ell) = -f_1(\ell) = \frac{F}{2} \quad f_0(\ell) = 0$$

for $\ell = 2, ..., N-1$ and

$$f_3(1) = -f_1(N) = \frac{F}{2} \quad f_0(1) = f_0(N) = 0$$

Therefore

$$r_N - r_1 = \sum_{\ell=2}^{N} r_\ell - r_{\ell-1} = \sum_{\ell=2}^{N} \frac{\Delta^0}{N-1} + f_3(\ell) - f_1(\ell-1) = \Delta^0 + (N-1)F$$

For the same external force and same total rest lenght, the deformation is now much larger, as illustrated in Fig. 4.

9.2 A 2D model

The same static deformation calculation can be performed for a simple 2D solid with four particles labeled A, B, C and D. Fig. 5 shows the system. The upper-left particle is A, the upper-right is B, the lower-right is D and the lowe-left is C.

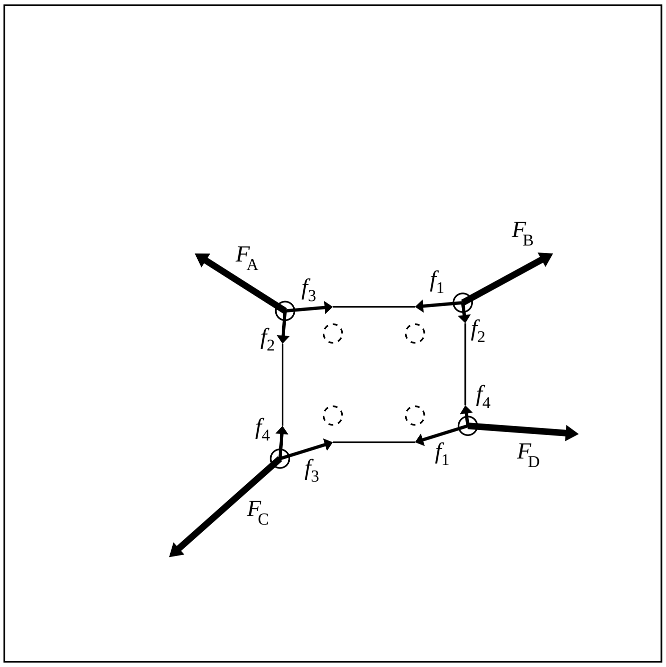

Figure 5: Deformation of a simple 2D solid. The original and final particle positions are shown, as well as the internal forces (thin arrows) and external forces (fat arrows).

Here we restrict the calculation to the case where $M_0 = 0$. Each particle has two links, thus $K = 2$. We denote the external forces as $\vec{F}_A$, $\vec{F}_B$, $\vec{F}_C$, and $\vec{F}_D$ and we assume that

$$\vec{F}_A + \vec{F}_B + \vec{F}_C + \vec{F}_D = 0$$

which is a necessary condition to be consistent with $\vec{r}_{\vec{\ell}}(t+\tau) = \vec{r}_{\vec{\ell}}(t)$

One has to compute $\vec{f}_2(A)$, $\vec{f}_3(A)$, $\vec{f}_1(D)$ and $\vec{f}_4(D)$ since, in the stationary state $\vec{f}_4(C) = -\vec{f}_2(A)$, $\vec{f}_3(C) = -\vec{f}_1(D)$, $\vec{f}_1(B) = -\vec{f}_3(A)$ and $\vec{f}_2(B) = -\vec{f}_4(D)$.

The calculation follows the same lines as in the previous section. However, an extra condition is needed to solve the system of equation. One has to take into account the fact that the four particles form a closed loop, namely that following the deformations from $\vec{r}_A$ through $\vec{r}_B$, $\vec{r}_D$ and $\vec{r}_D$, one ends up again in $\vec{r}_A$.

Using eq. (30) for each particles and noting that $\sum_i \Delta_i^0 =$, one has the condition

$$-\vec{f}_4(D) + \vec{f}_1(D) - \vec{f}_2(A) + \vec{f}_3(A) = 0 \tag{35}$$

After some algebra, the solution is

$$\vec{f}_3(A) = \frac{1}{2}\left[-\frac{1}{2}\vec{F}_A + \frac{1}{4}\vec{F}_B - \frac{1}{4}\vec{F}_C\right] \tag{36}$$

$$\vec{f}_4(D) = \frac{1}{2}\left[\frac{1}{2}\vec{F}_A + \frac{3}{4}\vec{F}_B + \frac{1}{4}\vec{F}_C\right] \tag{37}$$

$$\vec{f}_2(A) = \frac{1}{2}\left[-\frac{1}{2}\vec{F}_A - \frac{1}{4}\vec{F}_B + \frac{1}{4}\vec{F}_C\right] \quad (38)$$

$$\vec{f}_1(D) = \frac{1}{2}\left[\frac{1}{2}\vec{F}_A + \frac{1}{4}\vec{F}_B + \frac{3}{4}\vec{F}_C\right] \quad (39)$$

$$(40)$$

And the deformations read

$$\vec{r}_B - \vec{r}_A - \Delta^0_{AB} = 2\vec{f}_3(A) = \left[-\frac{1}{2}\vec{F}_A + \frac{1}{4}\vec{F}_B - \frac{1}{4}\vec{F}_C\right] \quad (41)$$

$$\vec{r}_C - \vec{r}_A - \Delta^0_{AC} = 2\vec{f}_2(A) = \left[-\frac{1}{2}\vec{F}_A - \frac{1}{4}\vec{F}_B + \frac{1}{4}\vec{F}_C\right] \quad (42)$$

$$\vec{r}_D - \vec{r}_C - \Delta^0_{CD} = -2\vec{f}_1(D) = \left[-\frac{1}{2}\vec{F}_A - \frac{1}{4}\vec{F}_B - \frac{3}{4}\vec{F}_C\right] \quad (43)$$

$$\vec{r}_D - \vec{r}_B - \Delta^0_{BD} = -2\vec{f}_4(D) = \left[-\frac{1}{2}\vec{F}_A - \frac{3}{4}\vec{F}_B - \frac{1}{4}\vec{F}_C\right] \quad (44)$$

$$(45)$$

To express these results in the formalism of elasticity theory, we define the stress tensor S_{xy} as (α denote the x or y component)

$$S_{x\alpha} = F_{A\alpha} + F_{C\alpha} = F_{B\alpha} + F_{D\alpha}$$

and

$$S_{y\alpha} = F_{A\alpha} + F_{B\alpha} = F_{C\alpha} + F_{D\alpha}$$

The strain tensor e_{xy} (deformation tensor) is defined as

$$e_{x\alpha} = \frac{1}{2}(u_{B\alpha} - u_{A\alpha}) + \frac{1}{2}(u_{D\alpha} - u_{C\alpha})$$

and

$$e_{y\alpha} = \frac{1}{2}(u_{A\alpha} - u_{C\alpha}) + \frac{1}{2}(u_{B\alpha} - u_{D\alpha})$$

where

$$(\vec{u}_B - \vec{u}_A) = \vec{r}_B - \vec{r}_A - \Delta^0_{AB}$$

After some algebra, we obtain that

$$S_{\alpha\beta} = 2e_{\alpha\beta}$$

Therefore, only one elasticity constant exist in this model and it has a fixed value for a given number of particles making up the solid.

10 Problems and conclusions

Having M_0 non zero seems to offer new possibilities. It changes the speed of sound in the solid (see [1], for instance) and should allow us to tune the elasticity constant. Moreover, making M_0 a matrix gives a formal way to couple the x and y deformation. The role of M_0 needs more investigation.

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