ICFP – Soft Matter

Stress tensor from microscopic configurations

Anke Lindner, Vincent Démery

The stress tensor $\sigma_{\mu\nu}$ is usually used as a mesoscopic quantity in continuum mechanics. However, both for conceptual reasons or for applications, it is desirable to have a microscopic definition of the stress tensor. Conceptually, we would like to know how the stress emerges from the elementary interactions. This knowledge is needed to measure the stress in molecular dynamics simulations. In this tutorial, we show how to define the stress tensor from the microscopic configuration of a system.

We consider an assembly of particles with an isotropic pair interaction. First, we define the stress tensor as the momentum current and identify the ideal gas and pair interaction contributions. Second, we average the ideal gas contribution over the velocities to recover the ideal gas law. Third, we show that the pair interaction contribution gives the variation of total pair energy upon a global deformation of the system. Last, we relate the spatial average of the stress to the pair correlation function in an homogeneous system.

We consider N particles of mass m in a box of volume V; we denote $\boldsymbol{x}_i$ and $\boldsymbol{p}_i = m\dot{\boldsymbol{x}}_i$ the position and momentum of the particle i. The particles interact through the isotropic pair potential $v(x)$, which can result from any elementary interaction (contact, electrostatic, Van der Waals, etc.).

Technical note: questions requiring calculations are indicated with asterisks: no asterisk for less than three lines of calculations, one for less than 10 lines, and two for longer calculations.

1 Stress tensor as the current of momentum

We define the density $\rho(\boldsymbol{x})$ and density of momentum $\boldsymbol{\pi}(\boldsymbol{x})$ in this system by

$$\rho(\boldsymbol{x}) = \sum_i \delta(\boldsymbol{x} - \boldsymbol{x}_i), \tag{1}$$

$$\boldsymbol{\pi}(\boldsymbol{x}) = \sum_i \boldsymbol{p}_i \delta(\boldsymbol{x} - \boldsymbol{x}_i). \tag{2}$$

1. Show that the time derivative of the density, $\partial_t \rho(\boldsymbol{x}, t)$, can be written as the divergence of the momentum density.

From continuum mechanics, the evolution of the momentum density is given by the stress tensor $\boldsymbol{\sigma}(\boldsymbol{x})$:

$$\partial_t \boldsymbol{\pi}(\boldsymbol{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{x}, t). \tag{3}$$

2. * Using the second Newton law for the particles, compute the evolution of the momentum density, $\partial_t \pi_\mu$ (we use greek indices for the coordinates and the Einstein convention for summation over repeated indices). Identify a kinetic and a pair interaction term. Write the kinetic term as a divergence, $\partial_\nu \sigma^{\mathrm{id}}_{\nu\mu}$ of the ideal gas contribution to the stress tensor, $\sigma^{\mathrm{id}}_{\nu\mu}$.

3. ** Write the pair interaction term as a sum over pairs $\langle i, j\rangle$. Then write this term as the divergence of the pair contribution to the stress tensor, $\sigma^{\mathrm{pair}}_{\nu\mu}$. To do so, you can first show that

$$\delta(\boldsymbol{x} - \boldsymbol{x}_i) - \delta(\boldsymbol{x} - \boldsymbol{x}_j) = \partial_\nu \left[x_{ij\nu} \int_0^1 \delta(\boldsymbol{x} - \boldsymbol{x}_i - \lambda[\boldsymbol{x}_j - \boldsymbol{x}_i])\mathrm{d}\lambda \right], \tag{4}$$

where $\boldsymbol{x}_{ij} = \boldsymbol{x}_j - \boldsymbol{x}_i$. You can use the action of the Dirac distribution on a test function $\phi(\boldsymbol{x})$. To keep simpler expressions in the following we denote $\delta_{[\boldsymbol{x}_i, \boldsymbol{x}_j]}(\boldsymbol{x}) = \int_0^1 \delta(\boldsymbol{x} - \boldsymbol{x}_i - \lambda[\boldsymbol{x}_j - \boldsymbol{x}_i])\mathrm{d}\lambda$.

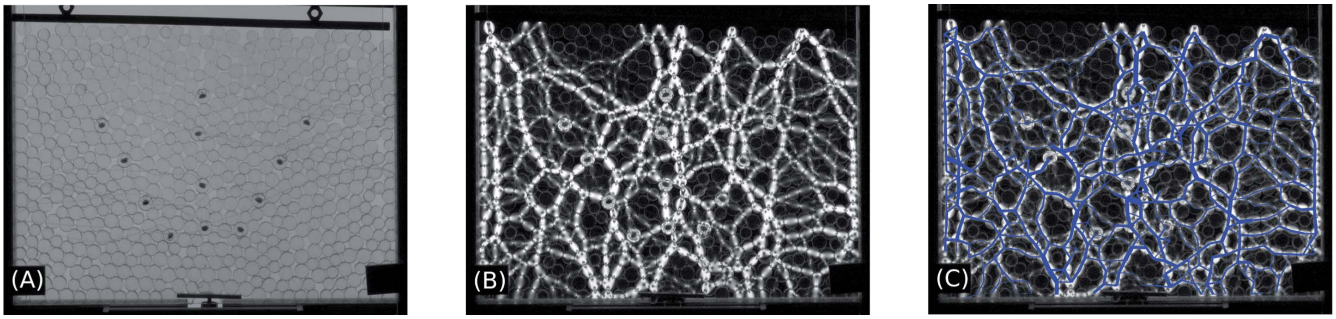

Figure 1: Forces in a two-dimensional granular packing measured by photoelasticity. Adapted from Ref. [2].

You have obtained the Irving-Kirkwood formula [1]. Notice the relation between this expression for the stress and the representation of force chains in granular packings: the blue network in Fig. 1 is actually the stress tensor.

2 Ideal gas contribution

4. Assuming a Maxwell distribution for the velocities of the particles, compute the average of the ideal gas contribution over the velocities and recover the perfect gas law (note that the stress tensor still depends on the positions of the particles).

3 Response to a deformation

5. ** Write the energy of the pair interactions, U_{pair}. How does it change when a small displacement $\boldsymbol{u}(\boldsymbol{x})$ is applied on the system, so that the particle i moves from $\boldsymbol{x}_i$ to $\boldsymbol{x}'_i = \boldsymbol{x}_i + \boldsymbol{u}(\boldsymbol{x}_i)$? Express this variation as a function of the strain tensor $\epsilon_{\mu\nu} = (\partial_\mu u_\nu + \partial_\nu u_\mu)/2$, and recover the pair contribution to the stress tensor $\sigma_{\mu\nu}$. In a first step, you can assume that $\epsilon_{\mu\nu}$ is uniform.

4 Spatial average and pair correlation

The two-particle density is defined by

$$\rho_2(\boldsymbol{x}, \boldsymbol{x}') = \sum_{i \neq j} \delta(\boldsymbol{x} - \boldsymbol{x}_i)\delta(\boldsymbol{x}' - \boldsymbol{x}_j). \tag{5}$$

When the system is uniform, $\rho_2(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{y})$ does not depend on $\boldsymbol{x}$, and we define the pair correlation $g(\boldsymbol{y}) = \rho_2(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{y})/\bar{\rho}^2$.

6. * Compute the spatial average of the stress in a uniform system,

$$\bar{\sigma}_{\mu\nu}^{\text{pair}} = \frac{1}{V} \int \sigma_{\mu\nu}^{\text{pair}}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}, \tag{6}$$

and express it with the pair correlation $g(\boldsymbol{y})$. Comment its dependence on $\bar{\rho}$. What happens if the pair correlation is isotropic?

References

[1] J. H. Irving and John G. Kirkwood. The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics. *The Journal of Chemical Physics*, 18(6):817–829, 1950.

[2] Danielle S. Bassett, Eli T. Owens, Mason A. Porter, M. Lisa Manning, and Karen E. Daniels. Extraction of force-chain network architecture in granular materials using community detection. *Soft Matter*, 11(14):2731–2744, 2015.