Two recent works on molecular systems out of equilibrium

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ENPC and INRIA

joint work with M. Dobson, T. Lelièvre, G. Stoltz (ENPC and INRIA),

A. Iacobucci and S. Olla (Dauphine).

CECAM workshop: *Free energy calculations: From theory to applications*

Outline of the talk

- Derivation of a nonequilibrium Langevin dynamics for a large particle immersed in a background flow field

  Motivation: multiscale simulations of liquids, coupling atomistic (Molecular Dynamics) and continuum (Navier-Stokes) descriptions

- Energy transport properties of a one-dimensional chain of particles, subjected to thermal and mechanical forcings. Each forcing induces a nonequilibrium steady state.

  In the system considered here, non-trivial interplay between thermal and mechanical forcings!

Langevin Dynamics in a nonzero Background Flow Field

joint work with M. Dobson, T. Lelièvre and G. Stoltz,
arXiv 1203.3773

Motivation

Macroscopic evolution of a fluid: Navier-Stokes equation:

$$\begin{aligned} \rho\left(\partial_t u + u\cdot\nabla u\right) &= f + \mathrm{div}\,\sigma, \\ \mathrm{div}\,u &= 0, \\ \sigma &= -p\mathrm{Id} + \tau \end{aligned}$$

where u is the velocity field, σ is the stress field, and p is the pressure field associated to the incompressibility constraint.

To close the system, we need a constitutive law, e.g. τ as a function of u:

- Newtonian fluids:

  $$\sigma = -p\mathrm{Id} + \eta\left(\nabla u + \nabla u^T\right)$$

  where η is the viscosity.

- Can we close the system on the basis of an atomistic model (thereby circumventing the difficulty to postulate a constitutive law at the macroscale)?

Our (long-term!) aim

Solve

$$\begin{aligned} \rho\,(\partial_t u + u \cdot \nabla u) &= f + \text{div}\ \sigma, \\ \text{div}\ u &= 0, \end{aligned}$$

where, in each/some macro grid, the relation

$$\text{field } \nabla u \mapsto \text{field } \sigma(\nabla u, T)$$

is computed on the basis of an atomistic model.

Since ∇u is a macroscopic quantity, we assume, at the atomistic scale, that

∇u is constant (in time) and uniform (in space).

Microscopic description of the system

- N point particles, with positions $q_i \in \mathcal{D}$, momentum p_i and unit mass.
- Hamiltonian $H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q_1, \ldots, q_N)$
- Canonical measure: density $\psi_{\mathrm{G}}(q,p) = Z^{-1}\, \mathrm{e}^{-\beta H(q,p)}$, with $\beta = \frac{1}{k_{\mathrm{B}} T}$
- Equilibrium properties are given by

$$\langle A \rangle = \int_{\mathcal{D}^N \times \mathbb{R}^{dN}} A(q,p)\, \psi_{\mathrm{G}}(q,p)\, dq\, dp$$

- Pressure observable: $A(q,p) = \frac{1}{d|\mathcal{D}|} \sum_{i=1}^{N} \left(p_i^2 - q_i \cdot \nabla_i V(q) \right)$

Such a setting classically allows to compute the pressure, as a function of ρ and T, at equilibrium (in particular, $\langle p_i \rangle = 0$).

One possible way to compute $\langle A \rangle$ is to use the Langevin dynamics:

- Stochastic perturbation of the Hamiltonian dynamics

$$\begin{aligned} dq_i &= p_i \, dt \\ dp_i &= -\nabla_i V(q) \, dt - \gamma p_i \, dt + \sigma \, dW_i \end{aligned}$$

- Fluctuation/dissipation relation: $\sigma^2 = \dfrac{2}{\beta}\gamma$ (for σ and γ scalar)
- Ergodic averages to compute average properties:

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T A(q(t), p(t)) \, dt = \int A(q,p) \, \psi_{\mathrm{G}}(q,p) \, dq \, dp$$

How to modify this setting to compute the stress tensor
at a given ∇u, given by the macroscopic code?

Some references

There has been many works along this line:
– Hadjiconstantinou 2005
– O'Connell and Thompson 1995
– Ren and E 2005
– Werder, Walther and Koumoutsakos 2005
– . . .

SLLOD and g-SLLOD equations of motion are a way to (partially) address this question.

Typical issue: appropriately control the temperature,
– in a way that is consistent with the imposed flow field,
– such that there is no energy drift.

Modified Langevin dynamics

A natural idea is to replace the standard Langevin equation

$$dq_i = p_i\,dt, \qquad dp_i = -\nabla_i V(q)\,dt - \gamma p_i\,dt + \sqrt{2\gamma/\beta}\,dW_i$$

by

$$dq_i = p_i\,dt, \qquad dp_i = -\nabla_i V(q)\,dt - \gamma(p_i - \nabla u\,q_i)\,dt + \sqrt{2\gamma/\beta}\,dW_i \qquad (1)$$

It amounts to consider a friction defined from the relative velocity of the particle, equal to the difference between

- its velocity p_i
- and the macroscopic velocity that we want to impose at point q_i, which is equal to $\nabla u\,q_i$ (recall that $u(x) = \nabla u\,x$ since ∇u is constant).

The modified Langevin equation (1) can also be obtained by applying a Langevin thermostat to the g-SLLOD equations.

Questions

$$dq_i = p_i \, dt, \qquad dp_i = -\nabla_i V(q) \, dt - \gamma(p_i - \nabla u \, q_i) \, dt + \sqrt{2\gamma/\beta} \, dW_i \qquad (2)$$

- in general, the invariant measure of this dynamics is not known. In particular, the density

$$Z^{-1} \exp\left[-\beta \left(V(q) + \sum_{i=1}^{N} \frac{(p_i - \nabla u \, q_i)^2}{2}\right)\right]$$

  is NOT left invariant.

- it may be the case that

$$\mathbb{E}\left[p_i | \text{position } q\right] = \frac{\int p\psi(q,p) \, dp}{\int \psi(q,p) \, dp} \neq \nabla u \, q.$$

  In particular, if ∇u is symmetric, then $\mathbb{E}\left[p_i | \text{position } q\right] = 0$.

As a consequence,

- the properties of the dynamics (2) need to be numerically explored
- interesting to further motivate the dynamics (2)

Numerical exploration

- Shear flow: $\nabla u = \begin{bmatrix} 0 & s & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ for various parameters s.
- $N = 1000$ particles interacting through a Lennard-Jones potential:

$$V(q) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \phi_{\mathrm{LJ}}(|q_i - q_j|)$$

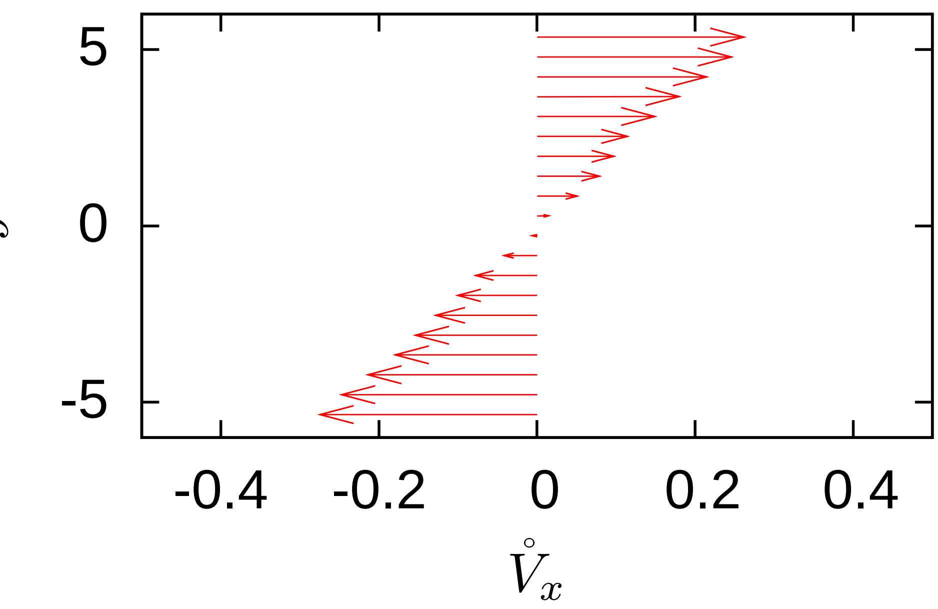
- Lees-Edwards boundary conditions
- Density and temperature chosen such that the particles are in a fluid regime.

Due to the choice of ∇u, we expect the flow to be uniform in x and z directions. We thus define slices R_k in the y direction:

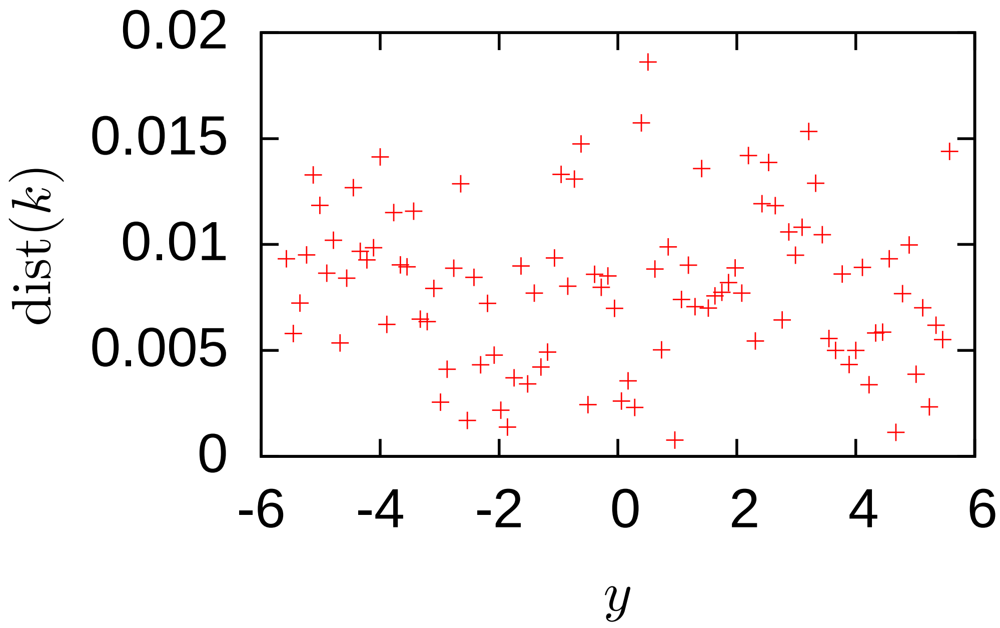
$$R_k = \mathcal{D} \cap \{k\Delta y \leq y \leq (k+1)\Delta y\}.$$

Average velocity: in agreement with background flow

Mean flow



Distance to background flow



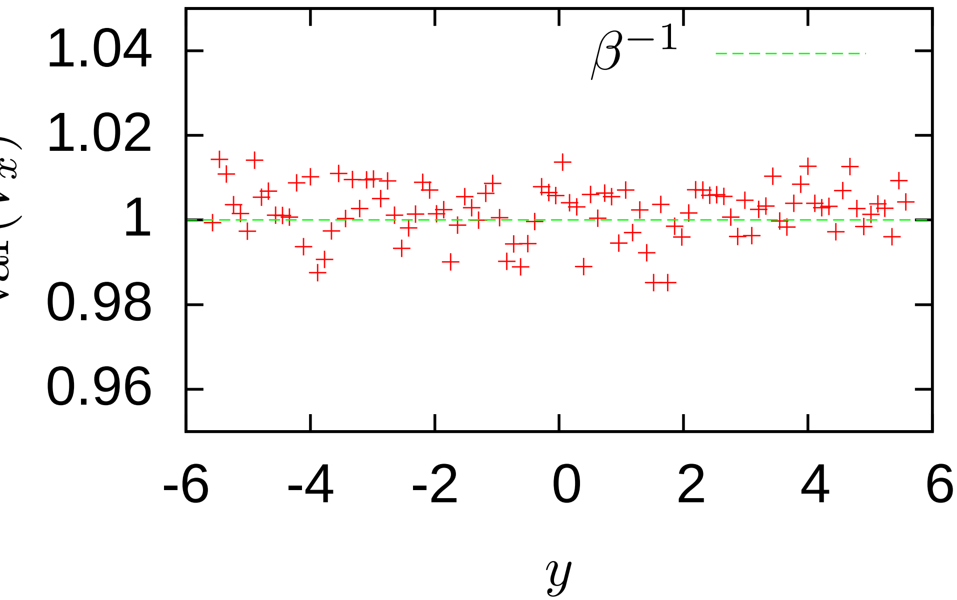
$$\mathring{\mathbf{V}}(k) = \frac{\sum_n \sum_{i=1}^N p_i^n \, \mathbf{1}_{R_k}(q_i^n)}{\sum_n \sum_{i=1}^N \mathbf{1}_{R_k}(q_i^n)} = \text{avg velocity (over time and particles) in slice } R_k$$

$$\mathrm{dist}(k) = \left\| \mathring{\mathbf{V}}(k) - u_{\mathrm{bkgrd}}(R_k) \right\| = \left[\left(\mathring{V}_x(k) - s\, y_{R_k} \right)^2 + \left(\mathring{V}_y(k) \right)^2 + \left(\mathring{V}_z(k) \right)^2 \right]^{1/2}$$

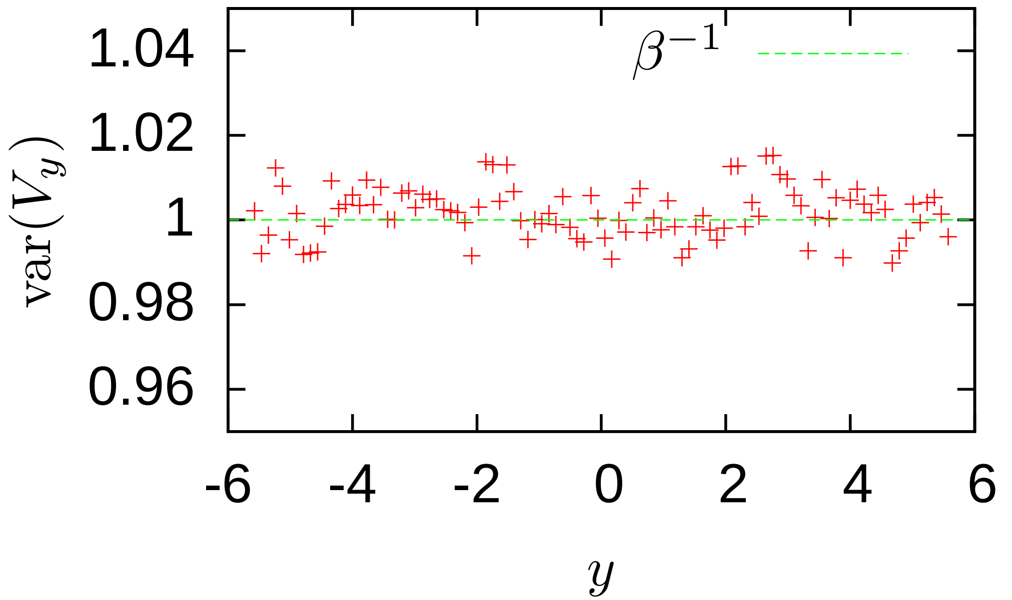
We indeed observe that $\mathring{\mathbf{V}}(k) \approx u_{\mathrm{bkgrd}}(R_k)$.

Velocity variance: in agreement with imposed temperature

Variance in V_x



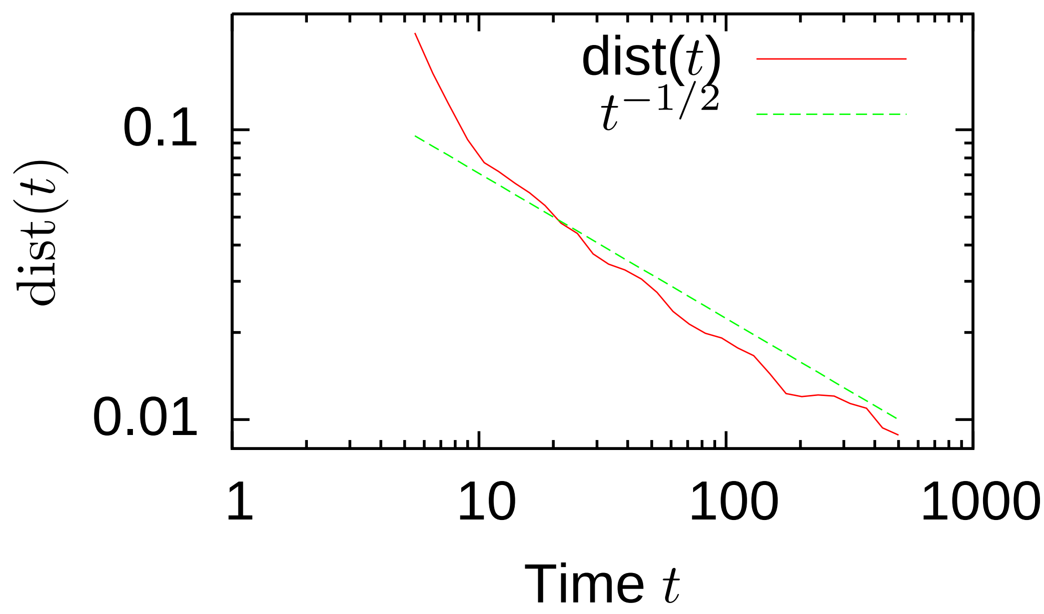
Variance in V_y



Variance of particle velocity as a function of y (we average in x, z and t). Results for V_x and V_z are similar.

All three variances are well centered around β^{-1}.

Convergence of mean flow to background

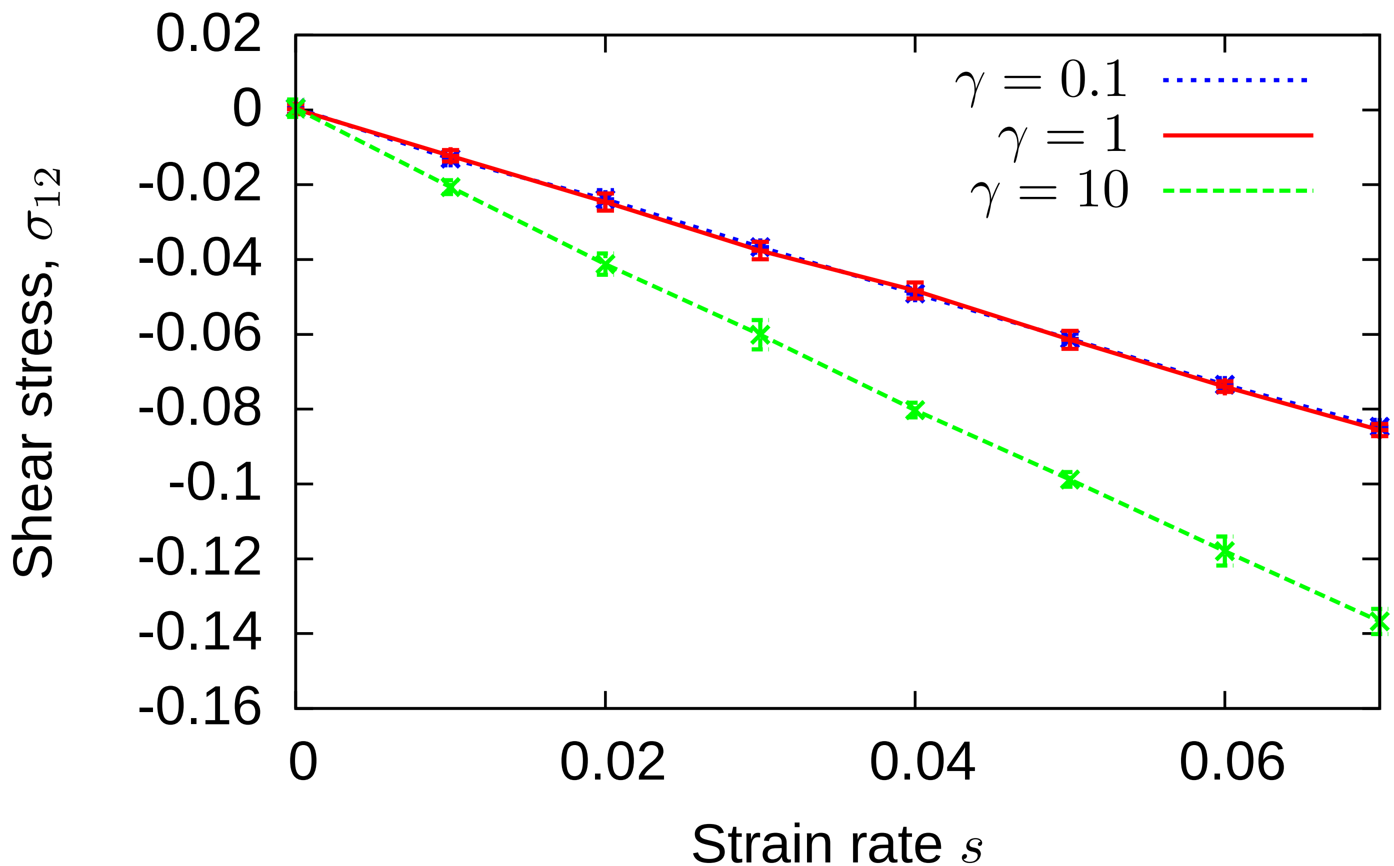


$$\mathrm{dist}(t) = \left[\frac{1}{K} \sum_{k=1}^{K} \left[\left(\mathring{V}_x(k,t) - s\, y_{R_k} \right)^2 + \left(\mathring{V}_y(k,t) \right)^2 + \left(\mathring{V}_z(k,t) \right)^2 \right] \right]^{1/2}$$

where $\mathring{\mathbf{V}}(k,t)$ is the average velocity in slice R_k over the time window $[0,t]$.

We check that convergence rate is $O(t^{-1/2})$.

Shear stress as a function of strain rate



$$\boldsymbol{\sigma}^n = \frac{1}{|\mathcal{D}|} \sum_{i=1}^{N} \left((p_i^n - \nabla u \, q_i^n) \otimes (p_i^n - \nabla u \, q_i^n) + \frac{1}{2} \sum_{j \neq i} (q_i^n - q_j^n) \otimes f^{(ij)} \right)$$

Shear viscosity $\eta = -\sigma_{12}/s$ for $\gamma = 0.1$ is consistent with values reported elsewhere (e.g. by [Rowley and Painter, 1997]).

Midway summary

$$dq_i = p_i\, dt, \qquad dp_i = -\nabla_i V(q)\, dt - \gamma(p_i - \nabla u\, q_i)\, dt + \sqrt{2\gamma/\beta}\, dW_i.$$

We have numerically checked that:

- this dynamics successfully simulates a system out of equilibrium
- the computed viscosity is consistent with previous computations, for Lennard-Jones fluids subjected to shear flow

Can we now further motivate this modified Langevin dynamics?

Midway summary

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Can we now further motivate this modified Langevin dynamics?

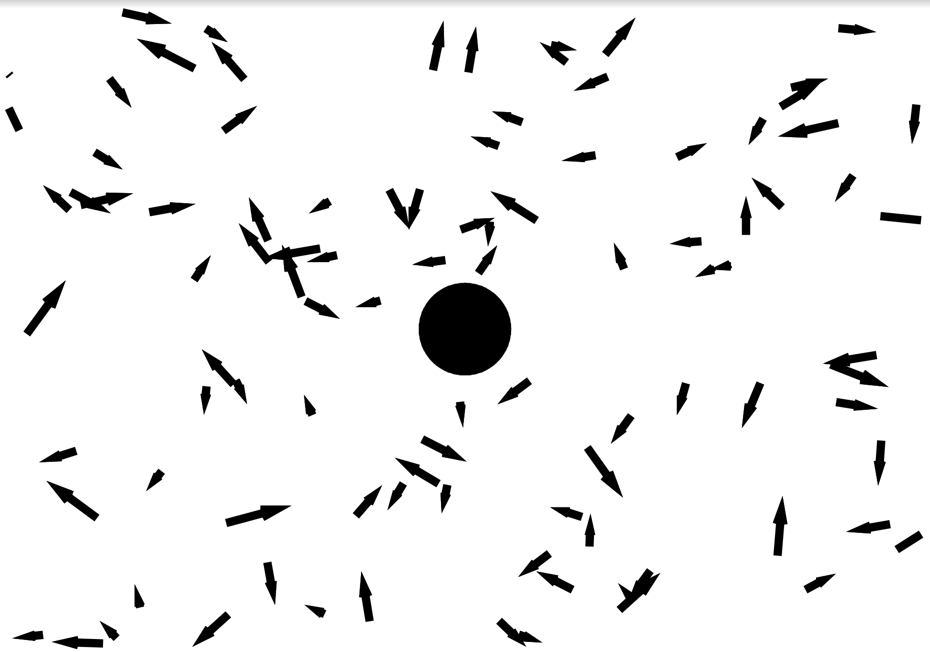
Idea: rather than seeing this as an adhoc modification of the Langevin equation, let's take a step back:

- where does the Langevin dynamics come from?

  Review the work of Durr, Goldstein and Lebowitz [CMP 1981], on the derivation of the Langevin dynamics in an equilibrium setting.

- adapt this derivation when a background flow field is imposed

Derivation of the Langevin dynamics - 1 (dynamics)



Consider a single, distinguished particle (of unit mass and radius R) immersed in a heat bath of light atoms (of mass $m \ll 1$ and zero radius).

- random initial condition, then deterministic evolution
- except for collisions, the particle and the heat bath atoms move ballistically
- elastic collisions between the particle and each heat bath atom (no interaction between the heat bath atoms)

Derivation of the Langevin dynamics - 2 (initial condition)

There are infinitely many bath atoms, with i.i.d. initial conditions. The initial position x and velocity v of each bath atom is drawn according to the density

$$d\mu_m = m^{(d-1)/2} f(m^{1/2} v) dx dv, \quad x \in \mathbb{R}^d, \ v \in \mathbb{R}^d$$

with f which is invariant by rotation:

- position is “uniformly” distributed in space
- velocity orientation is uniformly distributed
- typical example for the velocity magnitude: $f(v) = Z^{-1} \exp\left(-\beta |v|^2/2\right)$.

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The scaling ensures that, at the initial condition:

- the average kinetic energy per bath atom is constant when $m \to 0$ (large velocity, small mass)
- the number of bath atoms in a given volume scales as $1/\sqrt{m}$.

The measure $d\mu_m$ is invariant under the bath dynamics (in the absence of collisions).

Derivation of the Langevin dynamics - 3 (convergence result)

- Each (random) initial condition of the heat bath atoms corresponds to one trajectory of the distinguished particle.
- Durr, Goldstein and Lebowitz [CMP 1981]:
  When $m \to 0$, the trajectory $(q_m(t), p_m(t))$ of the distinguished particle converges to $(q(t), p(t))$, solution to the Langevin equation

$$dq = p\,dt, \qquad dp = -\gamma_{\mathrm{DGL}}\, p\,dt + \sigma_{\mathrm{DGL}}\, dW$$

  where γ_{DGL} and σ_{DGL} are given by analytical formulas (depending on the radius R of the particle, some properties of f, ...).
- Under some conditions on f, the Fluctuation-Dissipation Relation

$$\sigma_{\mathrm{DGL}} = \sqrt{2\gamma_{\mathrm{DGL}}\beta^{-1}}$$

  is satisfied. In particular, $f(v) = Z^{-1}\exp\left(-\frac{\beta}{2}|v|^2\right)$ OK.

Generalization to a nonzero background flow

Given some ∇u, we want to find

- a heat bath dynamics
- a measure $d\mu_m$ for the initial condition (x, v) of each heat bath atom

so that

- the heat bath initial condition is consistent with the background flow field:

$$\mathbb{E}_{\mu_m}(v|x) = \nabla u \, x$$

- the measure $d\mu_m(x, v)$ is invariant under the bath dynamics in the absence of collisions.

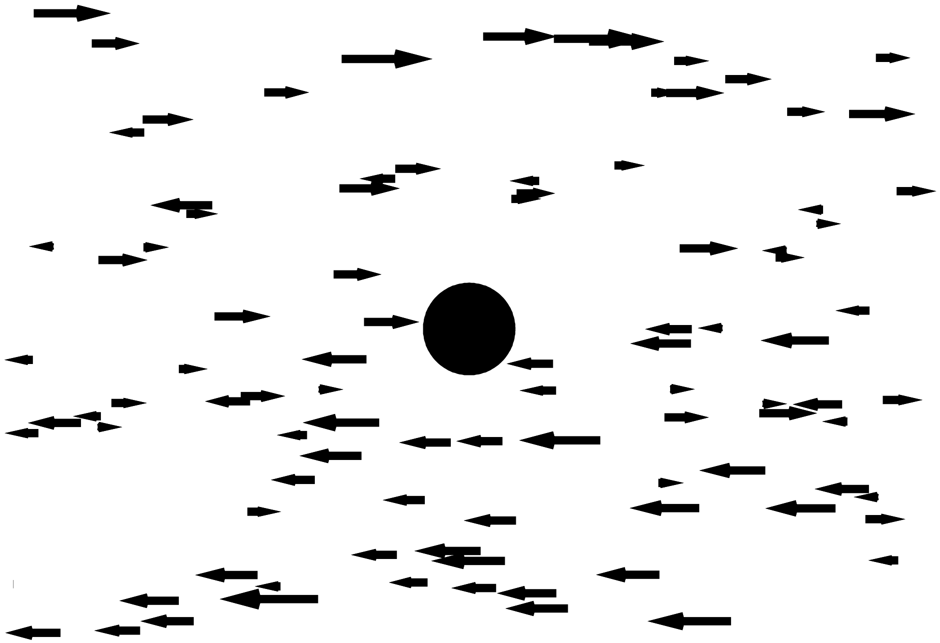
It is not completely trivial to find this . . .

Consider the specific case of shear flow: $\nabla u = \begin{bmatrix} 0 & s & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$

Simple idea: choose the heat bath atoms initial condition according to

$$d\mu_m(x,v) = Z^{-1} \exp\left(-\frac{\beta}{2} m (v_1 - s x_2)^2\right) \delta(v_2)\delta(v_3)\, dx\, dv,$$

and assume that the heat bath atoms follow ballistic motion.



Laminar flow models - 2

Again, elastic collision between the large particle and each heat bath atom. Then, when $m \to 0$, the large particle dynamics converges to

$$dq = p\,dt, \quad dp = -\gamma(p - \nabla u\, q)dt + \sigma dW,$$

where γ and σ are both anisotropic. Flaws:

- the dynamics does not satisfy a standard fluctuation-dissipation relation
- in the case when the shear flow is zero ($\nabla u = 0$), the above dynamics does not reduce to Langevin dynamics

  $$dq = p\,dt, \quad dp = -\gamma_{\mathrm{DGL}} p\,dt + \sigma_{\mathrm{DGL}} dW$$

  derived by Durr, Goldstein and Lebowitz [CMP 1981].

Rk: these flaws are not fixed if we consider the superposition of 3 heat baths, each with initial velocity according to the direction e_i.

Non-Hamiltonian bath dynamics

Satisfactory results are obtained with

- initial condition of the heat bath atoms distributed according to

$$d\mu_m(x,v) = m^{(d-1)/2} f\Big(m^{1/2}(v - \nabla u\, x)\Big)\, dx\, dv, \quad x \in \mathbb{R}^d,\ v \in \mathbb{R}^d$$

with $f(v)$ rotationally invariant. We then have $\mathbb{E}_{\mu_m}(v|x) = \nabla u\, x$.

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  with $f(v)$ rotationally invariant. We then have $\mathbb{E}_{\mu_m}(v|x) = \nabla u\, x$.

- the bath atoms follow the non-Hamiltonian dynamics

$$dx = v dt, \quad dv = \nabla u\, x\, dt$$

  and do not interact with one another.

  Under the assumption that $\mathrm{Tr}\,\nabla u = 0$ (incompressible background flow: div $u = 0$), the distribution $d\mu_m(x,v)$ is invariant under the dynamics.

In term of the relative velocity $\overline{v} = v - \nabla u\, x$, the above dynamics reads

$$dx = (\nabla u\, x + \overline{v})dt, \quad d\overline{v} = 0.$$

Convergence result

- initial condition and dynamics of the heat bath atoms as above
- ballistic motion of the large particle in-between collisions
- no interaction between the heat bath atoms
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Then, in the limit $m \to 0$, the large particle dynamics converges to the nonequilibrium Langevin dynamics

$$dq = p\,dt, \quad dp = -\gamma(p - \nabla u\, q)dt + \sigma dW,$$

where γ and σ are analytically known and scalar.

Under some assumptions on f, this dynamics satisfies a standard fluctuation-dissipation relation with temperature equal to the bath's temperature. In particular, $f(v) = Z^{-1} \exp\left(-\beta |v|^2/2\right)$ is OK.

When $\nabla u = 0$, we recover the limiting dynamics identified by Durr, Goldstein and Lebowitz [CMP 1981].

Summary

- introducing a heat bath model consistent with a non-zero incompressible background flow, we have shown that the dynamics of the distinguished large particle converges to

$$dq = pdt, \quad dp = -\gamma(p - \nabla u\, q)dt + \sigma dW$$

- this helps justifying the introduction of this modified Langevin equation
- our derivation is limited to the case of a single large particle (the case of several large particles, even if $\nabla u = 0$, is known to be very challenging)

- we have next considered the generalization of the dynamics to many large particles:

$$dq_i = p_i\, dt, \qquad dp_i = -\nabla_i V(q)\, dt - \gamma(p_i - \nabla u\, q_i)\, dt + \sigma\, dW_i$$

and checked that it yields interesting results.

M. Dobson, FL, T. Lelièvre and G. Stoltz, arXiv 1203.3773

A system with negative thermal conductivity

joint work with A. Iacobucci, S. Olla and G. Stoltz,
Phys. Rev. E 84 (2011)

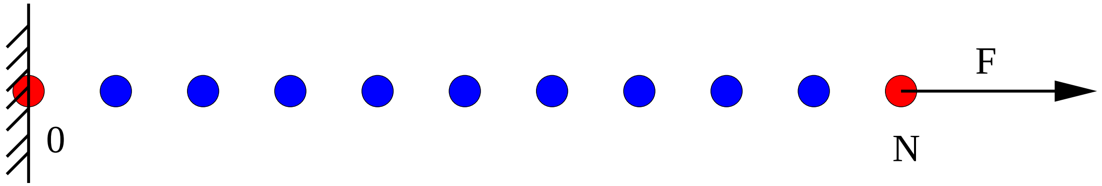
Aim

Study thermal transport under mechanical forcing:

- consider a simple one-dimensional system:

$$H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} v(q_i - q_{i-1}), \quad q_0 = 0.$$

- thermalize both ends at different temperatures
- put a non-gradient mechanical force at the right hand
- monitor the energy current



If $F = 0$, this is a very classical question (validation of Fourier law at the microscopic scale, ...). The consideration of both forcings is less classical!

Non-equilibrium dynamics

Two non-equilibrium settings:

- impose different temperatures on the two ends:

$$\begin{cases} dq_i = p_i \, dt, \qquad dp_i = -\dfrac{\partial V}{\partial q_i}(q)\, dt, \qquad i \neq 1, N, \\ dq_1 = p_1 \, dt, \qquad dp_1 = -\dfrac{\partial V}{\partial q_1}(q)\, dt - \gamma p_1 \, dt + \sqrt{2\gamma T_{\mathrm{L}}}\, dW_t^1, \\ dq_N = p_N \, dt, \qquad dp_N = -\dfrac{\partial V}{\partial q_N}(q)\, dt - \gamma p_N \, dt + \sqrt{2\gamma T_{\mathrm{R}}}\, dW_t^N, \quad T_{\mathrm{R}} \neq T_{\mathrm{L}} \end{cases}$$

- non-gradient forces (periodic potential V, $q \in \mathbb{T}$)

$$dq = p\, dt, \qquad dp = (-\nabla V(q) + F)\, dt - \gamma p\, dt + \sqrt{2\gamma T}\, dW_t$$

- Nonequilibrium dynamics are characterized by
  - the existence of non-zero currents in the system
  - the non-reversibility of the dynamics with respect to the invariant measure (entropy production, ...)

Linear response

Assume $T_{\rm L} = T_{\rm R} + \Delta T$ with $\Delta T \ll 1$. Then it is possible to use a perturbative approach:

- Equilibrium dynamics ($T_{\rm L} = T_{\rm R}$): invariant measure $\psi_0 = \exp(-\beta H(q,p))$
- Nonequilibrium dynamics: look for an invariant measure of the form

$$\psi_{\Delta T} = f_{\Delta T} \psi_0, \qquad f_{\Delta T} = 1 + \Delta T \mathrm{f}_1 + (\Delta T)^2 \mathrm{f}_2 + \dots$$

- Insert this expansion in the Fokker-Planck equation and use $\Delta T \ll 1$ to obtain useful relations for f_1, f_2, ...

A similar perturbative approach is possible in the case $F \ll 1$.

Assume that $H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} v(q_i - q_{i-1}), \quad q_0 = 0.$

Introduce the local energy

$$\varepsilon_i = \frac{p_i^2}{2} + \frac{1}{2}\Big(v(q_{i+1} - q_i) + v(q_i - q_{i-1})\Big), \qquad \frac{d\varepsilon_i}{dt} = j_{i-1,i} - j_{i,i+1},$$

where $j_{i,i+1} = -v'(q_{i+1} - q_i)\dfrac{p_i + p_{i+1}}{2}$ is the energy current.

- Total energy current $J = \sum_{i=1}^{N-1} j_{i,i+1}$
- Linear response: after some (non trivial) manipulations,

$$\text{thermal conductivity} := \lim_{\Delta T \to 0} \frac{\langle J \rangle_{\Delta T}}{\Delta T} = \frac{2\beta^2}{N-1} \int_0^{+\infty} \mathbb{E}\Big(J(q_t,p_t)J(q_0,p_0)\Big)\,dt$$

When the system is far from equilibrium, linear response does not hold anymore. There is no general theory.

In the following, we consider a chain of rotors subjected to a temperature gradient and a non-gradient mechanical force:

- Hamiltonian: $H(q,p) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + (1 - \cos(q_i - q_{i-1})) \right], \quad q_0 = 0.$
- Dynamics:

$$
\begin{cases}
dq_i = p_i \, dt, & dp_i = -\dfrac{\partial V}{\partial q_i}(q)\, dt, \qquad i \neq 1, N, \\
dq_1 = p_1 \, dt, & dp_1 = -\dfrac{\partial V}{\partial q_1}(q)\, dt - \gamma p_1 \, dt + \sqrt{2\gamma T_{\mathrm{L}}}\, dW_t^1, \\
dq_N = p_N \, dt, & dp_N = \left(F - \dfrac{\partial V}{\partial q_N}(q) \right) dt - \gamma p_N \, dt + \sqrt{2\gamma T_{\mathrm{R}}}\, dW_t^N
\end{cases}
$$

Non-equilibrium mechanisms

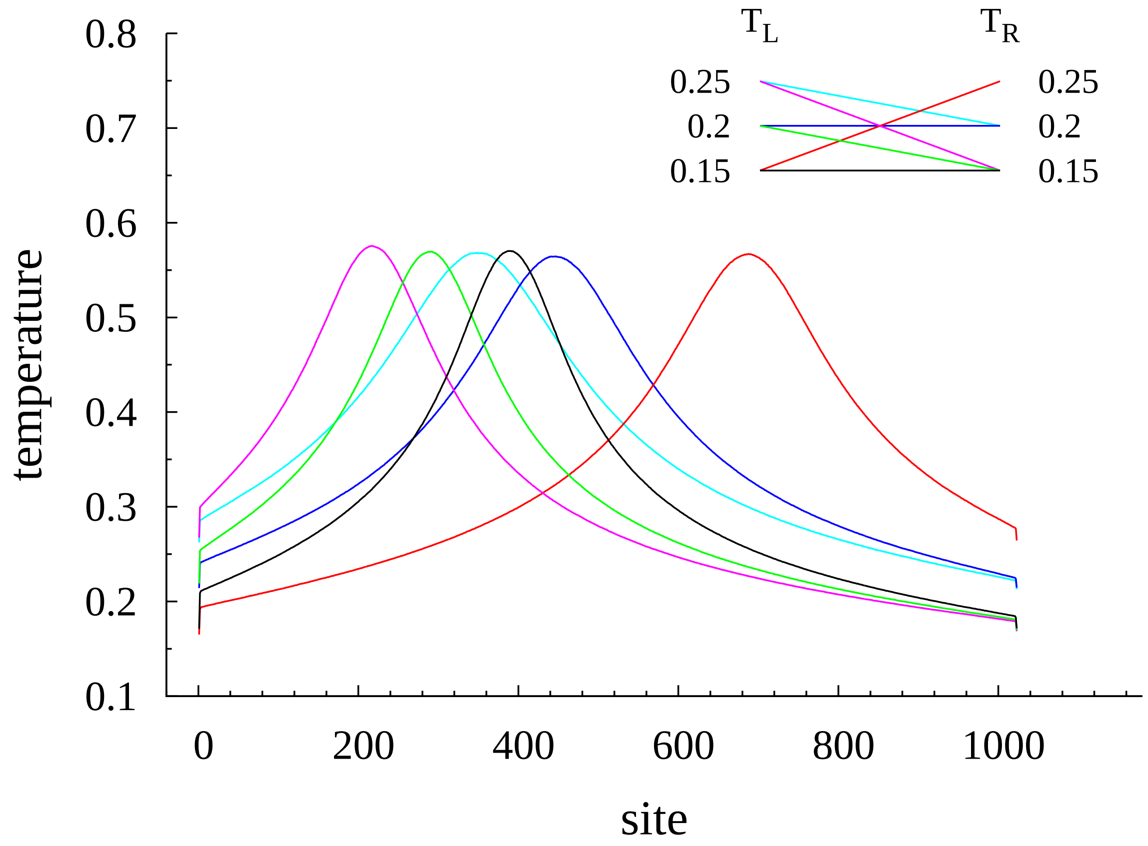
- when $T_{\mathrm{L}} = T_{\mathrm{R}}$, the presence of a mechanical force, $F \neq 0$, induces an energy current towards the left
- when $F = 0$, the presence of a temperature gradient induces an energy current (directed towards the left if $T_{\mathrm{L}} < T_{\mathrm{R}}$).

When $F = 0$:

- well studied system: Giardina et al 2000, Gendelman and Savin 2000 and 2005, Yang and Hu 2005.
- simple system with finite thermal conductivity
- the conductivity depends on T, and dramatically decreases when $T \geq 0.5$.

We are going to see that the two mechanims (thermal and mechanical) are not additive, and that one may reduce the effect of the other!

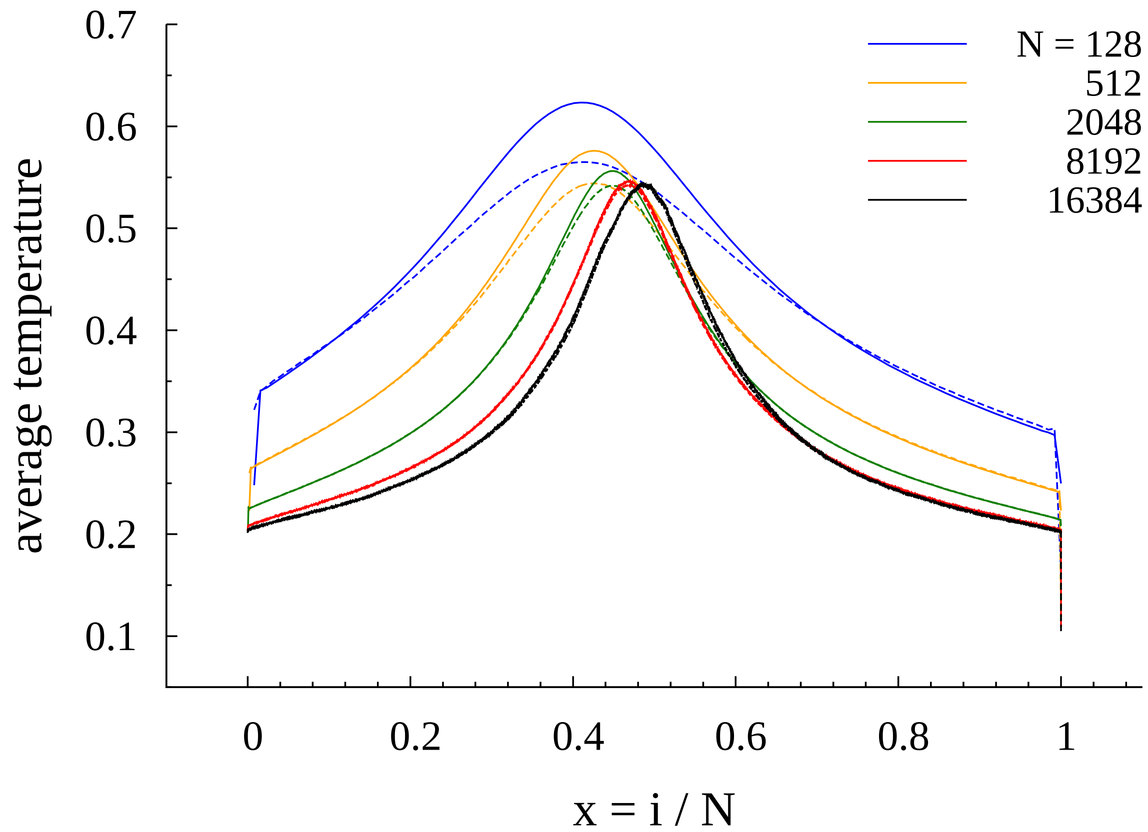
Kinetic temperature profiles (large $F = 1.6$)



Kinetic temperature := variance of momentum

The internal energy is larger in the middle of the system (nonlocal response!)

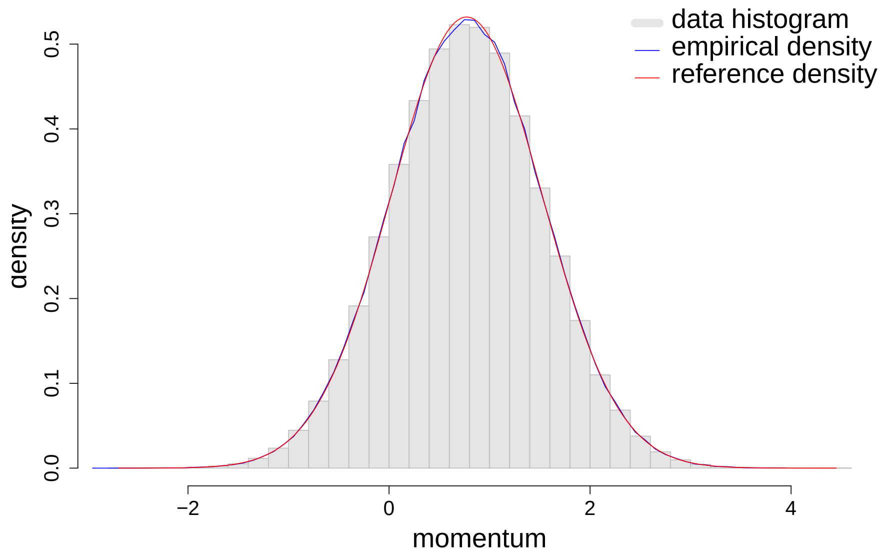
Local equilibrium (large $F = 1.6$, temperatures $T_{\mathrm{L}} = T_{\mathrm{R}} = 0.2$) - 1



Kinetic temperature (solid lines) and potential temperature (dashed lines) well agree one to each other in the thermodynamic limit.

Largest disagreement in the middle of the system.

Local equilibrium (large $F = 1.6$, temperatures $T_\mathrm{L} = T_\mathrm{R} = 0.2$) - 2

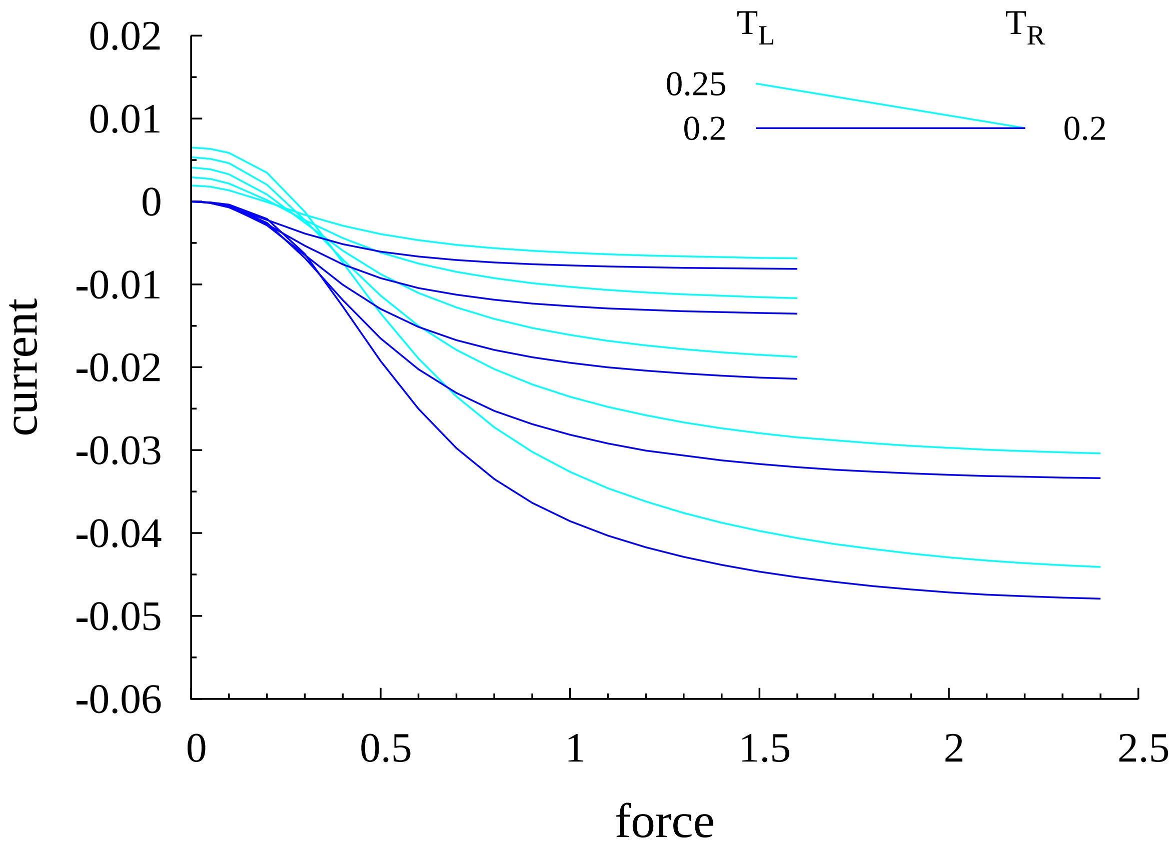


For a chain of length $N = 1024$, comparison of the empirical distribution of momentum at the middle site i_c with the local Gibbs equilibrium at the identified kinetic temperature.

Excellent agreement: local equilibrium holds!
Similar results for the distribution of $r_{i_c} = q_{i_c} - q_{i_c - 1}$ of the middle site

In addition, p_{i_c} and r_{i_c} appear to be independent (joint law = product of distributions).

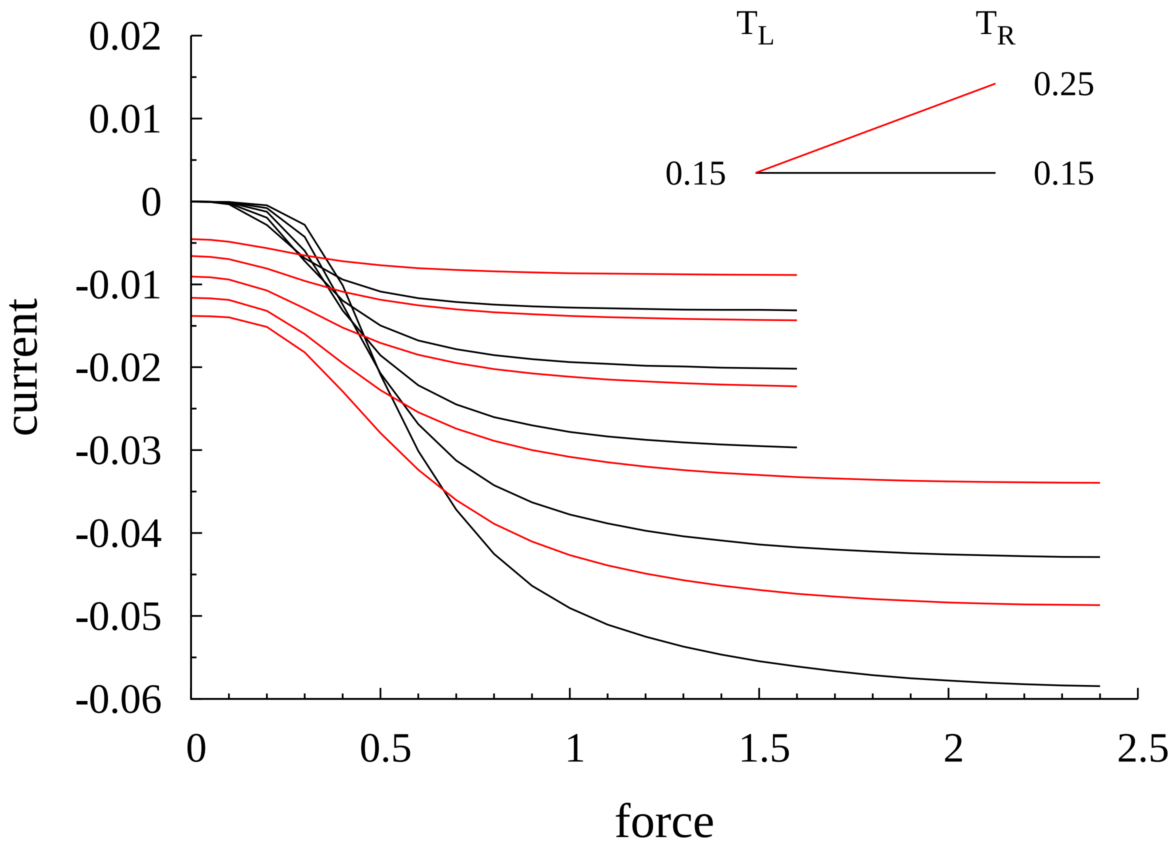
Energy currents for fixed right temperature T_R



From top to bottom: decreasing system sizes $N = 2048, 1024, 512, 256, 128$

When $T_\mathrm{L} = T_\mathrm{R}$, the force F induces a current towards the left.
If $T_\mathrm{L} > T_\mathrm{R}$, the opposite thermal gradient reduces this current, as expected.

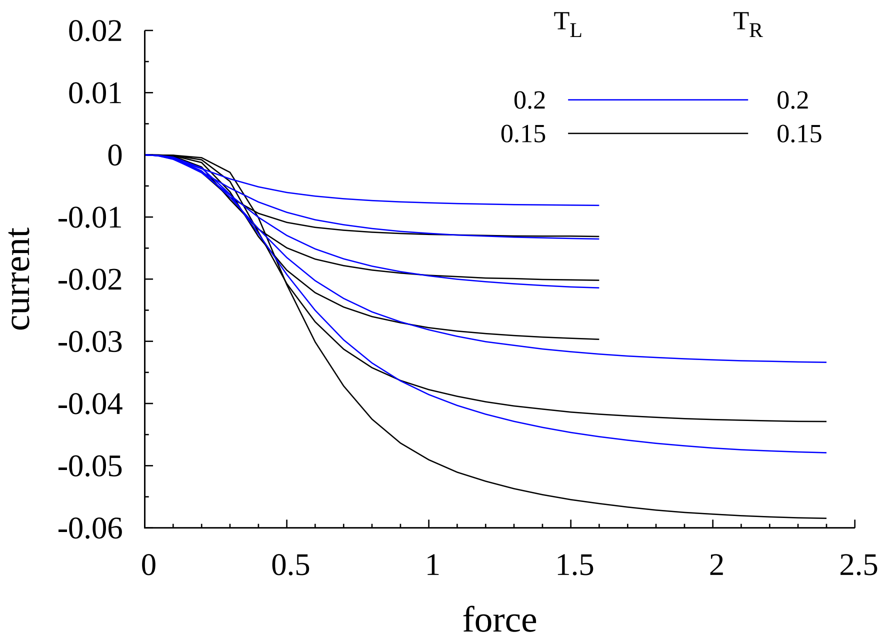
Energy currents for fixed left temperature $T_{\rm L}$

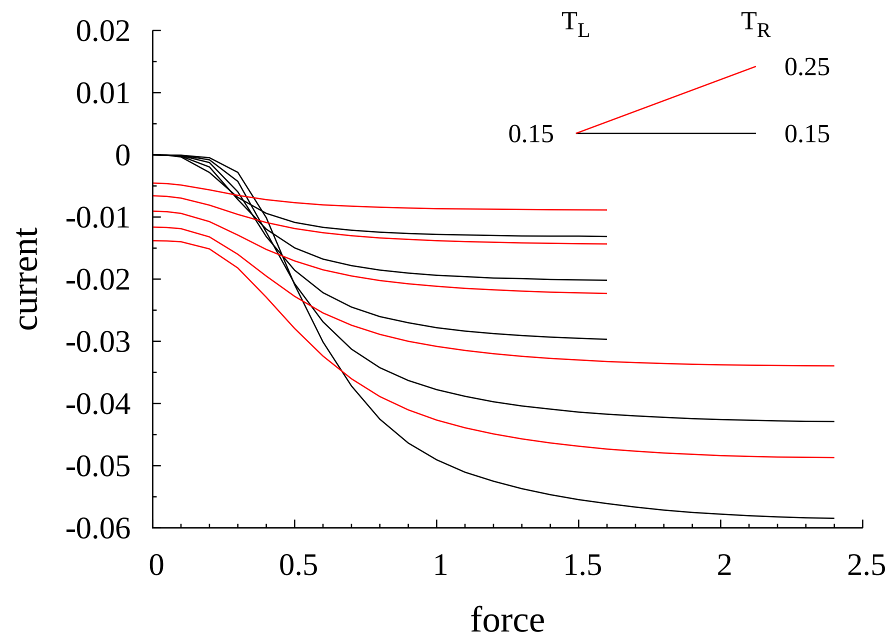


From top to bottom: decreasing system sizes $N = 2048, 1024, 512, 256, 128$.

When $T_{\rm L} = T_{\rm R}$, the force F induces a current towards the left.
If $T_{\rm L} < T_{\rm R}$, the thermal gradient reduces this current, although it is oriented in the same direction: COUNTER-INTUITIVE!

A possible explanation





When F is large, the thermal conductivity is a decreasing function of the temperature (left figure: larger temperature, smaller current).

Right figure: if $T_{\rm R}$ is raised, the thermal conductivity at the right-end is decreased, and the system is less sensitive to F. The increase in thermal current may be dominated by the decrease in mechanical current.

Conclusions

- We have considered a system far from equilibrium.
- This system shows nonlocal effects!
- Although the system is (globally) far from equilibrium, local equilibrium holds for long enough chains.
- Non-trivial interplay between the currents created by the temperature gradient and the mechanical forcing. These currents may not add up! This leads to counter-intuitive results.

A. Iacobucci, FL, S. Olla and G. Stoltz, Phys. Rev. E 84 (2011)