Computation of transport coefficients in molecular dynamics
A mathematical perspective, and an application to shear viscosity

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Outline of the talk

- Computation of equilibrium (static) properties
- Transport properties and linear response theory
  - Nonequilibrium dynamics
  - Linear response theory
  - Some standard examples
- A specific example: computation of shear viscosity with Langevin dynamics
  - Description of the dynamics
  - Definition of the viscosity
  - Asymptotics with respect to the friction coefficient
  - Numerical results

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Equilibrium Langevin dynamics
Microscopic description of a classical system

- Positions \( q \) (configuration), momenta \( p = M \dot{q} \) (\( M \) diagonal mass matrix)
- Microscopic description of a classical system (\( N \) particles):
  \[
  (q,p) = (q_1, \ldots, q_N, p_1, \ldots, p_N) \in \mathcal{E} = \mathcal{D}^N \times \mathbb{R}^{dN}
  \]
- Hamiltonian \( H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(q_1, \ldots, q_N) \) (all the physics in \( V \! \) !)

 Canonical measure: density \( \psi_0(q,p) = Z^{-1} e^{-\beta H(q,p)} \), with \( \beta = \frac{1}{k_B T} \)
- Equilibrium (static) properties: compute approximations of the high dimensional integral
  \[
  \langle A \rangle = \int_{\mathcal{E}} A(q,p) \psi_0(q,p) \, dq \, dp
  \]
- Pressure observable: \( A(q,p) = \frac{1}{d|\mathcal{D}|} \sum_{i=1}^{N} \left( \frac{p_i^2}{m_i} - q_i \cdot \nabla_{q_i} V(q) \right) \)
Langevin dynamics (1)

- **Stochastic perturbation of the Hamiltonian dynamics**
  \[
  \begin{cases}
    dq_t = M^{-1}p_t \, dt \\
    dp_t = -\nabla V(q_t) \, dt - \gamma M^{-1}p_t \, dt + \sigma \, dW_t
  \end{cases}
  \]

- **Fluctuation/dissipation relation** \( \sigma \sigma^T = \frac{2}{\beta} \gamma \)

- When \( V \) smooth: \( \psi_0 \) is the unique invariant measure

- **Ergodic averages to compute average properties:**
  \[
  \lim_{T \to +\infty} \frac{1}{T} \int_0^T A(q_t, p_t) \, dt = \int_E A(q, p) \psi_0(q, p) \, dq \, dp \quad \text{a.s.}
  \]

- **Reference space** \( L^2(\psi_0) \) with the scalar product
  \[
  \langle f, g \rangle_{L^2(\psi_0)} := \int_E f(q, p)g(q, p) \psi_0(q, p) \, dq \, dp.
  \]

- **Generator** \( A_0 = A_{\text{ham}} + A_{\text{thm}} \) with \( A_{\text{ham}}^* = -A_{\text{ham}} \) and \( A_{\text{thm}}^* = A_{\text{thm}} \)
Langevin dynamics (2)

- Precise expressions of the generators:

\[ A_{\text{ham}} = \frac{p}{m} \cdot \nabla q - \nabla V(q) \cdot \nabla p, \quad A_{\text{thm}} = A_{x,\text{thm}} + A_{y,\text{thm}} \]

with \( A_{\alpha,\text{thm}} = \gamma_{\alpha} \left( -\frac{p_{\alpha}}{m} \cdot \nabla p_{\alpha} + \frac{1}{\beta} \Delta p_{\alpha} \right) = -\frac{1}{\beta} \sum_{i=1}^{N} (\partial p_{\alpha i})^* \partial p_{\alpha i} \)

- Note that \([\partial p_{\alpha i}, A_{\text{ham}}] = \frac{1}{m} \partial q_{\alpha i}\) (where \([A, B] = AB - BA\))

- Standard results of hypocoercivity\(^a\) show that \( \text{Ker}(A_0) = \text{Span}(1), \)

\[ \| e^{tA_0^*} \|_{\mathcal{B}(H^1(\psi_0) \cap \mathcal{H})} \leq Ce^{-\lambda t} \]

and \( A_0^{-1} \) compact on \( \mathcal{H} = \left\{ f \in L^2(\psi_0) \left| \int_{\mathcal{D}^N \times \mathbb{R}^dN} f\psi_0 = 0 \right. \right\} = L^2(\psi_0) \cap \{1\}^\perp \)

Transport properties and linear response theory
There are three main types of techniques

- **Equilibrium** techniques: Green-Kubo formula (autocorrelation)
- **Transient** methods
- **Steady-state nonequilibrium** techniques
  - boundary driven
  - bulk driven

The determination of transport coefficients relies on an analogy with macroscopic evolution equations

First mathematical questions:

- For equilibrium techniques: integrability of the autocorrelation function
- For steady-state techniques: existence and uniqueness of an invariant probability measure (the thermodynamic ensemble is well defined)
  → usually only results for bulk driven dynamics (except systems with very simple geometries)
We consider **perturbations of equilibrium** dynamics through

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

\[
\begin{align*}
    dq_t &= M^{-1} p_t \, dt \\
    dp_t &= \left( -\nabla V(q_t) + \xi F \right) dt - \gamma M^{-1} p_t \, dt + \sqrt{\frac{2\gamma}{\beta}} \, dW_t
\end{align*}
\]

- **fluctuation terms with different temperatures**

\[
\begin{align*}
    dq_i &= p_i \, dt, \\
    dp_i &= \left( v'(q_{i+1} - q_i) - v'(q_i - q_{i-1}) \right) dt, \quad i \neq 1, N, \\
    dp_1 &= v'(q_2 - q_1) \, dt - \gamma p_1 \, dt + \sqrt{2\gamma T_L} \, dW_t^1, \\
    dp_N &= -v'(q_N - q_{N-1}) \, dt - \gamma p_N \, dt + \sqrt{2\gamma T_R} \, dW_t^N,
\end{align*}
\]

**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, non self-adjointness of the generator)
Nonequilibrium dynamics: General formalism

- Equilibrium dynamics: invariant measure $\psi_0$, generator $A_0$
- Nonequilibrium dynamics: generator $A_0 + \xi A_1$, invariant measure

$$\psi_\xi = f_\xi \psi_0, \quad f_\xi = 1 + \xi f_1 + \xi^2 f_2 + \ldots$$

solution of $(A_0^* + \xi A_1^*) f_\xi = 0$, where adjoints are considered on $L^2(\psi_0)$:

$$\int_\mathcal{E} f (A_0 g) \psi_0 = \int_\mathcal{E} (A_0^* f) g \psi_0$$

- Formally, $f_\xi = \left(1 + \xi (A_0^*)^{-1} A_1\right)^{-1} 1 = \left(1 + \sum_{n=1}^{+\infty} \xi^n \left[-(A_0^*)^{-1} A_1^*\right]^n\right) 1$

- To make such computations rigorous (for $\xi$ small enough): prove that
  - (properties of the equilibrium dynamics) $\text{Ker}(A_0^*) = 1$ and $A_0^*$ is invertible on $\mathcal{H} = 1^\perp$
  - (properties of the perturbation) $\text{Ran}(A_1^*) \subset \mathcal{H}$ and $(A_0^*)^{-1} A_1^*$ is bounded on $\mathcal{H}$. Typically, $\|A_1 \varphi\| \leq a \|A_0 \varphi\| + b \|\varphi\|$ for $\varphi \in \mathcal{H}$
Nonequilibrium dynamics: Linear response

- **Response property** $\mathcal{R} \in \mathcal{H}$, conjugated response $S = A_1^* \mathbf{1}$:

$$\alpha = \lim_{\xi \to 0} \frac{\langle R \rangle_{\xi}}{\xi} = \int_\mathcal{E} R f_1 \psi_0 = -\int_\mathcal{E} [A_0^{-1} R] [A_1^* \mathbf{1}] \psi_0$$

$$= \int_0^{+\infty} \mathbb{E} \left( R(x_t) S(x_0) \right) dt$$

where formally $-A_0^{-1} = \int_0^{+\infty} e^{tA_0} dt$ (as operators on $\mathcal{H}$)

- **Autocorrelation of $\mathcal{R}$** recovered for perturbations such that $A_1^* \mathbf{1} \propto \mathcal{R}$

- **In practice:**
  - Identify the **response** function
  - Construct a physically meaningful **perturbation**
  - Obtain the transport coefficient $\alpha$
  - It is then possible to construct non physical perturbations allowing to compute the same transport coefficient ("Synthetic NEMD")
Example 1: Autodiffusion

- Periodic potential $V$, constant external force $F$

\[
\begin{aligned}
    dq_t &= M^{-1} p_t \, dt \\
    dp_t &= \left( -\nabla V(q_t) + \xi F \right) dt - \gamma M^{-1} p_t \, dt + \sqrt{\frac{2\gamma}{\beta}} \, dW_t
\end{aligned}
\]

- In this case, $A_1 = F \cdot \partial_p$ and so $A_1^* \mathbf{1} = -\beta F \cdot M^{-1} p$

- Response: $R(q,p) = F \cdot M^{-1} p = \text{average velocity in the direction } F$

- Linear response result: defines the mobility

\[
\lim_{\xi \to 0} \frac{\langle F \cdot M^{-1} p \rangle}{\xi} = \beta \int_0^{+\infty} \mathbb{E}\left( (F \cdot M^{-1} p_t)(F \cdot M^{-1} p_0) \right) \, dt = \beta \lim_{T \to +\infty} \frac{\left( F \cdot \mathbb{E}(q_T - q_0) \right)^2}{2T}
\]

since

\[
\left[ F \cdot \mathbb{E}(q_T - q_0) \right]^2 = 2T \int_0^T \mathbb{E}\left( (F \cdot M^{-1} p_t)(F \cdot M^{-1} p_0) \right) \left( 1 - \frac{t}{T} \right) \, dt
\]
Example 2: Thermal transport

- Consider $T_L = T + \Delta T$ and $T_R = T - \Delta T$ so that $\xi = \Delta T$

- Reference dynamics = Langevin with thermostats at temperature $T$ at the boundaries, generator of the perturbation $A_1 = \gamma (\partial_{p_1}^2 - \partial_{p_N}^2)$

- Invariant measure for the equilibrium dynamics

$$\psi_0(q,p) = Z^{-1} e^{-\beta H(q,p)} \, dq \, dp, \quad H(q,p) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N-1} v(q_{i+1} - q_i)$$

- Ergodicity (up to global translations) can be proven under some conditions on the interaction potential $v$

- Response function: energy current (local variations of the energy)

$$\varepsilon_i = \frac{p_i^2}{2} + \frac{1}{2} \left( v(q_{i+1} - q_i) + v(q_i - q_{i-1}) \right), \quad \frac{d\varepsilon_i}{dt} = j_{i-1,i} - j_{i,i+1},$$
Example 2: Thermal transport (continued)

- Total energy current $J = \sum_{i=1}^{N-1} j_{i+1,i}$ with $j_{i+1,i} = -v' (q_{i+1} - q_i) \frac{p_i + p_{i+1}}{2}$

- Linear response: after some (non trivial) manipulations,

\[
\lim_{\Delta T \to 0} \frac{\langle J \rangle_{\Delta T}}{\Delta T} = -\beta^2 \gamma \int_0^{+\infty} \int_0^{\infty} (e^{-t A_0} J) (p_1^2 - p_N^2) \psi_0 \, dt
\]

\[
= \frac{2\beta^2}{N-1} \int_0^{+\infty} \mathbb{E} \left( J(q_t, p_t) J(q_0, p_0) \right) \, dt
\]

- Synthetic dynamics: fixed temperatures of the thermostats but external forcings $\to$ bulk driven dynamics (convergence may be faster)
  - Non-gradient perturbation $-\xi \left( v' (q_{i+1} - q_i) + v' (q_i - q_{i-1}) \right)$
  - Hamiltonian perturbation $H_0 + \xi H_1$ with $H_1(q, p) = \sum_{i=1}^{N} i \varepsilon_i$

In both cases, $A^*_1 = -A_1 + cJ$
Time-dependent forcings (Fourier transforms of autocorrelations, stochastic resonance)

Constrained nonequilibrium systems (computation of transport properties for systems with molecular constraints)

Variance reduction (in particular, importance sampling) for nonequilibrium dynamics is difficult since the invariant measure depends non-trivially on the dynamics

Simple one-dimensional example: \( q \in \mathbb{T} \) and \( V \) periodic,

\[
dx_t = \left( -V'(x_t) + F \right) dt + \sqrt{2} dW_t
\]

The unique invariant probability measure is

\[
\psi_\infty(x) = Z^{-1} \int_0^1 e^{V(x+y)-V(x)-Fy} dy
\]

Local perturbations of \( V \) are felt globally.
Nonequilibrium Langevin dynamics for shear computations
A picture of the nonequilibrium forcing

2D system to simplify notation: $\mathcal{D} = L_x T \times L_y T$
The nonequilibrium dynamics

- Add a smooth nongradient force in the $x$ direction, depending on $y$:

$$
\begin{aligned}
    dq_{i,t} &= \frac{p_{i,t}}{m} \, dt, \\
    dp_{xi,t} &= -\nabla q_{xi} V(q_t) \, dt + \xi F(q_{yi,t}) \, dt - \gamma_x \frac{p_{xi,t}}{m} \, dt + \sqrt{\frac{2\gamma_x}{\beta}} \, dW_{xi}^t, \\
    dp_{yi,t} &= -\nabla q_{yi} V(q_t) \, dt - \gamma_y \frac{p_{yi,t}}{m} \, dt + \sqrt{\frac{2\gamma_y}{\beta}} \, dW_{yi}^t,
\end{aligned}
$$

- For any $\xi \in \mathbb{R}$, existence/uniqueness of a smooth invariant measure with density $\psi_\xi \in C^\infty(\mathcal{D}^N \times \mathbb{R}^{2N})$ provided $\gamma_x, \gamma_y > 0$

- Series expansion: there exists $\xi^* > 0$ such that, for any $\xi \in (-\xi^*, \xi^*)$,

$$
\psi_\xi = f_\xi \psi_0, \quad f_\xi = 1 + \sum_{k \geq 1} \xi^k f_k, \quad \|f_k\|_{L^2(\psi_0)} \leq C(\xi^*)^{-k}
$$

- Use $\|B\varphi\|^2 \leq |\langle \varphi, A_0 \varphi \rangle|$, define $f_{k+1} = - (A_0^*)^{-1} B^* f_k$ so $(A_0 + \xi B)^* f_\xi = 0$

- Averages with respect to the measure $\psi_\xi$: $\langle h \rangle_\xi = \langle h, f_\xi \rangle_{L^2(\psi_0)}$
Local conservation of the longitudinal velocity

- **Linear response** result: 
  \[ \lim_{\xi \to 0} \frac{\langle A_0 h \rangle_{\xi}}{\xi} = -\frac{\beta}{m} \left( h, \sum_{i=1}^{N} p_{xi} F(q_{yi}) \right) \]  
  \[ L^2(\psi_0) \]

- Can be applied to \( A_0^{-1} h \) for a function \( h \in \mathcal{H} \) (otherwise consider \( h - \langle h \rangle_0 \))

- **Average longitudinal velocity** 
  \[ u_x(Y) = \lim_{\varepsilon \to 0} \lim_{\xi \to 0} \frac{\langle U_x^\varepsilon(Y, \cdot) \rangle_{\xi}}{\xi} \] 
  where

  \[ U_x^\varepsilon(Y, q, p) = \frac{L_y}{Nm} \sum_{i=1}^{N} p_{xi} \chi^\varepsilon(q_{yi} - Y) \]

- **Average off-diagonal stress** 
  \[ \sigma_{xy}(Y) = \lim_{\varepsilon \to 0} \lim_{\xi \to 0} \frac{\langle \ldots \rangle_{\xi}}{\xi} \] 
  where \( \ldots = \)

  \[ \frac{1}{L_x} \left( \sum_{i=1}^{N} \frac{p_{xi}p_{yi}}{m} \chi^\varepsilon(q_{yi} - Y) - \sum_{1 \leq i < j \leq N} V'(|q_i - q_j|) \frac{q_{xi} - q_{xj}}{|q_i - q_j|} \int_{q_{yj}}^{q_{yi}} \chi^\varepsilon(s - Y) \, ds \right) \]

- **Local conservation law**
  \[ \frac{d\sigma_{xy}(Y)}{dY} + \gamma_x \bar{\rho} u_x(Y) = \bar{\rho} F(Y) \]  
  (with \( \bar{\rho} = N/|D| \))

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Definition of the viscosity and asymptotics (1)

- **Definition** \( \sigma_{xy}(Y) := -\eta(Y) \frac{du_x(Y)}{dY} \)

- **Closure assumption** \( \eta(Y) = \eta > 0 \)

- **Closed equation on the longitudinal velocity**: basis for numerics
  \[-\eta u''_x(Y) + \gamma_x \bar{u}_x(Y) = \bar{\rho} F(Y)\]

- **Asymptotic behavior of the viscosity** for large frictions: understand the limit of the longitudinal velocity field as \( \gamma_x \) or \( \gamma_y \to +\infty \)
  \[u_{x}^{\alpha,\varepsilon}(Y) := \lim_{\xi \to 0} \frac{\langle U_{x}^{\varepsilon}(Y, \cdot) \rangle_{\xi}}{\xi} = \frac{\beta}{m} \left\langle \sum_{i=1}^{N} p_{xi} F(q_{yi}), U^{\varepsilon}(Y, q, p) \right\rangle_{L^2(\psi_0)}\]
  with \(-A_0 U^{\varepsilon}(Y, \cdot) = U_{x}^{\varepsilon}(Y, \cdot)\) and \(A_0 = A_{\text{ham}} + \gamma_x A_{x, \text{thm}} + \gamma_y A_{y, \text{thm}}\)

- **Behavior of solutions to the Poisson equation** \(-A_0 f = \sum_{i=1}^{N} p_{xi} G(q_{yi})?\)

- **Formal solution** \( f = f^0 + \gamma_{1}^{-1} f^1 + \gamma_{\alpha}^2 f^2 + \ldots \)
Definition of the viscosity and asymptotics (2)

- Infinite transverse friction: $\gamma_y \to +\infty$
  
  - $f_{\gamma_y}$ unique solution in $\mathcal{H}$ of the equation $-A_0(\gamma_y)f_{\gamma_y} = \sum_{i=1}^{N} p_{xi} G(q_{yi})$
  
  - for all $\gamma_y \geq \gamma_x$, $\|f_{\gamma_y} - f^0\|_{H^1(\psi_0)} \leq \frac{C}{\gamma_y}$
  
  - the function $f^0$ is of the form $f^0(q, p) = \sum_{i=1}^{N} G(q_{yi}) \phi_i(q_x, q_y, p_x)$
  
  - a finite limit is obtained for the longitudinal velocity ($G = \chi_\varepsilon(\cdot - Y)$)

- Infinite longitudinal friction: $\gamma_x \to +\infty$
  
  - $f_{\gamma_x} \in \mathcal{H}$ unique solution of $-A_0(\gamma_x)f_{\gamma_x} = \sum_{i=1}^{N} p_{xi} G(q_{yi})$
  
  - for all $\gamma_x \geq \gamma_y$, $\|f_{\gamma_x} - \gamma_x^{-1} f^1\|_{H^1(\psi_0)} \leq \frac{C}{\gamma_x^2}$
  
  - it holds $f^1(q, p) = m \sum_{i=1}^{N} p_{xi} G(q_{yi}) + \tilde{f}^1(q, p)$
  
  - vanishing longitudinal velocity: $\bar{u}_x(Y) = \lim_{\varepsilon \to 0} \lim_{\gamma_x \to +\infty} \gamma_x u_x^\varepsilon(Y) = F(Y)$
Definition of the viscosity and asymptotics (3)

- Idea of the proof in the case when $\gamma_y \to +\infty$

- Define $T_{qy} = p_x \cdot \nabla q_x - \nabla q_x V(q_x, q_y) \cdot \nabla p_x + \gamma_x A_{x,\text{thm}}$ acting on $L^2(\Psi_{qy})$

\[
\begin{align*}
A_{y,\text{thm}} f^0 &= 0, \\
A_{y,\text{thm}} f^1(q, p) &= -p_y \cdot \nabla q_y f^0(q, p_x) - \sum_{i=1}^N p_{xi} G(q_{yi}) - T_{qy} f^0(q, p_x)
\end{align*}
\]

- The first equation shows that $f^0 \equiv f^0(q, p_x)$

- Set $f^1 = \tilde{f}^1 + p_y \cdot \nabla q_y f^0$ so that $A_{y,\text{thm}} \tilde{f}^1 = -\sum_{i=1}^N p_{xi} G(q_{yi}) - T_{qy} f^0(q, p_x)$

- Solvability condition: $f^0(q, p) = -\sum_{i=1}^N G(q_{yi}) T_{qy}^{-1}(p_{xi})$ and $\tilde{f}^1 = 0$

- Uniform hypocoercivity estimates: useful for $\gamma_y \geq \gamma_x$:

\[
C \|u\|_{H^1(\psi_0)}^2 - (\gamma_y - \gamma_x) \langle \langle u, A_{y,\text{thm}} u \rangle \rangle \leq -\langle \langle u, A_0 u \rangle \rangle \geq 0
\]

- Finish the proof by considering $u = f_{\gamma_y} - f^0 - \gamma^{-1}_y f^1$
2D Lennard-Jones fluid $V_{\text{LJ}}(r) = 4\varepsilon_{\text{LJ}} \left( \left( \frac{d_{\text{LJ}}}{r} \right)^{12} - \left( \frac{d_{\text{LJ}}}{r} \right)^6 \right)$

($d_{\text{LJ}} = \varepsilon_{\text{LJ}} = 1$, smooth cut-off between 2.9 and 3)

Thermodynamic conditions: $\beta = 0.4$, $\rho = 0.69$ ($m = 1$)

Applied nongradient forces:

- sinusoidal: $F(y) = \sin \left( \frac{2\pi y}{L_y} \right)$;

- piecewise linear: $F(y) = \begin{cases} 
\frac{4}{L_y} \left( y - \frac{L_y}{4} \right), & 0 \leq y \leq \frac{L_y}{2}, \\
\frac{4}{L_y} \left( \frac{3L_y}{4} - y \right), & \frac{L_y}{2} \leq y \leq L_y;
\end{cases}$

- piecewise constant: $F(y) = \begin{cases} 
1, & 0 < y < \frac{L_y}{2}, \\
-1, & \frac{L_y}{2} < y < L_y.
\end{cases}$
Numerical implementation

- Numerical scheme: \( \alpha_{x,y} = \exp(-\gamma_{x,y} \Delta t) \), time step \( \Delta t = 0.005 \)
  \[
  \begin{align*}
  p^{n+1/4} &= p^n - \frac{\Delta t}{2} \nabla V(q^n), \\
  q^{n+1} &= q^n + \Delta t p^{n+1/4}, \\
  p^{n+1/2} &= p^{n+1/4} - \frac{\Delta t}{2} \nabla V(q^{n+1}), \\
  p_{x_i}^{n+1} &= \alpha_x p_{x_i}^{n+1/2} + \sqrt{\frac{1}{\beta} (1 - \alpha_x^2)} G_{x_i}^n + (1 - \alpha_x) \frac{\xi}{\gamma_x} F(q_{y_i}^{n+1}) \\
  p_{y}^{n+1} &= \alpha_y p_{y}^{n+1/2} + \sqrt{\frac{1}{\beta} (1 - \alpha_y^2)} G_{y}^n,
  \end{align*}
  \]

- Well behaved in the limits \( \gamma \to \) and/or \( \gamma \to +\infty \)

- Binning procedure to obtain averages as a function of the altitude \( Y \)

- Fourier series analysis to estimate the viscosity \( U_k = \frac{F_k}{\eta \left( \frac{2\pi}{L_y} \right)^2 k^2 + \gamma_x} \)
Numerical results: Validation of the closure (1)

Velocity profile and off diagonal component of the stress tensor for the *sinusoidal* nongradient force.
Numerical results: Validation of the closure (2)

Velocity profile and off diagonal component of the stress tensor for the piecewise linear nongradient force.
Numerical results: Validation of the closure (3)

Velocity profile and off diagonal component of the stress tensor for the piecewise constant nongradient force.
Numerical results: Infinite transverse friction

Left: Convergence of the velocity profile for increasing values of the transverse friction $\gamma_y$.
Right: Shear viscosity $\eta$ as function of $\gamma_y$ in the case $\gamma_x = 1$, for the sinusoidal nongradient force.
Numerical results: Infinite longitudinal friction

Left: Convergence of the rescaled velocity profile for increasing values of the transverse friction $\gamma_x$.
Right: Shear viscosity $\eta$ as function of $\gamma_x$ in the case $\gamma_y = 1$, for the sinusoidal nongradient force.