# *Computation of transport properties by molecular dynamics*

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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[a]
  - Description of the dynamics
  - Definition of the viscosity
  - Asymptotics with respect to the friction coefficient
  - Numerical results

[a] R. Joubaud and G. Stoltz, Nonequilibrium shear viscosity computations with Langevin dynamics, *arXiv preprint* **1106.0633** (2011), to appear in SIAM MMS

# 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):

$$(q,p) = (q_1,\dots,q_N,\ p_1,\dots,p_N) \in \mathcal{E} = \mathcal{D}^N \times \mathbb{R}^{dN}$$

- Hamiltonian $H(q,p) = \displaystyle\sum_{i=1}^N \frac{p_i^2}{2m_i} + V(q_1,\dots,q_N)$ (all the physics in $V$!)
- Canonical measure: density $\psi_0(q,p) = Z^{-1}\,\mathrm{e}^{-\beta H(q,p)}$, with $\beta = \dfrac{1}{k_\mathrm{B} T}$
- 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: $A(q,p) = \dfrac{1}{d|\mathcal{D}|} \displaystyle\sum_{i=1}^N \left( \frac{p_i^2}{m_i} - q_i \cdot \nabla_{q_i} V(q) \right)$

- 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:

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T A(q_t, p_t)\, dt = \int_{\mathcal{E}} A(q,p)\, \psi_0(q,p)\, dq\, dp \qquad \text{a.s.}$$

- Reference space $L^2(\psi_0)$ with the scalar product

$$\langle f, g \rangle_{L^2(\psi_0)} := \int_{\mathcal{E}} f(q,p) g(q,p)\, \psi_0(q,p)\, dq\, dp.$$

- Generator $\mathcal{A}_0 = \mathcal{A}_{\mathrm{ham}} + \mathcal{A}_{\mathrm{thm}}$ with $\mathcal{A}_{\mathrm{ham}}^* = -\mathcal{A}_{\mathrm{ham}}$ and $\mathcal{A}_{\mathrm{thm}}^* = \mathcal{A}_{\mathrm{thm}}$

## *Langevin dynamics (2)*

- Precise expressions of the generators:

$$\mathcal{A}_{\mathrm{ham}} = \frac{p}{m} \cdot \nabla_q - \nabla V(q) \cdot \nabla_p, \qquad \mathcal{A}_{\mathrm{thm}} = \mathcal{A}_{x,\mathrm{thm}} + \mathcal{A}_{y,\mathrm{thm}}$$

with $\mathcal{A}_{\alpha,\mathrm{thm}} = \gamma_\alpha \left( -\frac{p_\alpha}{m} \cdot \nabla_{p_\alpha} + \frac{1}{\beta} \Delta_{p_\alpha} \right) = -\frac{1}{\beta} \sum_{i=1}^{N} (\partial_{p_{\alpha i}})^* \, \partial_{p_{\alpha i}}$

- Note that $[\partial_{p_{\alpha i}}, \mathcal{A}_{\mathrm{ham}}] = \frac{1}{m} \partial_{q_{\alpha i}}$ (where $[A,B] = AB - BA$)
- Standard results of hypocoercivity[a] show that $\mathrm{Ker}\,(\mathcal{A}_0) = \mathrm{Span}(1)$,

$$\left\| \mathrm{e}^{t\mathcal{A}_0^*} \right\|_{\mathcal{B}(H^1(\psi_0) \cap \mathcal{H})} \le C \mathrm{e}^{-\lambda t}$$

and $\mathcal{A}_0^{-1}$ compact on $\mathcal{H} = \left\{ f \in L^2(\psi_0) \;\middle|\; \int_{\mathcal{D}^N \times \mathbb{R}^{dN}} f \psi_0 = 0 \right\} = L^2(\psi_0) \cap \{1\}^\perp$

[a] Villani, *Trans. AMS* **950** (2009); Pavliotis and Hairer, *J. Stat. Phys.* **131** (2008); Ottobre and Pavliotis, *Nonlinearity* **24** (2011)

# Transport properties and linear response theory

## *Computation of transport properties*

- 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) $\rightarrow$ usually only results for bulk driven dynamics (except systems with very simple geometries)

# Nonequilibrium dynamics: Zoology

- We consider perturbations of equilibrium dynamics through
  - non-gradient forces (periodic potential $V$, $q \in \mathbb{T}$)

$$\begin{cases} dq_t = M^{-1} p_t \, dt \\ dp_t = \Big( -\nabla V(q_t) + \xi F \Big) dt - \gamma M^{-1} p_t \, dt + \sqrt{\frac{2\gamma}{\beta}} \, dW_t \end{cases}$$

  - fluctuation terms with different temperatures

$$\begin{cases} dq_i = p_i \, dt, \\ dp_i = \Big( v'(q_{i+1} - q_i) - v'(q_i - q_{i-1}) \Big) dt, \qquad i \neq 1, N, \\ dp_1 = v'(q_2 - q_1) \, dt - \gamma p_1 \, dt + \sqrt{2\gamma T_{\mathrm{L}}} \, dW_t^1, \\ dp_N = -v'(q_N - q_{N-1}) \, dt - \gamma p_N \, dt + \sqrt{2\gamma T_{\mathrm{R}}} \, dW_t^N, \end{cases}$$

- 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)

# Nonequilibrium dynamics: General formalism

- Equilibrium dynamics: invariant measure $\psi_0$, generator $\mathcal{A}_0$
- Nonequilibrium dynamics: generator $\mathcal{A}_0 + \xi \mathcal{A}_1$, invariant measure

$$\psi_\xi = f_\xi \psi_0, \qquad f_\xi = 1 + \xi \mathrm{f}_1 + \xi^2 \mathrm{f}_2 + \dots$$

solution of $(\mathcal{A}_0^* + \xi \mathcal{A}_1^*)\, f_\xi = 0$, where adjoints are considered on $L^2(\psi_0)$:

$$\int_{\mathcal{E}} f\,(\mathcal{A}_0 g)\ \psi_0 = \int_{\mathcal{E}} (\mathcal{A}_0^* f)\, g\, \psi_0$$

- Formally, $f_\xi = \left(1 + \xi\,(\mathcal{A}_0^*)^{-1} \mathcal{A}_1\right)^{-1} \mathbf{1} = \left(1 + \sum_{n=1}^{+\infty} \xi^n \left[(\mathcal{A}_0^*)^{-1} \mathcal{A}_1^*\right]^n\right) \mathbf{1}$
- To make such computations rigorous (for $\xi$ small enough): prove that
  - (properties of the equilibrium dynamics) $\mathrm{Ker}(\mathcal{A}_0^*) = \mathbf{1}$ and $\mathcal{A}_0^*$ is invertible on $\mathcal{H} = \mathbf{1}^\perp$
  - (properties of the perturbation) $\mathrm{Ran}(\mathcal{A}_1^*) \subset \mathcal{H}$ and $(\mathcal{A}_0^*)^{-1} \mathcal{A}_1^*$ is bounded on $\mathcal{H}$. Typically, $\|\mathcal{A}_1 \varphi\| \leq a \|\mathcal{A}_0 \varphi\| + b \|\varphi\|$ for $\varphi \in \mathcal{H}$

- Response property $R \in \mathcal{H}$, conjugated response $S = \mathcal{A}_1^* \mathbf{1}$:

$$\alpha = \lim_{\xi \to 0} \frac{\langle R \rangle_\xi}{\xi} = \int_{\mathcal{E}} R \, \mathrm{f}_1 \, \psi_0 = \int_{\mathcal{E}} \left[\mathcal{A}_0^{-1} R\right] \left[\mathcal{A}_1^* \mathbf{1}\right] \psi_0$$
$$= -\int_0^{+\infty} \mathbb{E}\Big(R(x_t) S(x_0)\Big) dt$$

where formally $-\mathcal{A}_0^{-1} = \int_0^{+\infty} \mathrm{e}^{t\mathcal{A}_0} \, dt$ (as operators on $\mathcal{H}$)

- Autocorrelation of $R$ recovered for perturbations such that $\mathcal{A}_1^* \mathbf{1} \propto R$
- 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 $F$

$$\begin{cases} dq_t = M^{-1} p_t \, dt \\ dp_t = \Big( -\nabla V(q_t) + \xi F \Big) dt - \gamma M^{-1} p_t \, dt + \sqrt{\dfrac{2\gamma}{\beta}} \, dW_t \end{cases}$$

- In this case, $\mathcal{A}_1 = F \cdot \partial_p$ and so $\mathcal{A}_1^* \mathbf{1} = -\beta F \cdot M^{-1} p$
- Response: $R(q,p) = F \cdot M^{-1} p$ = average velocity in the direction $F$
- Linear response result: defines the mobility

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

since $\left[ F \cdot \mathbb{E}(q_T - q_0) \right]^2 = 2T \displaystyle\int_0^T \mathbb{E}\Big( (F \cdot M^{-1} p_t)(F \cdot M^{-1} p_0) \Big) \left( 1 - \frac{t}{T} \right) dt$

# Example 2: Thermal transport

- Consider $T_{\mathrm{L}} = T + \Delta T$ and $T_{\mathrm{R}} = T - \Delta T$ so that $\xi = \Delta T$
- Reference dynamics = Langevin with thermostats at temperature $T$ at the boundaries, generator of the perturbation $\mathcal{A}_1 = \gamma(\partial^2_{p_1} - \partial^2_{p_N})$
- Invariant measure for the equilibrium dynamics

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

- 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)

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

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

$$\lim_{\Delta T \to 0} \frac{\langle J \rangle_{\Delta T}}{\Delta T} = -\beta^2 \gamma \int_0^{+\infty} \int_{\mathcal{E}} \left(\mathrm{e}^{-t\mathcal{A}_0} J\right) (p_1^2 - p_N^2) \psi_0 \, dt$$
$$= \frac{2\beta^2}{N-1} \int_0^{+\infty} \mathbb{E}\Big( J(q_t, p_t) J(q_0, p_0) \Big) \, dt$$

- Synthetic dynamics: fixed temperatures of the thermostats but external forcings → bulk driven dynamics (convergence may be faster)
  - Non-gradient perturbation $-\xi\Big(v'(q_{i+1} - q_i) + v'(q_i - q_{i-1})\Big)$
  - Hamiltonian perturbation $H_0 + \xi H_1$ with

$$H_1(q,p) = \sum_{i=1}^{N} (i - i_0) \frac{p_i^2}{2} + \sum_{i=1}^{N-1} \left( i - i_0 - \frac{1}{2} \right) v(q_i - q_{i-1}),$$

In both cases, $\mathcal{A}_1^* = -\mathcal{A}_1 + cJ$

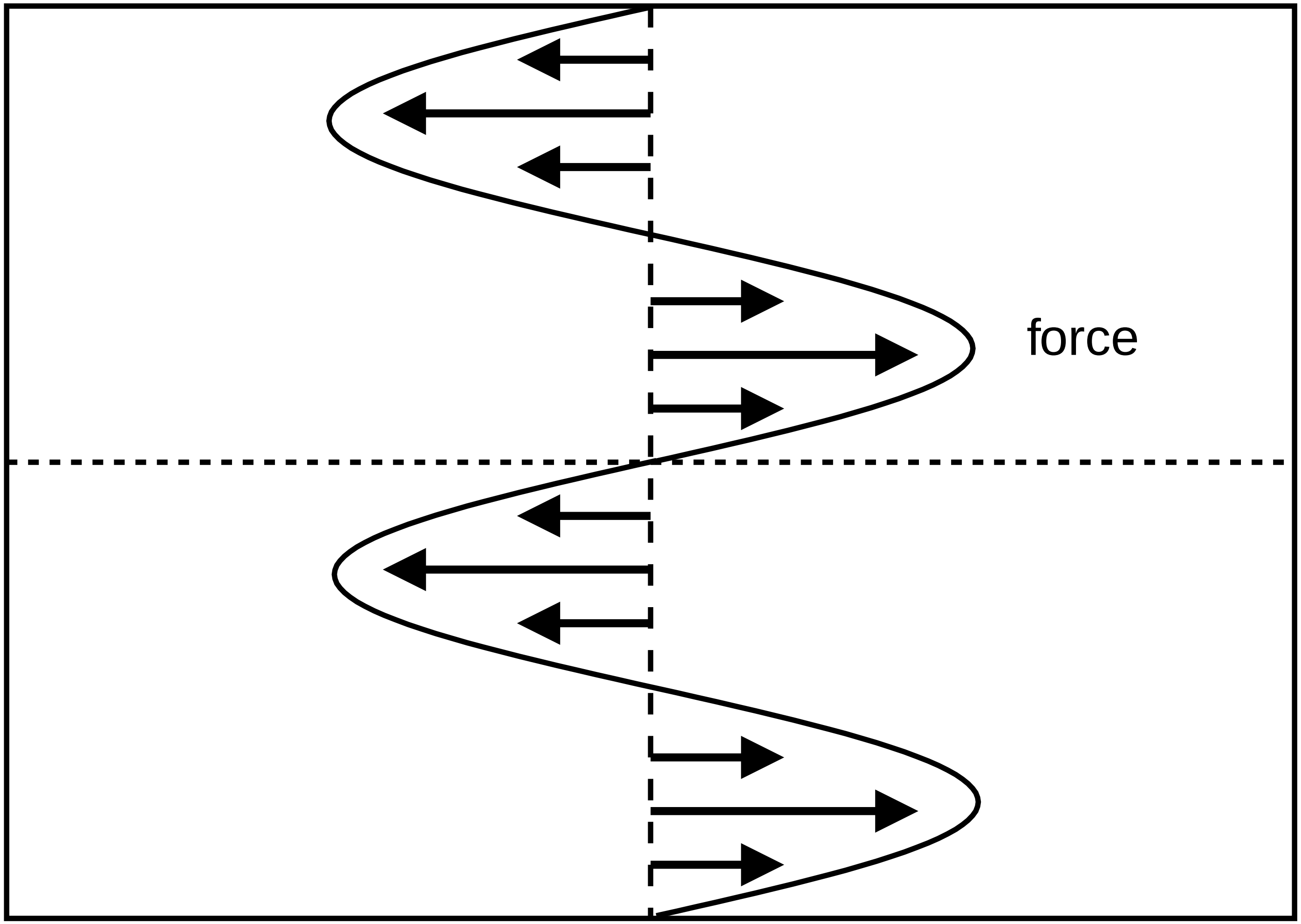
# *Extensions*

- 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

# Nonequilibrium Langevin dynamics for shear computations

# A picture of the nonequilibrium forcing

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



## The nonequilibrium dynamics

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

$$\begin{cases} dq_{i,t} = \dfrac{p_{i,t}}{m}\,dt, \\ dp_{xi,t} = -\nabla_{q_{xi}} V(q_t)\,dt + \xi F(q_{yi,t})\,dt - \gamma_x \dfrac{p_{xi,t}}{m}\,dt + \sqrt{\dfrac{2\gamma_x}{\beta}}\,dW_t^{xi}, \\ dp_{yi,t} = -\nabla_{q_{yi}} V(q_t)\,dt - \gamma_y \dfrac{p_{yi,t}}{m}\,dt + \sqrt{\dfrac{2\gamma_y}{\beta}}\,dW_t^{yi}, \end{cases}$$

- 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 $\xi \in (-\xi^*, \xi^*)$,

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

- Use $\|\mathcal{B}\varphi\|^2 \leq |\langle \varphi, \mathcal{A}_0\varphi\rangle|$, define $\mathrm{f}_{k+1} = -\left(\mathcal{A}_0^*\right)^{-1} \mathcal{B}^* \mathrm{f}_k$ so $(\mathcal{A}_0 + \xi\mathcal{B})^* f_\xi = 0$
- 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: $\displaystyle \lim_{\xi\to 0} \frac{\langle \mathcal{A}_0 h\rangle_\xi}{\xi} = -\frac{\beta}{m}\left\langle h, \sum_{i=1}^N p_{xi} F(q_{yi})\right\rangle_{L^2(\psi_0)}$
- Can be applied to $\mathcal{A}_0^{-1} h$ for a function $h \in \mathcal{H}$ (otherwise consider $h - \langle h\rangle_0$)
- Average longitudinal velocity $\displaystyle u_x(Y) = \lim_{\varepsilon\to 0}\lim_{\xi\to 0} \frac{\langle U_x^\varepsilon(Y,\cdot)\rangle_\xi}{\xi}$ where

$$U_x^\varepsilon(Y,q,p) = \frac{L_y}{Nm}\sum_{i=1}^N p_{xi}\chi_\varepsilon\left(q_{yi}-Y\right)$$

- Average off-diagonal stress $\displaystyle \sigma_{xy}(Y) = \lim_{\varepsilon\to 0}\lim_{\xi\to 0} \frac{\langle \dots\rangle_\xi}{\xi}$ where ... =

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

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

[a] Irving and Kirkwood, *J. Chem. Phys.* **18** (1950)

# Definition of the viscosity and asymptotics (1)

- Definition $\sigma_{xy}(Y) := -\eta(Y)\dfrac{du_x(Y)}{dY}$
- Closure assumption $\eta(Y) = \eta > 0$
- Closed equation on the longitudinal velocity: basis for numerics

$$-\eta u_x''(Y) + \gamma_x \overline{\rho} u_x(Y) = \overline{\rho} F(Y)$$

- Asymptotic behavior of the viscosity for large frictions: understand the limit of the longitudinal velocity field as $\gamma_x$ or $\gamma_y \to +\infty$

$$u_x^{\gamma_\alpha,\varepsilon}(Y) := \lim_{\xi \to 0} \frac{\langle U_x^\varepsilon(Y,\cdot)\rangle_\xi}{\xi} = -\frac{\beta}{m}\left\langle \sum_{i=1}^N p_{xi} F(q_{yi}), \mathscr{U}^\varepsilon(Y,q,p) \right\rangle_{L^2(\psi_0)}$$

with $-\mathcal{A}_0 \mathscr{U}^\varepsilon(Y,\cdot) = U_x^\varepsilon(Y,\cdot)$ and $\mathcal{A}_0 = \mathcal{A}_{\mathrm{ham}} + \gamma_x \mathcal{A}_{x,\mathrm{thm}} + \gamma_y \mathcal{A}_{y,\mathrm{thm}}$

- Behavior of solutions to the Poisson equation $-\mathcal{A}_0 f = \sum_{i=1}^N p_{xi} G(q_{yi})$?
- Formal solution $f = f^0 + \gamma_\alpha^{-1} f^1 + \gamma_\alpha^2 f^2 + \dots$

## 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 $-\mathcal{A}_0(\gamma_y) f_{\gamma_y} = \sum_{i=1}^{N} p_{xi} G(q_{yi})$
  - for all $\gamma_y \geq \gamma_x$, $\left\| f_{\gamma_y} - f^0 - \gamma_y^{-1} f^1 \right\|_{H^1(\psi_0)} \leq \dfrac{C}{\gamma_y}$
  - 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 $-\mathcal{A}_0(\gamma_x) f_{\gamma_x} = \sum_{i=1}^{N} p_{xi} G(q_{yi})$
  - for all $\gamma_x \geq \gamma_y$, $\left\| f_{\gamma_x} - \gamma_x^{-1} f^1 - \gamma_x^{-2} f^2 \right\|_{H^1(\psi_0)} \leq \dfrac{C}{\gamma_x^2}$
  - it holds $f^1(q,p) = m \sum_{i=1}^{N} p_{xi} G(q_{yi}) + \widetilde{f}^1(q, p_y)$
  - vanishing longitudinal velocity: $\overline{u}_x(Y) = \lim_{\varepsilon \to 0} \lim_{\gamma_x \to +\infty} \gamma_x u_x^\varepsilon(Y) = F(Y)$

- Idea of the proof in the case when $\gamma_y \to +\infty$
- Define $\mathcal{T}_{q_y} = p_x \cdot \nabla_{q_x} - \nabla_{q_x} V(q_x, q_y) \cdot \nabla_{p_x} + \gamma_x \mathcal{A}_{x,\mathrm{thm}}$ acting on $L^2(\Psi_{q_y})$

$$\begin{cases} \mathcal{A}_{y,\mathrm{thm}} f^0 = 0, \\ \mathcal{A}_{y,\mathrm{thm}} f^1(q,p) = -p_y \cdot \nabla_{q_y} f^0(q,p_x) - \sum_{i=1}^N p_{xi} G(q_{yi}) - \mathcal{T}_{q_y} f^0(q,p_x) \end{cases}$$

- The first equation shows that $f^0 \equiv f^0(q,p_x)$
- Set $f^1 = \widetilde{f}^1 + p_y \cdot \nabla_{q_y} f^0$ so that $\mathcal{A}_{y,\mathrm{thm}} \widetilde{f}^1 = -\sum_{i=1}^N p_{xi} G(q_{yi}) - \mathcal{T}_{q_y} f^0(q,p_x)$
- Solvability condition: $f^0(q,p) = -\sum_{i=1}^N G(q_{yi}) \mathcal{T}_{q_y}^{-1}(p_{xi})$ and $\widetilde{f}^1 = 0$
- Uniform hypocoercivity estimates: useful for $\gamma_y \geq \gamma_x$:

$$C\,\|u\|^2_{H^1(\psi_0)} - (\gamma_y - \gamma_x) \underbrace{\langle\langle u, \mathcal{A}_{y,\mathrm{thm}} u \rangle\rangle}_{\geq 0} \leq -\langle\langle u, \mathcal{A}_0 u \rangle\rangle$$

- Finish the proof by considering $u = f_{\gamma_y} - f^0 - \gamma_y^{-1} f^1$

## Numerical results: Description of the system

- 2D Lennard-Jones fluid $\mathcal{V}_{\rm LJ}(r) = 4\varepsilon_{\rm LJ}\left(\left(\frac{d_{\rm LJ}}{r}\right)^{12} - \left(\frac{d_{\rm LJ}}{r}\right)^{6}\right)$

  ($d_{\rm LJ} = \varepsilon_{\rm LJ} = 1$, 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: $F(y) = \begin{cases} \frac{4}{L_y}\left(y - \frac{L_y}{4}\right), & 0 \le y \le \frac{L_y}{2}, \\ \frac{4}{L_y}\left(\frac{3L_y}{4} - y\right), & \frac{L_y}{2} \le y \le L_y; \end{cases}$
  - piecewise constant: $F(y) = \begin{cases} 1, & 0 < y < \frac{L_y}{2}, \\ -1, & \frac{L_y}{2} < y < L_y. \end{cases}$

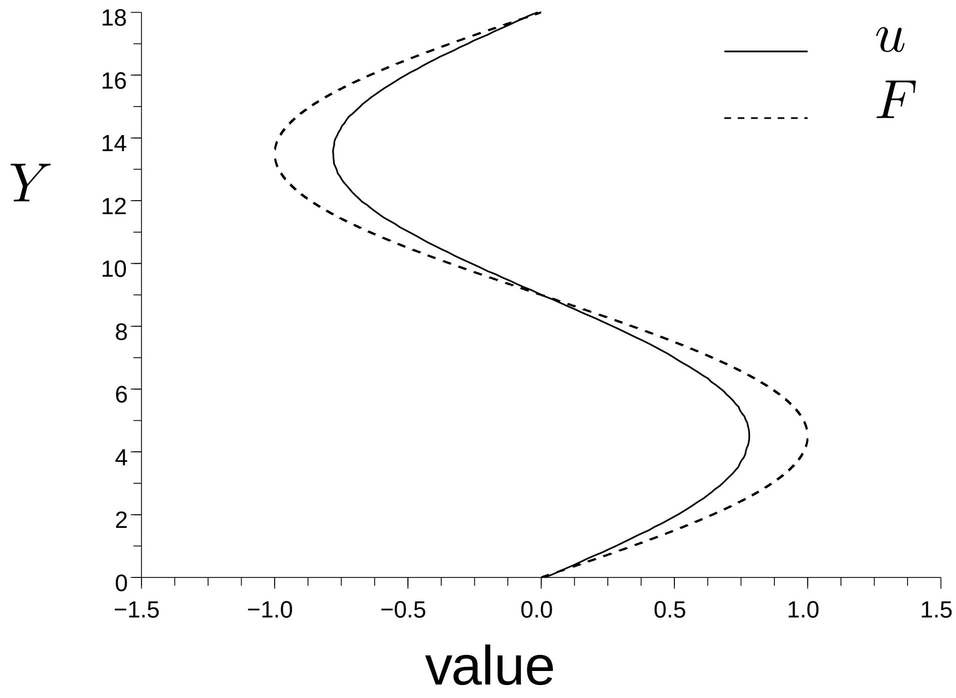
## Numerical implementation

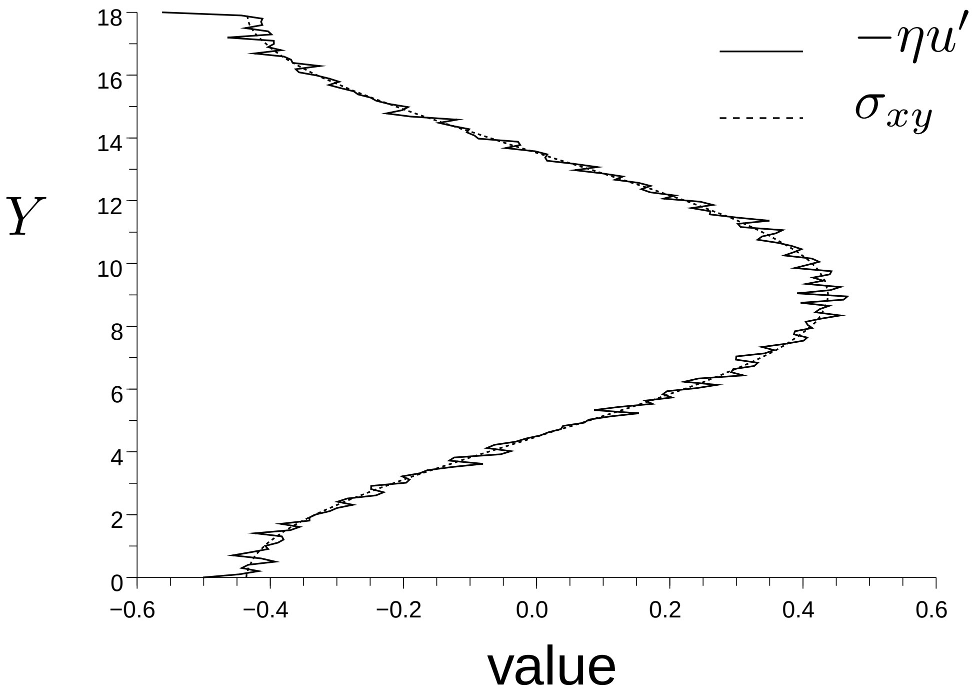
- Numerical scheme: $\alpha_{x,y} = \exp(-\gamma_{x,y}\Delta t)$, time step $\Delta t = 0.005$

$$
\begin{cases}
p^{n+1/4} = p^n - \dfrac{\Delta t}{2}\nabla V(q^n), \\
q^{n+1} = q^n + \Delta t\, p^{n+1/4}, \\
p^{n+1/2} = p^{n+1/4} - \dfrac{\Delta t}{2}\nabla V(q^{n+1}), \\
p_{xi}^{n+1} = \alpha_x p_{xi}^{n+1/2} + \sqrt{\dfrac{1}{\beta}(1-\alpha_x^2)}\, G_{xi}^n + (1-\alpha_x)\,\dfrac{\xi}{\gamma_x} F\left(q_{yi}^{n+1}\right) \\
p_{y}^{n+1} = \alpha_y p_{y}^{n+1/2} + \sqrt{\dfrac{1}{\beta}(1-\alpha_y^2)} G_y^n,
\end{cases}
$$

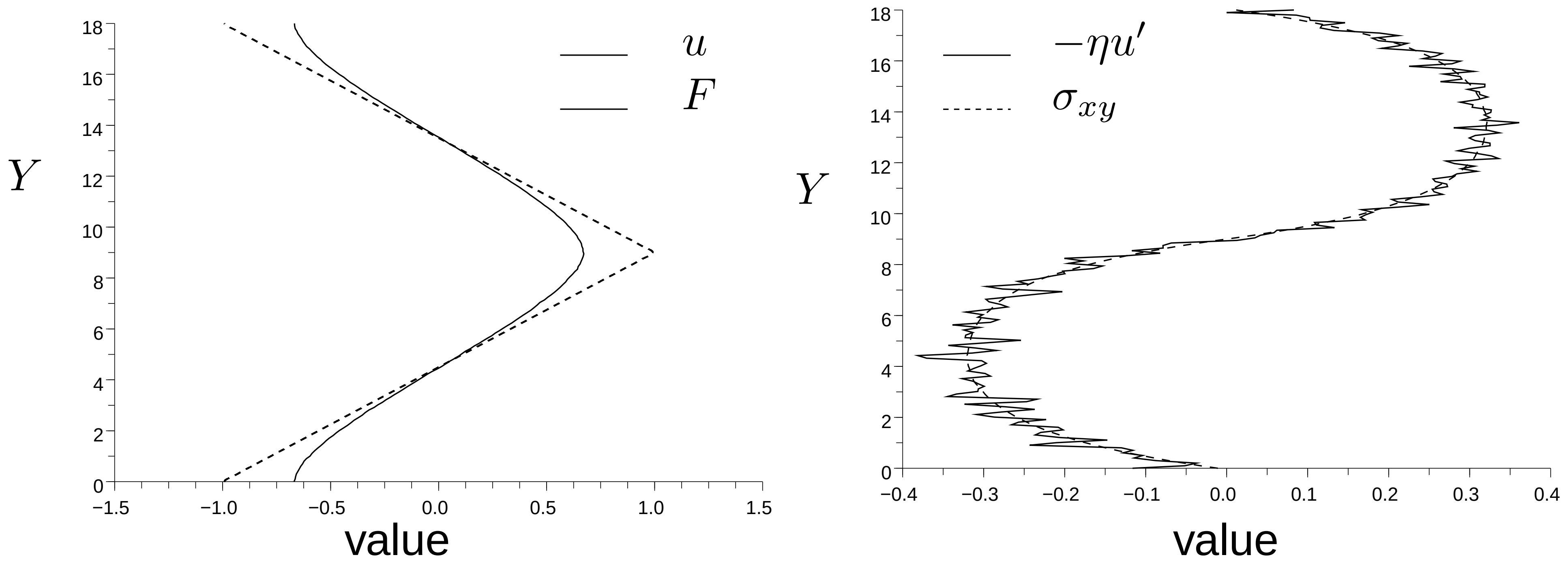
- Well behaved in the limits $\gamma \to$ and/or $\gamma \to +\infty$
- Binning procedure to obtain averages as a function of the altitude $Y$
- Fourier series analysis to estimate the viscosity $U_k = \dfrac{F_k}{\dfrac{\eta}{\rho}\left(\dfrac{2\pi}{L_y}\right)^2 k^2 + \gamma_x}$

## Numerical results: Validation of the closure (1)

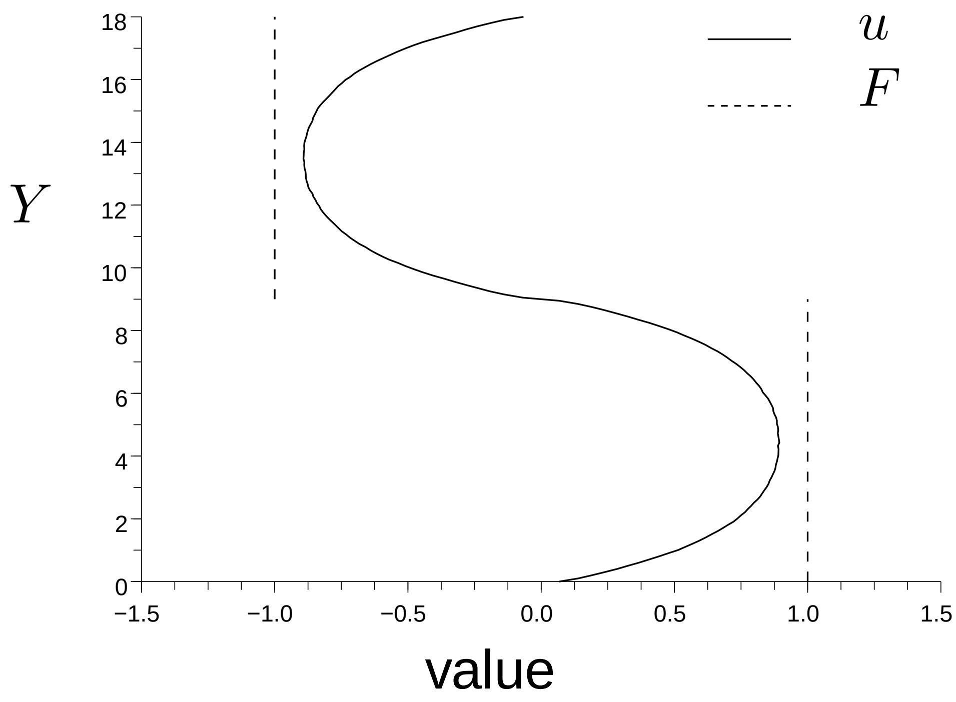


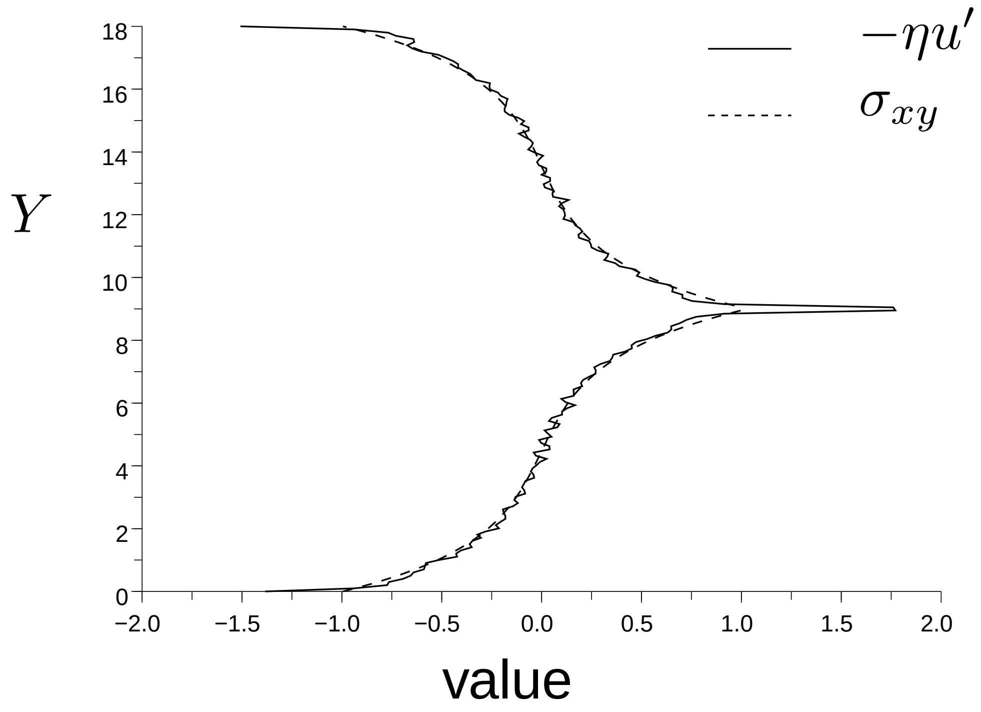




Velocity profile and off diagonal component of the stress tensor for the sinusoidal nongradient force.



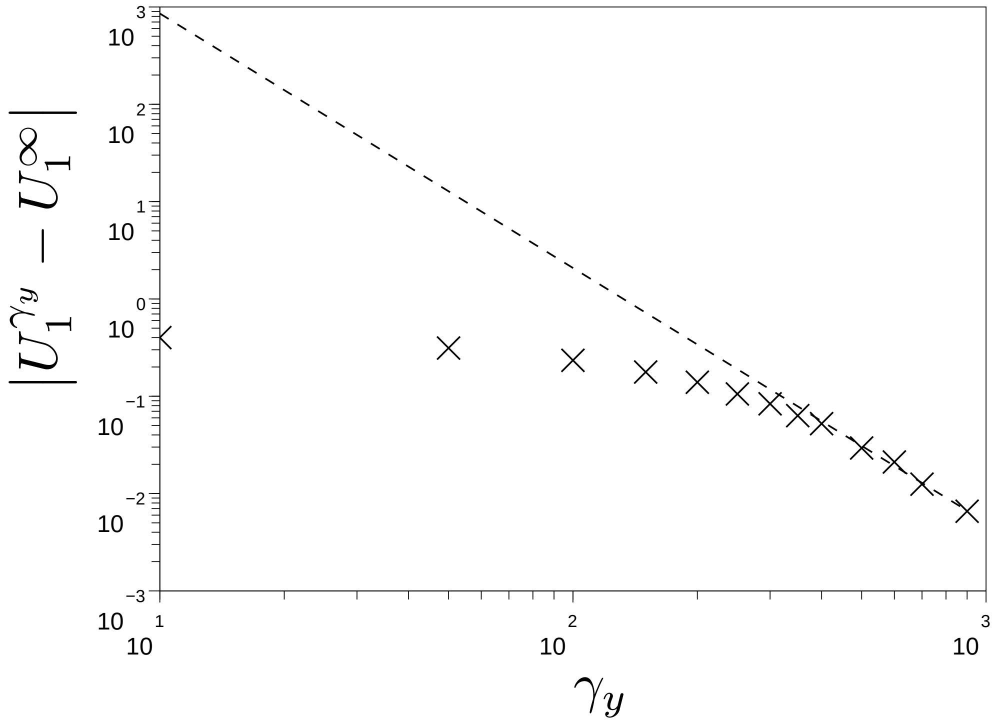

Velocity profile and off diagonal component of the stress tensor for the piecewise linear nongradient force.

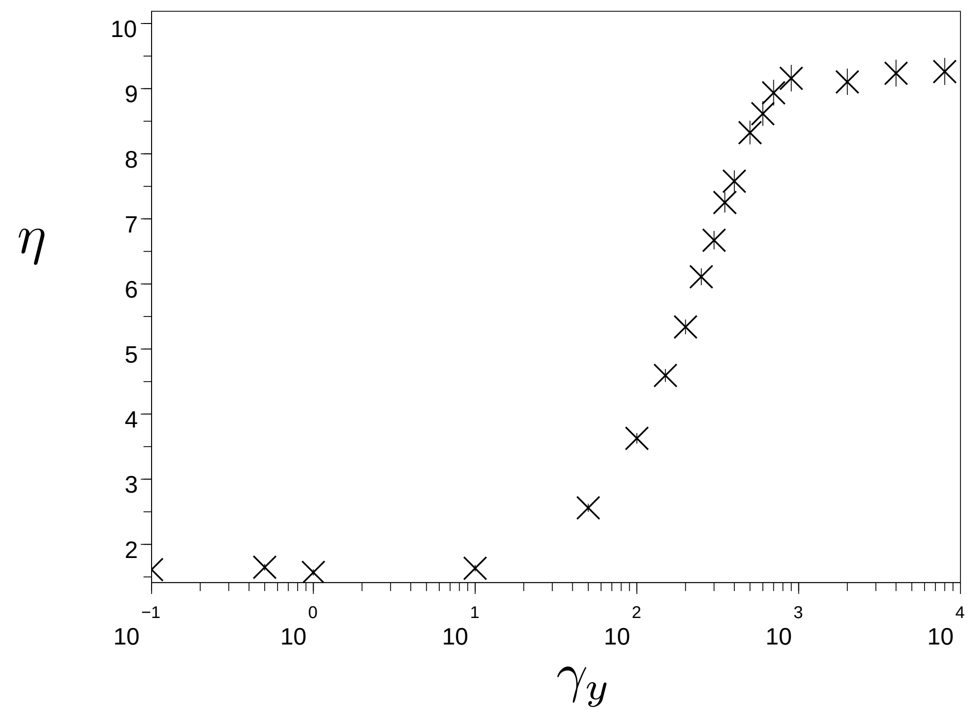



Velocity profile and off diagonal component of the stress tensor for the piecewise constant nongradient force.

# Numerical results: Infinite transverse friction

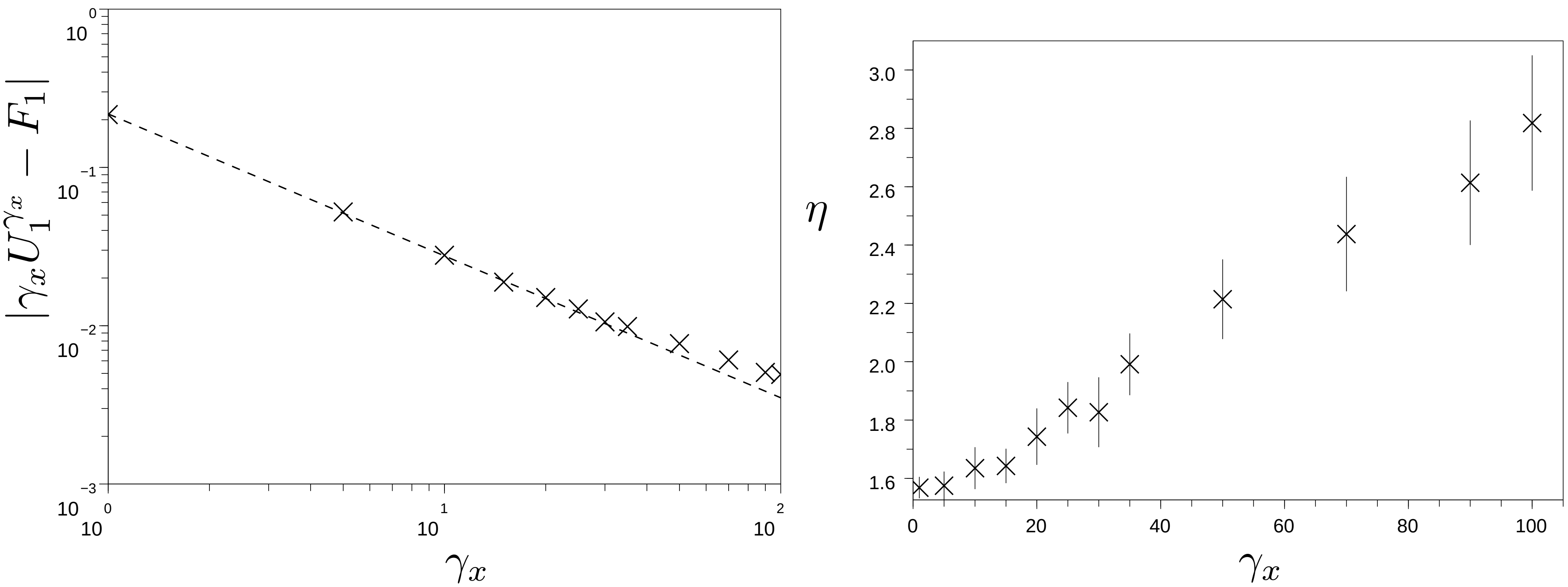



Left: Convergence of the velocity profile for increasing values of the transverse friction $\gamma_y$.

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.