

# *Computation of transport properties by molecular dynamics*

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- 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<sup>a</sup>
  - Description of the dynamics
  - Definition of the viscosity
  - Asymptotics with respect to the friction coefficient
  - Numerical results

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<sup>a</sup>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  $H(q, p) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V(q_1, \dots, q_N)$  (all the physics in  $V$ !)

- **Canonical** measure: density  $\psi_0(q, p) = Z^{-1} e^{-\beta H(q, p)}$ , 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:  $A(q, p) = \frac{1}{d|\mathcal{D}|} \sum_{i=1}^N \left( \frac{p_i^2}{m_i} - q_i \cdot \nabla_{q_i} V(q) \right)$

- **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:

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

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

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

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

- Precise expressions of the generators:

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

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

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

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

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

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<sup>a</sup>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

- 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**  $dq_t = \left( -\nabla V(q_t) + F \right) dt + \sqrt{\frac{2}{\beta}} dW_t$  and  $q_t \in \mathbb{T}$
- fluctuation terms with **different temperatures**

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

- 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

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

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

solution of  $(\mathcal{A}_0^* + \xi \mathcal{A}_1^*) f_\lambda = 0$ , 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**,  $f_\lambda = \left(1 + \xi (\mathcal{A}_0^*)^{-1} \mathcal{A}_1\right)^{-1} \mathbf{1} = \left(1 + \sum_{n=1}^{+\infty} \xi^n \left[(\mathcal{A}_0^*)^{-1} \mathcal{A}_1^*\right]^n\right) \mathbf{1}$
- To make such computations rigorous (for  $\xi$  small enough): prove that
  - **(properties of the equilibrium dynamics)**  $\text{Ker}(\mathcal{A}_0^*) = \mathbf{1}$  and  $\mathcal{A}_0^*$  is invertible on  $\mathcal{H} = \mathbf{1}^\perp$
  - **(properties of the perturbation)**  $\text{Ran}(\mathcal{A}_1^*) \subset \mathcal{H}$  and  $(\mathcal{A}_0^*)^{-1} \mathcal{A}_1^*$  is bounded on  $\mathcal{H}$ . Typically,  $\|\mathcal{A}_1 \varphi\| \leq a \|\mathcal{A}_0 \varphi\| + b \|\varphi\|$

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

$$\begin{aligned}\alpha &= \lim_{\xi \rightarrow 0} \frac{\langle R \rangle_\xi}{\xi} = \int_{\mathcal{E}} R f_1 \psi_0 = \int_{\mathcal{E}} [\mathcal{A}_0^{-1} R] [\mathcal{A}_1^* \mathbf{1}] \psi_0 \\ &= - \int_0^{+\infty} \mathbb{E} \left( R(x_t) S(x_0) \right) dt\end{aligned}$$

where formally  $-\mathcal{A}_0^{-1} = \int_0^{+\infty} e^{t\mathcal{A}_0} dt$  (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**  $F$

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

- 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**

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

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

## 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  $\mathcal{A}_1 = \gamma(\partial_{p_1}^2 - \partial_{p_N}^2)$
- 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 can be proven under some **conditions on the interaction** potential  $v$
- Response function: **energy current** (local variations of the energy)

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

## Example 2: Thermal transport (continued)

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

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

- **Synthetic dynamics:** fixed temperatures of the thermostats but external forcings  $\rightarrow$  **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

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

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

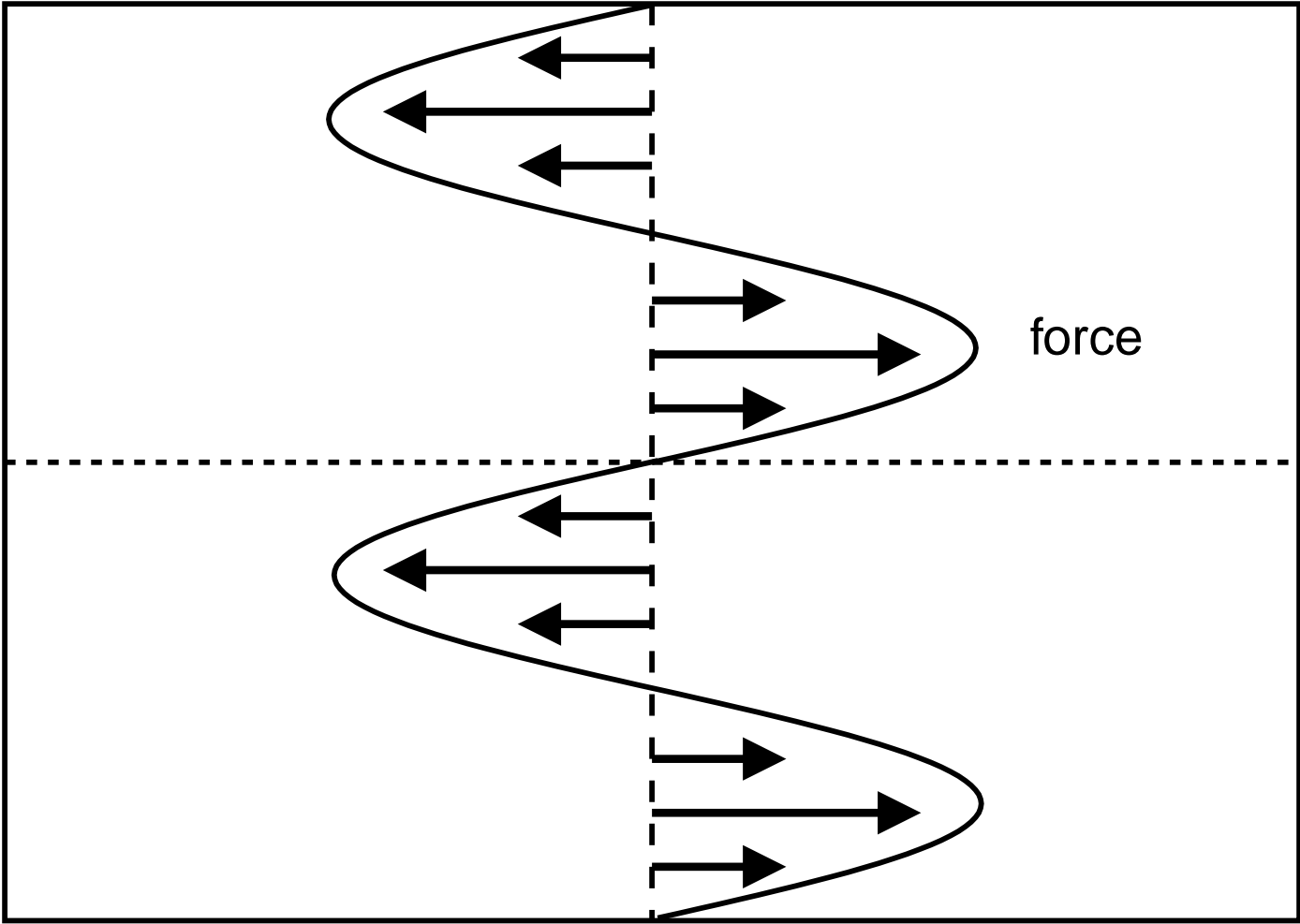
- **Time-dependent forcings** (Fourier transforms of autocorrelations, stochastic resonance)
- **Constrained nonequilibrium** systems (computation of transport properties for systems with molecular constraints)
- **Variance reduction** (in particular, importance sampling) for nonequilibrium dynamics

# Nonequilibrium Langevin dynamics for shear computations



# A picture of the nonequilibrium forcing

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



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

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

- 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  $\|\mathcal{B}\varphi\|^2 \leq |\langle \varphi, \mathcal{A}_0 \varphi \rangle|$ , define  $f_{k+1} = -(\mathcal{A}_0^*)^{-1} \mathcal{B}^* f_k$  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:  $\lim_{\xi \rightarrow 0} \frac{\langle \mathcal{A}_0 h \rangle_\xi}{\xi} = -\frac{\beta}{m} \left\langle h, \sum_{i=1}^N p_{xi} F(q_{yi}) \right\rangle_{L^2(\psi_0)}$
- 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**  $u_x(Y) = \lim_{\varepsilon \rightarrow 0} \lim_{\xi \rightarrow 0} \frac{\langle U_x^\varepsilon(Y, \cdot) \rangle_\xi}{\xi}$  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**  $\sigma_{xy}(Y) = \lim_{\varepsilon \rightarrow 0} \lim_{\xi \rightarrow 0} \frac{\langle \dots \rangle_\xi}{\xi}$  where ... =

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

- **Local conservation law**<sup>a</sup>  $\frac{d\sigma_{xy}(Y)}{dY} + \gamma_x \bar{\rho} u_x(Y) = \bar{\rho} F(Y)$  (with  $\bar{\rho} = N/|\mathcal{D}|$ )

<sup>a</sup>Irving and Kirkwood, *J. Chem. Phys.* **18** (1950)

## 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**

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

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

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

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

- 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:  $\gamma_y \rightarrow +\infty$

- $f_{\gamma_y}$  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  $\gamma_y \geq \gamma_x$ ,  $\|f_{\gamma_y} - f^0 - \gamma_y^{-1}f^1\|_{H^1(\psi_0)} \leq \frac{C}{\gamma_y}$
- 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:  $\gamma_x \rightarrow +\infty$

- $f_{\gamma_x} \in \mathcal{H}$  unique solution of  $-\mathcal{A}_0(\gamma_x)f_{\gamma_x} = \sum_{i=1}^N p_{xi}G(q_{yi})$
- for all  $\gamma_x \geq \gamma_y$ ,  $\|f_{\gamma_x} - \gamma_x^{-1}f^1 - \gamma_x^{-2}f^2\|_{H^1(\psi_0)} \leq \frac{C}{\gamma_x^2}$
- it holds  $f^1(q, p) = m \sum_{i=1}^N p_{xi}G(q_{yi}) + \tilde{f}^1(q, p_y)$
- **vanishing** longitudinal velocity:  $\bar{u}_x(Y) = \lim_{\varepsilon \rightarrow 0} \lim_{\gamma_x \rightarrow +\infty} \gamma_x u_x^\varepsilon(Y) = F(Y)$

- 2D Lennard-Jones fluid  $\mathcal{V}_{\text{LJ}}(r) = 4\varepsilon_{\text{LJ}} \left( \left( \frac{d_{\text{LJ}}}{r} \right)^{12} - \left( \frac{d_{\text{LJ}}}{r} \right)^6 \right)$   
( $d_{\text{LJ}} = \varepsilon_{\text{LJ}} = 1$ , 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 scheme:  $\alpha_{x,y} = \exp(-\gamma_{x,y}\Delta t)$ , time step  $\Delta t = 0.005$

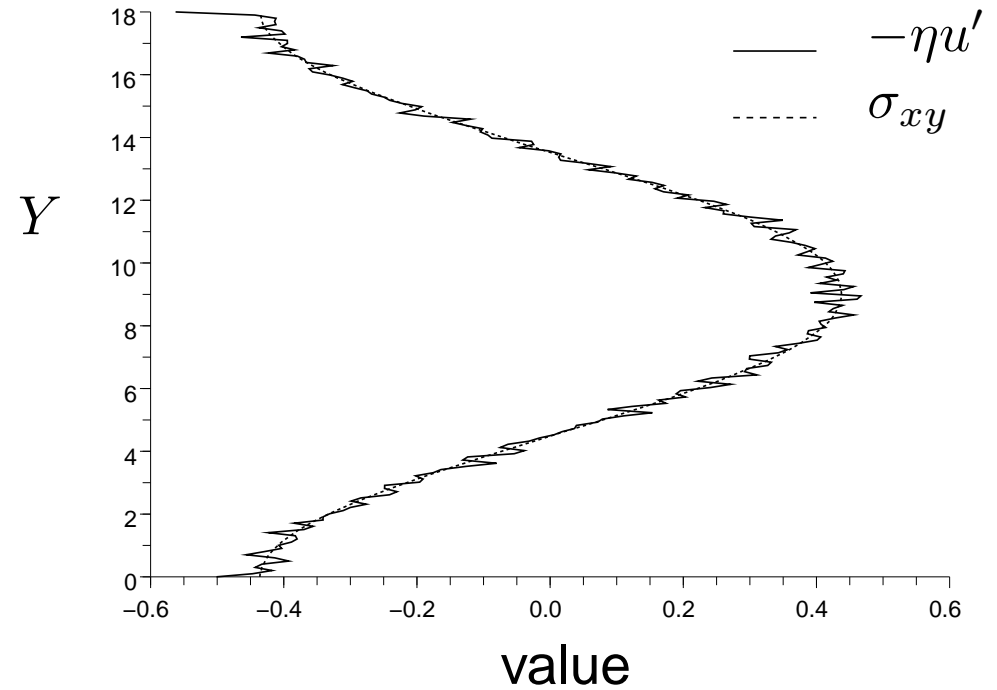
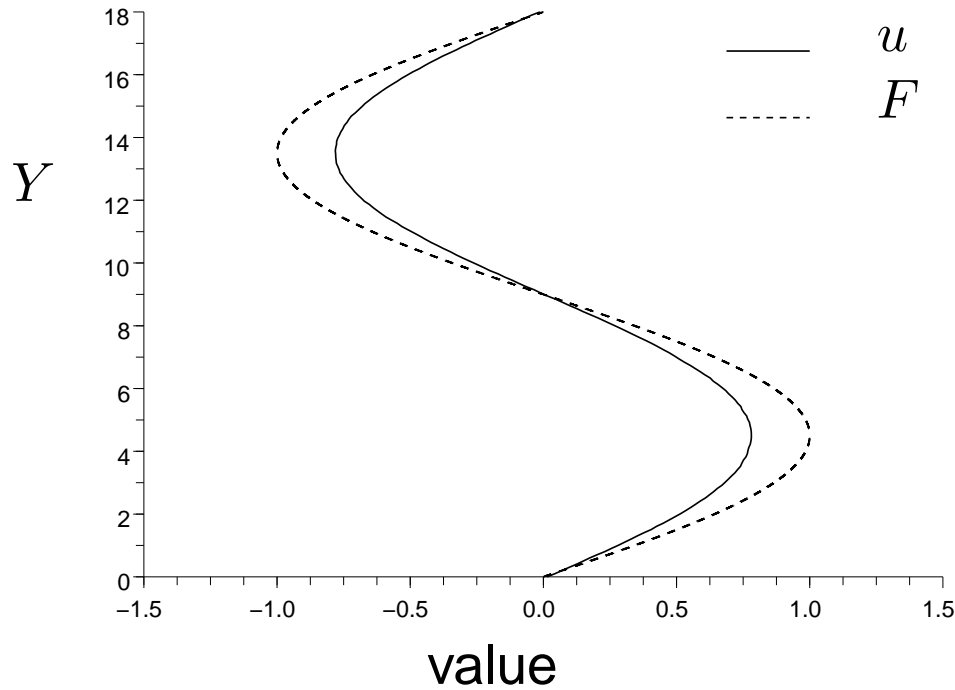
$$\left\{ \begin{array}{l} p^{n+1/4} = p^n - \frac{\Delta t}{2} \nabla V(q^n), \\ q^{n+1} = q^n + \Delta t p^{n+1/4}, \\ p^{n+1/2} = p^{n+1/4} - \frac{\Delta t}{2} \nabla V(q^{n+1}), \\ p_{xi}^{n+1} = \alpha_x p_{xi}^{n+1/2} + \sqrt{\frac{1}{\beta}(1 - \alpha_x^2)} G_{xi}^n + (1 - \alpha_x) \frac{\xi}{\gamma_x}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

- **Well behaved** in the limits  $\gamma \rightarrow 0$  and/or  $\gamma \rightarrow +\infty$

- **Binning** procedure to obtain averages as a function of the altitude  $Y$

- **Fourier series analysis** to estimate the viscosity  $U_k = \frac{F_k}{\frac{\eta}{\rho} \left(\frac{2\pi}{L_y}\right)^2 k^2 + \gamma_x}$

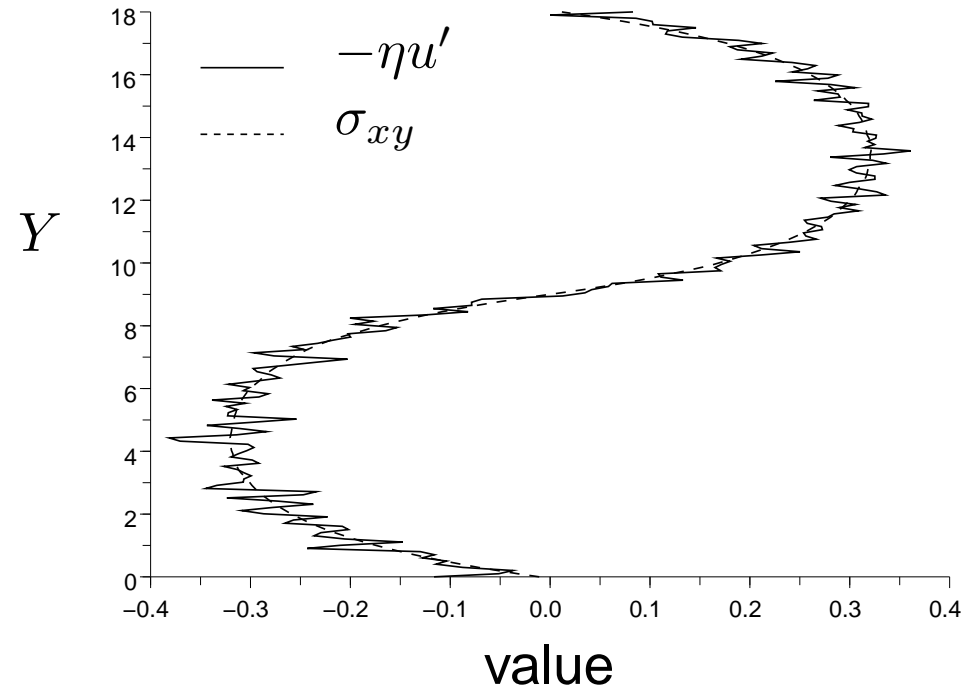
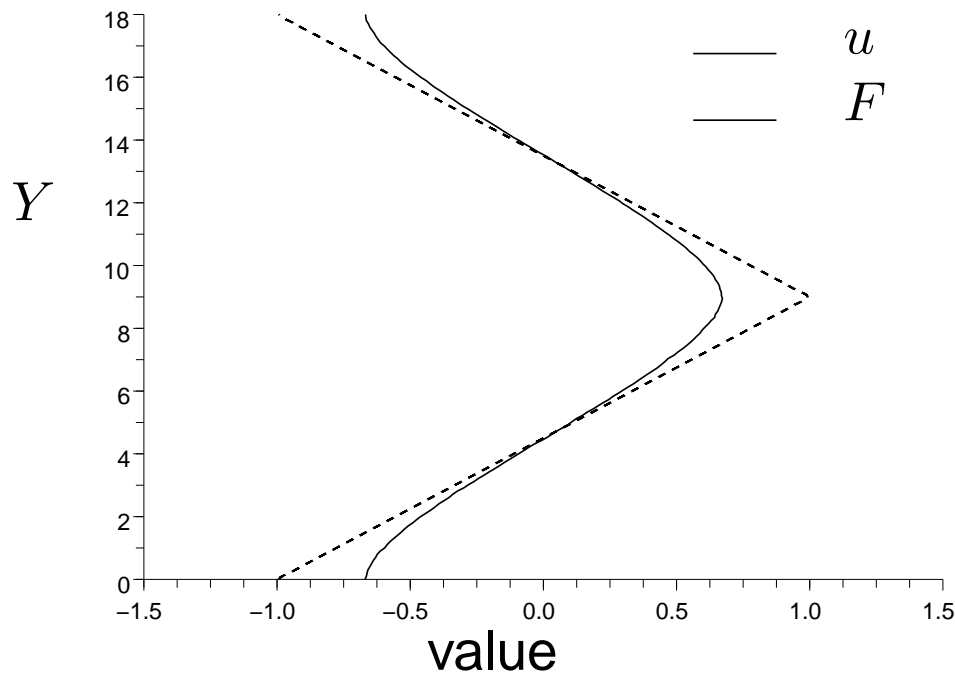
# Numerical results: Validation of the closure (1)



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

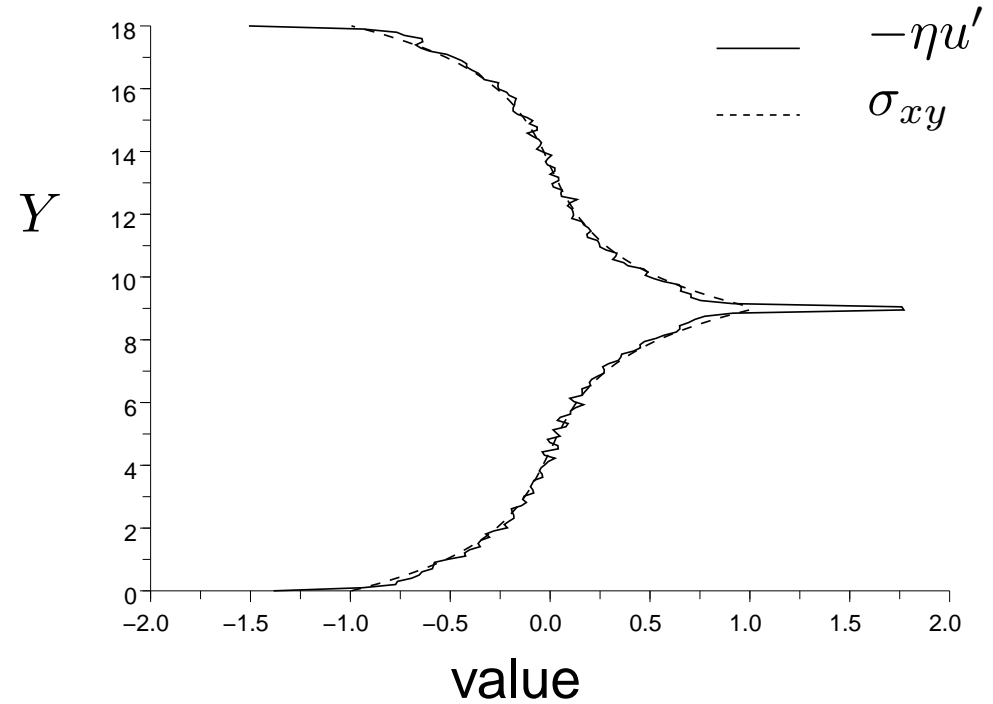
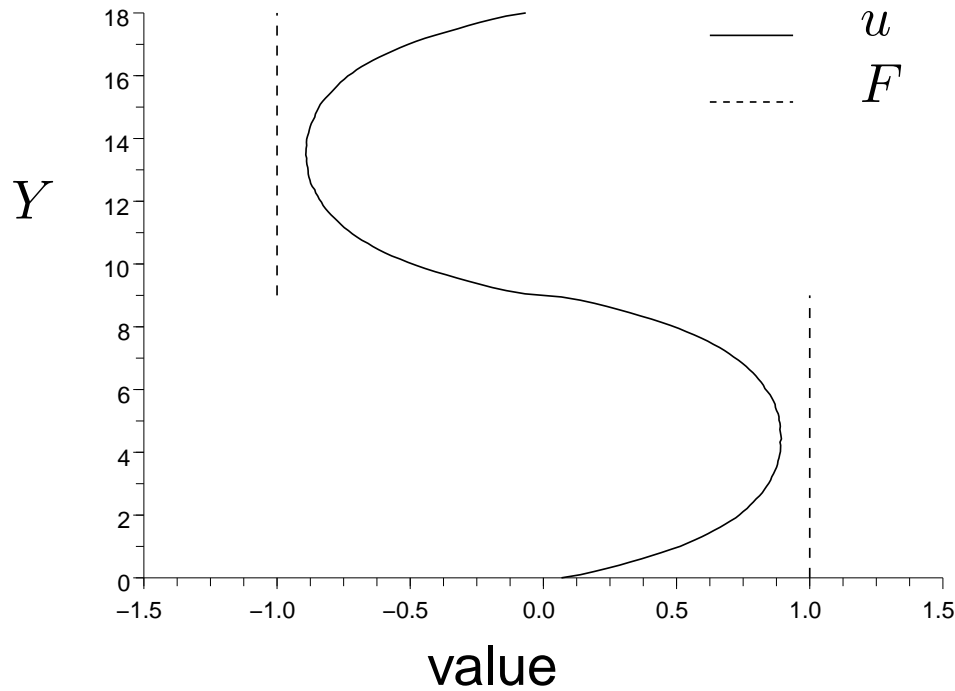


## Numerical results: Validation of the closure (2)



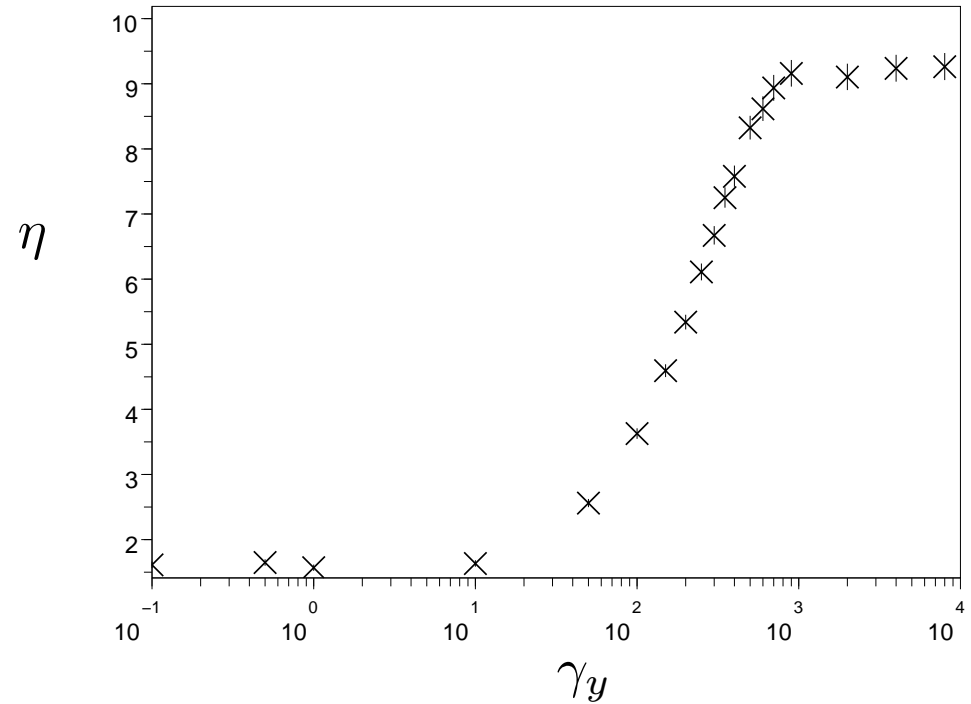
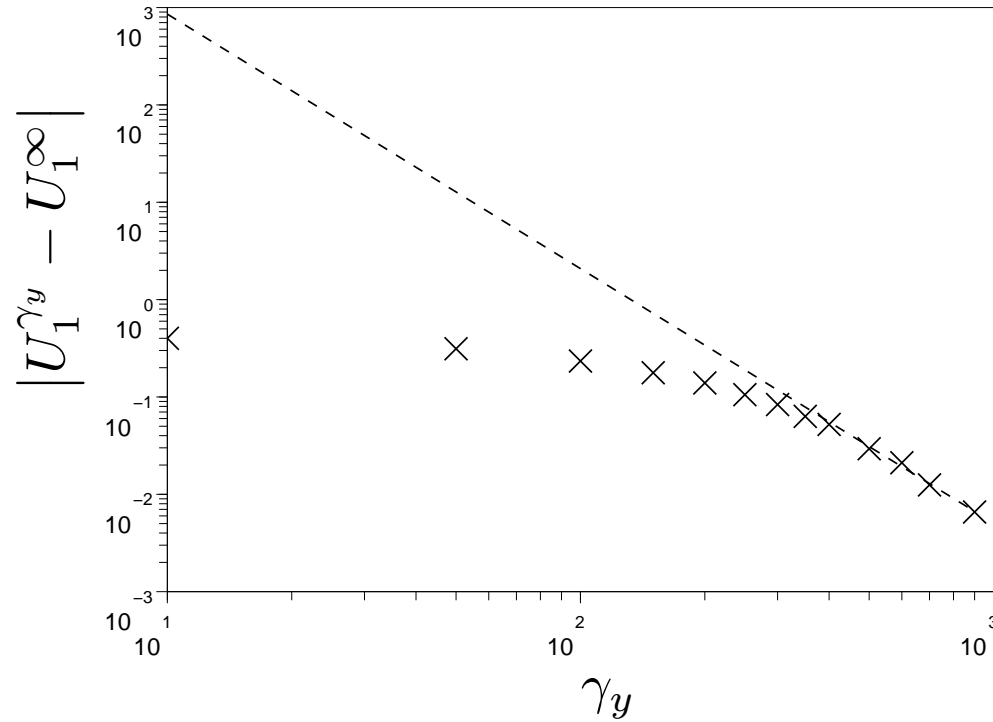
Velocity profile and off diagonal component of the stress tensor for the **piecewise linear** nongradient force.

# Numerical results: Validation of the closure (3)



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

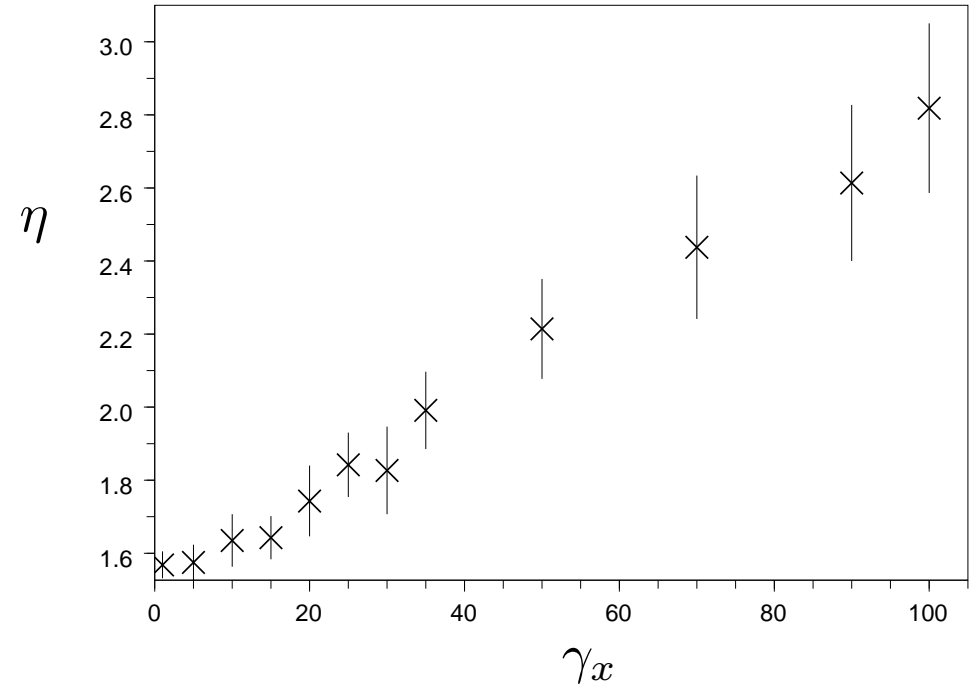
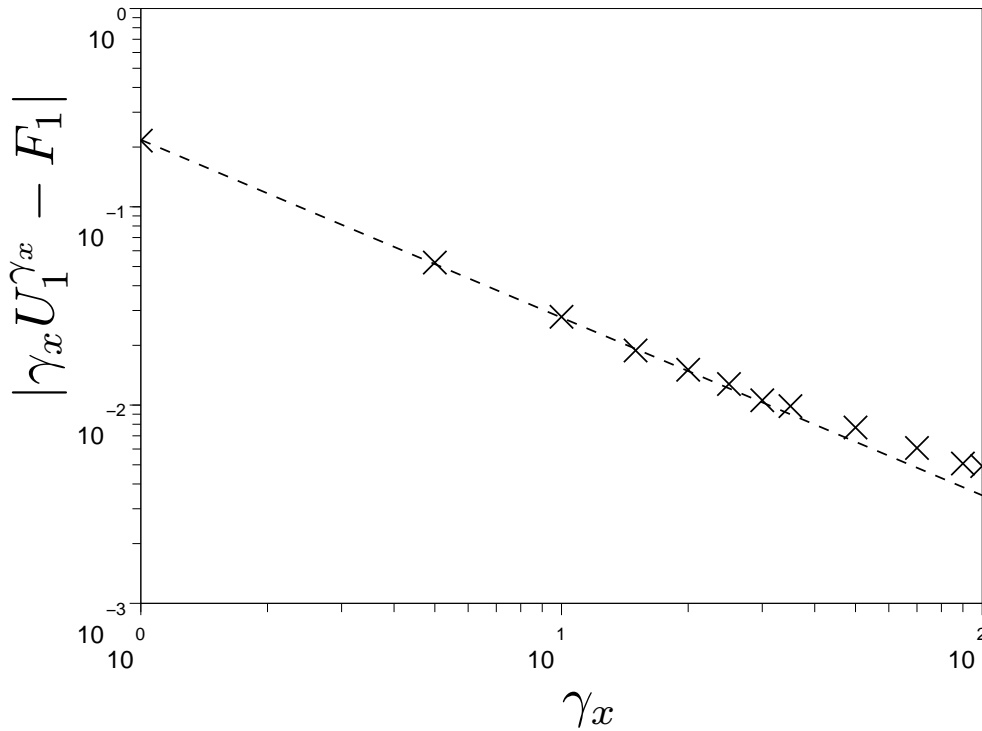
# Numerical results: Infinite transverse friction



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.