Norton Dynamics

Noé Blassel & Gabriel Stoltz

CERMICS lab, École des Ponts ParisTech - MATHERIALS team, Inria

December 14, 2022

Introduction

- Aim: compute transport coefficients (mobility, shear viscosity, thermal conductivity...). Proportionality constants in the linear response of a flux to a non-equilibrium perturbation by a force.

Introduction

- Aim: compute transport coefficients (mobility, shear viscosity, thermal conductivity...). Proportionality constants in the linear response of a flux to a non-equilibrium perturbation by a force.
- At the macroscopic level, fluxes and forces play symmetric and conjugate roles: fixing one determines the other.

Proposed by Denis Evans and coauthors in 1980s, but in a deterministic setting where ergodicity is dubious at best. Numerically shown to be correct, formal proofs, but no rigorous mathematical treatment. Goal: define a stochastic version of the method, easier to study theoretically, and more in phase with current numerical practice.

Introduction

- Aim: compute transport coefficients (mobility, shear viscosity, thermal conductivity...). Proportionality constants in the linear response of a flux to a non-equilibrium perturbation by a force.
- At the macroscopic level, fluxes and forces play symmetric and conjugate roles: fixing one determines the other.
- "Standard" NEMD approaches fix the force exactly at the microscopic level, and measure ergodic averages of the flux.

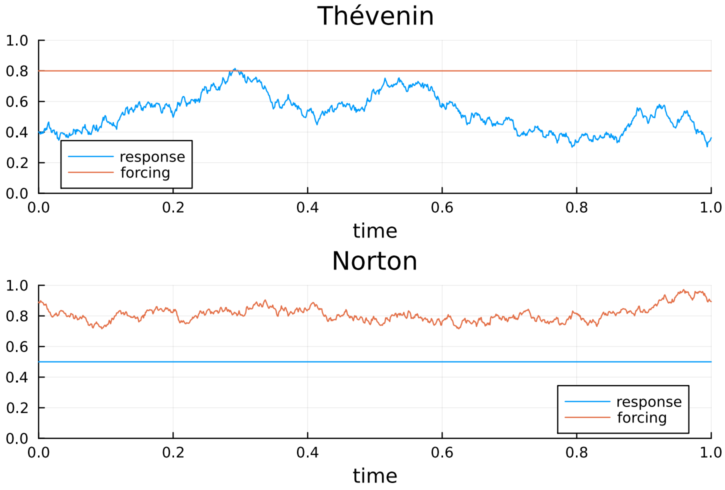
Proposed by Denis Evans and coauthors in 1980s, but in a deterministic setting where ergodicity is dubious at best. Numerically shown to be correct, formal proofs, but no rigorous mathematical treatment. Goal: define a stochastic version of the method, easier to study theoretically, and more in phase with current numerical practice.

Introduction

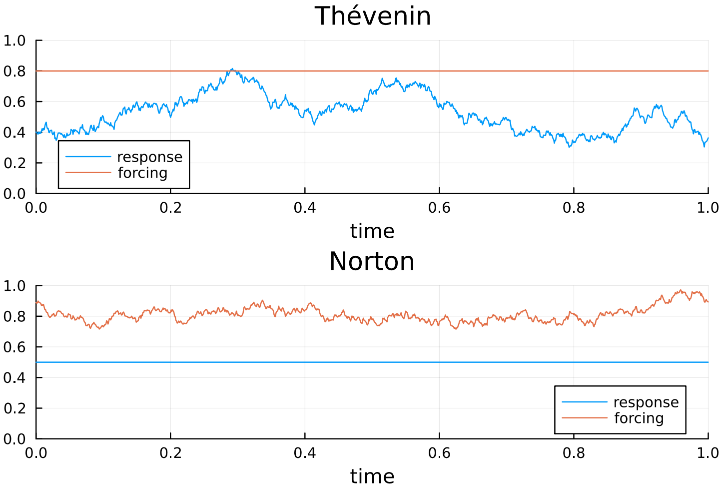
- Aim: compute transport coefficients (mobility, shear viscosity, thermal conductivity...). Proportionality constants in the linear response of a flux to a non-equilibrium perturbation by a force.
- At the macroscopic level, fluxes and forces play symmetric and conjugate roles: fixing one determines the other.
- "Standard" NEMD approaches fix the force exactly at the microscopic level, and measure ergodic averages of the flux.
- Instead, we can try to take the dual approach: fix the flux exactly, and measure ergodic averages of the forcing needed to sustain it.

Proposed by Denis Evans and coauthors in 1980s, but in a deterministic setting where ergodicity is dubious at best. Numerically shown to be correct, formal proofs, but no rigorous mathematical treatment. Goal: define a stochastic version of the method, easier to study theoretically, and more in phase with current numerical practice.

Illustration



Illustration



If the estimators for the average forcing have better statistical properties than estimators for the average response, choose Norton over Thévenin.

Standard NEMD dynamics

Fix a d-dimensional configuration space $\mathcal{X}$, a reference drift b and diffusion matrix σ. External forcing: $F : \mathcal{X} \to \mathbb{R}^d$, modulated in strength by $\eta \geq 0$.

- Standard NEMD/ "Thévenin":

$$\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t.$$

Standard NEMD dynamics

Fix a d-dimensional configuration space $\mathcal{X}$, a reference drift b and diffusion matrix σ. External forcing: $F : \mathcal{X} \to \mathbb{R}^d$, modulated in strength by $\eta \geq 0$.

- Standard NEMD/"Thévenin":

$$\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t.$$

- We measure averages of the response $R : \mathcal{X} \to \mathbb{R}$, with respect to the invariant mesure μ^η.

Standard NEMD dynamics

Fix a d-dimensional configuration space $\mathcal{X}$, a reference drift b and diffusion matrix σ. External forcing: $F : \mathcal{X} \to \mathbb{R}^d$, modulated in strength by $\eta \geq 0$.

- Standard NEMD/"Thévenin":

$$\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t.$$

- We measure averages of the response $R : \mathcal{X} \to \mathbb{R}$, with respect to the invariant mesure μ^η.
- Transport coefficient:

$$\rho_{R,F} = \lim_{\eta \to 0} \frac{1}{\eta} \left[\int_{\mathcal{X}} R\,\mathrm{d}\mu^\eta - \int_{\mathcal{X}} R\,\mathrm{d}\mu^0 \right].$$

Norton dynamics

Thévenin dynamics: $\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t$. Fix $r \geq 0$ the value of the response.

Norton dynamics

Thévenin dynamics: $\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t$. Fix $r \geq 0$ the value of the response.
For the Norton approach, we replace $\eta\,\mathrm{d}t$ by the increment of a stochastic process $\mathrm{d}\Lambda_t^r$.

- Norton dynamics:

$$\mathrm{d}Y_t^r = b(Y_t^r)\,\mathrm{d}t + \sigma(Y_t^r)\,\mathrm{d}W_t + F(Y_t^r)\,\mathrm{d}\Lambda_t^r.$$

Norton dynamics

Thévenin dynamics: $\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t$. Fix $r \geq 0$ the value of the response.
For the Norton approach, we replace $\eta\,\mathrm{d}t$ by the increment of a stochastic process $\mathrm{d}\Lambda_t^r$.

- Norton dynamics:

$$\mathrm{d}Y_t^r = b(Y_t^r)\,\mathrm{d}t + \sigma(Y_t^r)\,\mathrm{d}W_t + F(Y_t^r)\,\mathrm{d}\Lambda_t^r.$$

- The forcing process Λ_t^r is determined by the condition $R(Y_t^r) = r$ for all $t \geq 0$, and can be written as an adapted Itô process,

$$\mathrm{d}\Lambda_t^r = \lambda_t \mathrm{d}t + \mathrm{d}\widetilde{\Lambda}_t^r,$$

with $\widetilde{\Lambda}^r$ a martingale.

Norton dynamics

Thévenin dynamics: $\mathrm{d}X_t^\eta = b(X_t^\eta)\,\mathrm{d}t + \sigma(X_t^\eta)\,\mathrm{d}W_t + \eta F(X_t^\eta)\,\mathrm{d}t$. Fix $r \geq 0$ the value of the response.
For the Norton approach, we replace $\eta\,\mathrm{d}t$ by the increment of a stochastic process $\mathrm{d}\Lambda_t^r$.

- Norton dynamics:

$$\mathrm{d}Y_t^r = b(Y_t^r)\,\mathrm{d}t + \sigma(Y_t^r)\,\mathrm{d}W_t + F(Y_t^r)\,\mathrm{d}\Lambda_t^r.$$

- The forcing process Λ_t^r is determined by the condition $R(Y_t^r) = r$ for all $t \geq 0$, and can be written as an adapted Itô process,

$$\mathrm{d}\Lambda_t^r = \lambda_t \mathrm{d}t + \mathrm{d}\widetilde{\Lambda}_t^r,$$

  with $\widetilde{\Lambda}^r$ a martingale.
- Dynamics on the manifold

$$\Sigma_r = \{y \in \mathcal{X}, \quad R(y) = r\} = R^{-1}\{r\}.$$

Explicit form

By applying Itô's formula to the constraint, the SDE for Λ^r can be written explicitely, and the Norton dynamics can be written as

$$\mathrm{d}Y_t^r = \overline{P}_{F,\nabla R}(Y_t^r)\left[b(Y_t^r)\mathrm{d}t + \sigma(Y_t^r)\mathrm{d}W_t\right] - \frac{\left(\nabla^2 R : \Pi_{F,\nabla R,\sigma}\right) F}{2\nabla R \cdot F}(Y_t^r)\,\mathrm{d}t.$$

Explicit form

By applying Itô's formula to the constraint, the SDE for Λ^r can be written explicitely, and the Norton dynamics can be written as

$$\begin{aligned}\mathrm{d}Y_t^r = \overline{P}_{F,\nabla R}(Y_t^r)\left[b(Y_t^r)\mathrm{d}t + \sigma(Y_t^r)\mathrm{d}W_t\right] \\ - \frac{\left(\nabla^2 R : \Pi_{F,\nabla R,\sigma}\right) F}{2\nabla R \cdot F}(Y_t^r)\,\mathrm{d}t.\end{aligned}$$

The linear map $\overline{P}_{F,\nabla R}$ is a non-orthogonal projector onto $\nabla R^\perp$, $\Pi_{F,\nabla R,\sigma}$ is a covariation matrix.

Explicit form

By applying Itô's formula to the constraint, the SDE for Λ^r can be written explicitely, and the Norton dynamics can be written as

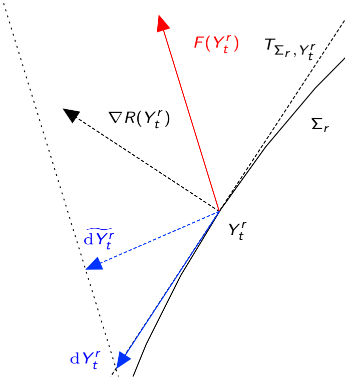
$$\begin{aligned}\mathrm{d}Y_t^r &= \overline{P}_{F,\nabla R}(Y_t^r)\left[b(Y_t^r)\mathrm{d}t + \sigma(Y_t^r)\mathrm{d}W_t\right] \\ &\quad - \frac{\left(\nabla^2 R : \Pi_{F,\nabla R,\sigma}\right) F}{2\nabla R \cdot F}(Y_t^r)\,\mathrm{d}t.\end{aligned}$$

The linear map $\overline{P}_{F,\nabla R}$ is a non-orthogonal projector onto $\nabla R^\perp$, $\Pi_{F,\nabla R,\sigma}$ is a covariation matrix.

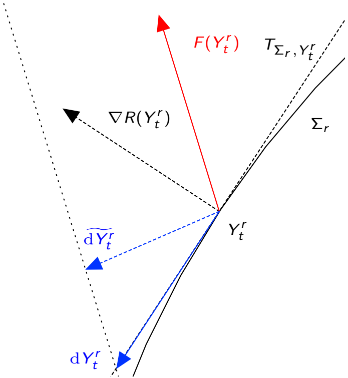
Expressions for the forcing terms: $\lambda_t = \lambda(Y_r^t)$, for some explicit $\lambda : \mathcal{X} \to \mathbb{R}$, and for the martingale part,

$$\mathrm{d}\widetilde{\Lambda}_t^r = -\frac{\nabla R(Y_t^r) \cdot \sigma(Y_t^r)\mathrm{d}W_t}{\nabla R(Y_t^r) \cdot F(Y_t^r)}.$$

Geometric picture

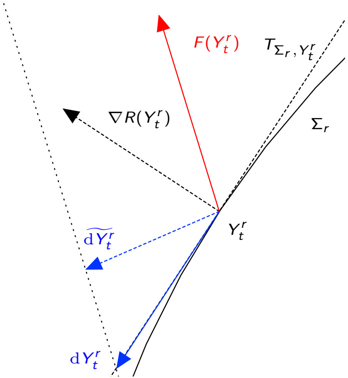


Geometric picture



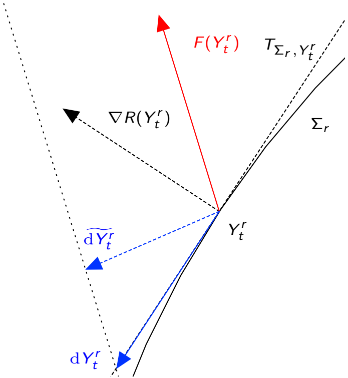
The increments get reprojected onto the tangent space, but with respect to F instead of ∇R.

Geometric picture



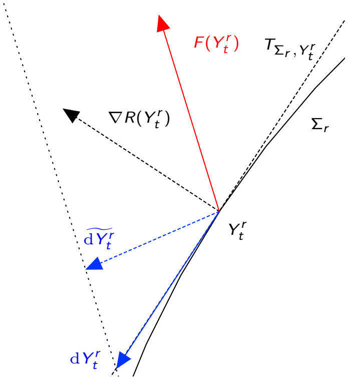
The increments get reprojected onto the tangent space, but with respect to F instead of ∇R.
"Controllability" condition: $F \cdot \nabla R \neq 0$ on Σ_r.

Geometric picture



The increments get reprojected onto the tangent space, but with respect to F instead of ∇R.
"Controllability" condition: $F \cdot \nabla R \neq 0$ on Σ_r.
In the case $F = \nabla R$, standard constrained dynamics.

Geometric picture



The increments get reprojected onto the tangent space, but with respect to F instead of ∇R.

"Controllability" condition: $F \cdot \nabla R \neq 0$ on Σ_r.

In the case $F = \nabla R$, standard constrained dynamics.

We are interested in the average magnitude with respect to $F(Y_t^r)$ of (the non-martingale part of) the recall force or Lagrange multiplier $\mathrm{d}\Lambda_t^r$.

straightforward generalizations

By very similar arguments, we can easily recover explicit expressions for the following generalizations:

- The case of constraints on multiple fluxes.
- The case of a time-dependent constraint $R(Y_t^r) = r_t$, with r_t deterministic or stochastic.
- A combination of these two.

Transport coefficients

Assuming that the Norton dynamics has a unique invariant probability measure ν^r for all r small enough, define the Norton analog of the transport coefficient:

$$\widetilde{\rho}_{R,F} = \lim_{r \to 0} \frac{r}{\int_{\Sigma_r} \lambda \, \mathrm{d}\nu^r - \int_{\Sigma_0} \lambda \, \mathrm{d}\nu^0}.$$

Transport coefficients

Assuming that the Norton dynamics has a unique invariant probability measure ν^r for all r small enough, define the Norton analog of the transport coefficient:

$$\widetilde{\rho}_{R,F} = \lim_{r \to 0} \frac{r}{\int_{\Sigma_r} \lambda \, \mathrm{d}\nu^r - \int_{\Sigma_0} \lambda \, \mathrm{d}\nu^0}.$$

Loosely: measure the reciprocal of the resistance of the system instead of the conductance.

Computing averages of λ in practice

In practice, compute discrete trajectory averages of Lagrange multipliers:

$$\begin{cases} \widetilde{X}^{n+1} = \Phi_{\Delta t}(X^n, G^n), \\ X^{n+1} = \widetilde{X}^{n+1} + \Lambda^{n,*} F(X^n), \end{cases} \tag{1}$$

with $\Phi_{\Delta t}$ a scheme for the reference dynamics, $\Lambda^{n,*}$ is taken so that $R(X^{n+1}) = r$.

Using the equation for $\mathrm{d}\widetilde{\Lambda}_t^r$, the martingale part can be corrected at dominant order:

$$\Lambda^n = \Lambda^{n,*} - \sqrt{\Delta t}\,\frac{\nabla R(X^n) \cdot \sigma(X^n) G^n}{\nabla R(X^n) \cdot F(X^n)}.$$

Then, estimate λ^n by

$$\lambda^n = \frac{1}{\Delta t} \Lambda^n.$$

Norton dynamics in the Langevin setting

We consider fluxes of the form

$$R(q,p) = G(q) \cdot p$$

and mechanical forcings acting on the momentum coordinates.

Norton dynamics in the Langevin setting

We consider fluxes of the form

$$R(q,p) = G(q) \cdot p$$

and mechanical forcings acting on the momentum coordinates.
Thévenin dynamics:

$$\begin{cases} \mathrm{d}q_t = M^{-1} p_t \mathrm{d}t, \\ \mathrm{d}p_t = -\nabla V(q_t)\,\mathrm{d}t - \gamma M^{-1} p_t\,\mathrm{d}t + \sqrt{\frac{2\gamma}{\beta}} \mathrm{d}W_t + \eta F(q_t)\,\mathrm{d}t, \end{cases} \quad (2)$$

Norton dynamics:

$$\begin{cases} \mathrm{d}q_t = M^{-1} p_t\,\mathrm{d}t, \\ \mathrm{d}p_t = \overline{P}_{F,G}(q_t) \left(-\nabla V(q_t)\,\mathrm{d}t - \gamma M^{-1} p_t\,\mathrm{d}t + \sqrt{\frac{2\gamma}{\beta}}\,\mathrm{d}W_t \right) \\ \qquad + \dfrac{\nabla G(q_t) p_t \cdot M^{-1} p_t}{F(q_t) \cdot G(q_t)} F(q_t)\,\mathrm{d}t. \end{cases} \quad (3)$$

Physical interpretation

The Norton dynamics satisfies an oblique Gauss's principle of least constraint: the Norton force minimizes the distance to the equilibrium force, with respect to a metric for which

$$F(q) \perp G(q)^{\perp} \quad \forall\, q.$$

If F is proportional to G, this is just the classical principle of least constraint, and corresponds to the original idea of Evans & al.

Splitting schemes

The generator for the Norton dynamics can be written as

$$\mathcal{L} = \mathcal{L}^{\mathrm{A}} + \mathcal{L}^{\mathrm{B}} + \gamma \mathcal{L}^{\mathrm{O}},$$

with

$$\begin{cases} \mathcal{L}^{\mathrm{A}} = M^{-1} p \cdot \nabla_q + \dfrac{\nabla G p \cdot M^{-1} p}{F \cdot G} F \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{B}} = -\overline{P}_{F,G} \nabla V \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{O}} = -\overline{P}_{F,G} M^{-1} p \cdot \nabla_p + \dfrac{1}{\beta} \overline{P}_{F,G} \overline{P}_{G,F} : \nabla_p^2. \end{cases} \tag{4}$$

These are the respective generators of dynamics which individually preserve the constant-response manifold Σ_r.

Splitting schemes

The generator for the Norton dynamics can be written as

$$\mathcal{L} = \mathcal{L}^{\mathrm{A}} + \mathcal{L}^{\mathrm{B}} + \gamma \mathcal{L}^{\mathrm{O}},$$

with

$$\begin{cases} \mathcal{L}^{\mathrm{A}} = M^{-1} p \cdot \nabla_q + \dfrac{\nabla G p \cdot M^{-1} p}{F \cdot G} F \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{B}} = -\overline{P}_{F,G} \nabla V \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{O}} = -\overline{P}_{F,G} M^{-1} p \cdot \nabla_p + \dfrac{1}{\beta} \overline{P}_{F,G} \overline{P}_{G,F} : \nabla_p^2. \end{cases} \tag{4}$$

These are the respective generators of dynamics which individually preserve the constant-response manifold Σ_r.
B dynamics: ballistic evolution.

Splitting schemes

The generator for the Norton dynamics can be written as

$$\mathcal{L} = \mathcal{L}^{\mathrm{A}} + \mathcal{L}^{\mathrm{B}} + \gamma\mathcal{L}^{\mathrm{O}},$$

with

$$\begin{cases} \mathcal{L}^{\mathrm{A}} = M^{-1}p \cdot \nabla_q + \dfrac{\nabla Gp \cdot M^{-1}p}{F \cdot G} F \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{B}} = -\overline{P}_{F,G} \nabla V \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{O}} = -\overline{P}_{F,G} M^{-1} p \cdot \nabla_p + \dfrac{1}{\beta} \overline{P}_{F,G} \overline{P}_{G,F} : \nabla_p^2. \end{cases} \tag{4}$$

These are the respective generators of dynamics which individually preserve the constant-response manifold Σ_r.

B dynamics: ballistic evolution.

O dynamics: projected Ornstein-Uhlenbeck process.

Splitting schemes

The generator for the Norton dynamics can be written as

$$\mathcal{L} = \mathcal{L}^{\mathrm{A}} + \mathcal{L}^{\mathrm{B}} + \gamma \mathcal{L}^{\mathrm{O}},$$

with

$$\begin{cases} \mathcal{L}^{\mathrm{A}} = M^{-1}p \cdot \nabla_q + \dfrac{\nabla G p \cdot M^{-1} p}{F \cdot G} F \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{B}} = -\overline{P}_{F,G} \nabla V \cdot \nabla_p, \\ \mathcal{L}^{\mathrm{O}} = -\overline{P}_{F,G} M^{-1} p \cdot \nabla_p + \dfrac{1}{\beta} \overline{P}_{F,G} \overline{P}_{G,F} : \nabla_p^2. \end{cases} \tag{4}$$

These are the respective generators of dynamics which individually preserve the constant-response manifold Σ_r.
B dynamics: ballistic evolution.
O dynamics: projected Ornstein-Uhlenbeck process.
A dynamics: not analytically solvable in general.

Splitting schemes

These individual dynamics can be combined in a sequence to give an approximation of the evolution operator over one time step. By combining the forcing contribution of each substep, possible to estimate λ from the integration step.

Splitting schemes

These individual dynamics can be combined in a sequence to give an approximation of the evolution operator over one time step. By combining the forcing contribution of each substep, possible to estimate λ from the integration step.
In the case $R = G \cdot p$, the Lagrange multiplier can be computed analytically.

Splitting schemes

These individual dynamics can be combined in a sequence to give an approximation of the evolution operator over one time step. By combining the forcing contribution of each substep, possible to estimate λ from the integration step.
In the case $R = G \cdot p$, the Lagrange multiplier can be computed analytically.
Because the O step is analytically solvable, the contribution of the Gaussian increment can be exactly cancelled.

Mobility

We take a constant force $F \in \mathbb{R}^{dN}$ (d =physical dimension, N=number of particles).

Mobility

We take a constant force $F \in \mathbb{R}^{dN}$ (d =physical dimension, N=number of particles).
The response is the velocity in the direction F,

$$R(q,p) = F \cdot M^{-1} p = M^{-1} F \cdot p.$$

Then $G = M^{-1}F$, $\nabla G = 0$, so the Norton dynamics is just given by

$$\begin{cases} \mathrm{d}q_t = M^{-1} p_t \,\mathrm{d}t, \\ \mathrm{d}p_t = \overline{P}_{F,M^{-1}F}(q_t) \left(-\nabla V(q_t)\,\mathrm{d}t - \gamma M^{-1} p_t \,\mathrm{d}t + \sqrt{\frac{2\gamma}{\beta}}\,\mathrm{d}W_t \right). \end{cases} \tag{5}$$

Shear viscosity

Take a F acting only on the x-components, but with a strength dictated by a y-profile. The response is the y-profile in the x-components of the velocity, which can be quantified by an empirical Fourier coefficient. In equations,

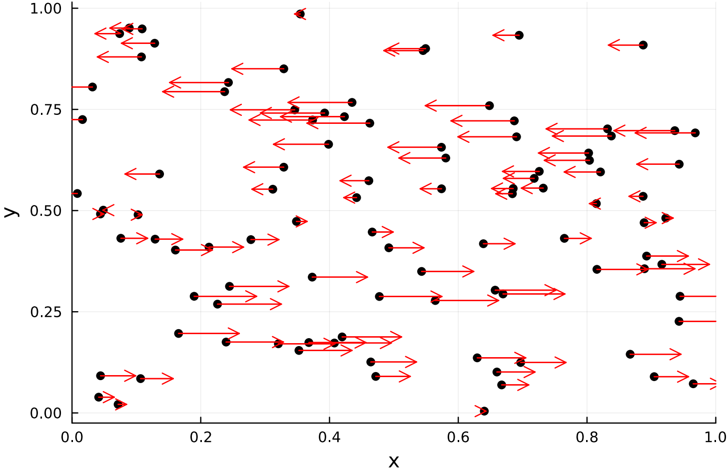
$$\forall\, 1 \leq i \leq N, \forall\, 2 \leq \alpha \leq d, \quad F(q)_{i1} = f_y(q_{i2}), \quad F(q)_{i\alpha} = 0,$$

with f_y a reference forcing profile, and

$$R(q,p) = \frac{1}{N} \sum_{i=1}^{N} \left(M^{-1} p \right)_{i1} \exp\left(\frac{2 i \pi q_{i2}}{L} \right). \tag{6}$$

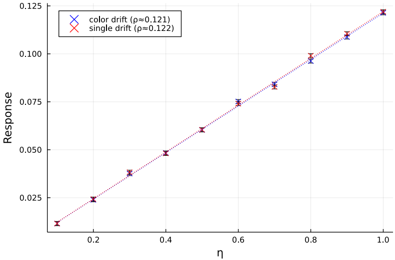
The shear viscosity can be related to the transport coefficient for this response, which is again of the form $G \cdot p$.

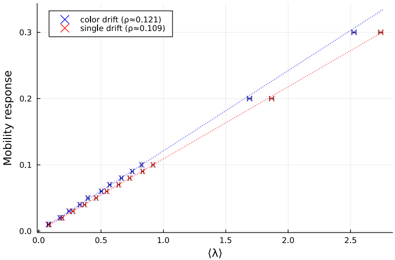
Shear viscosity



Numerical results: mobility

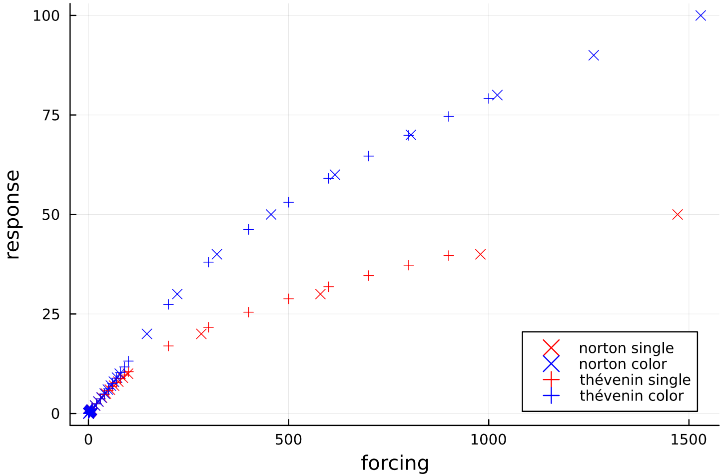
We apply the method to a Lennard-Jones fluid of 1000 particles. We observe agreement in the linear regime for the “color drift” forcing:





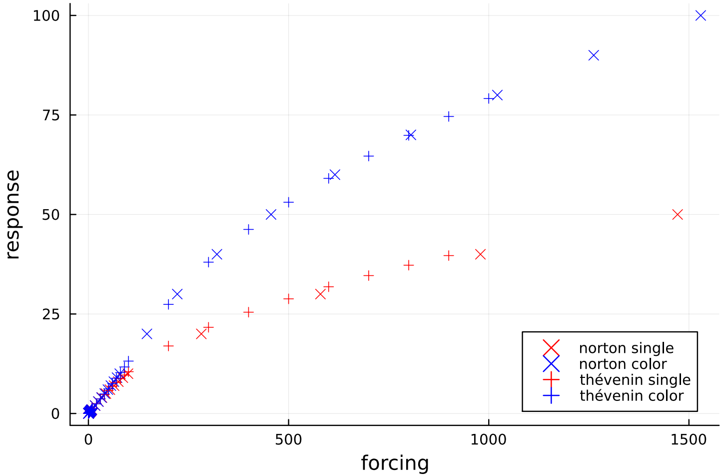
Numerical results: mobility

Agreement far into the non-linear regime



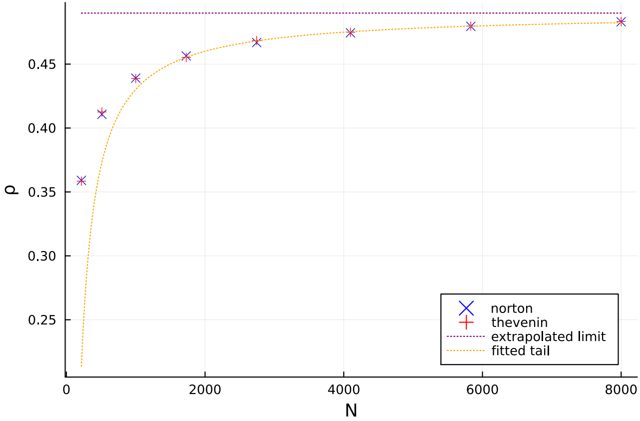
Numerical results:mobility

No gain in asymptotic variance for the mobility estimators.



Numerical results: shear viscosity

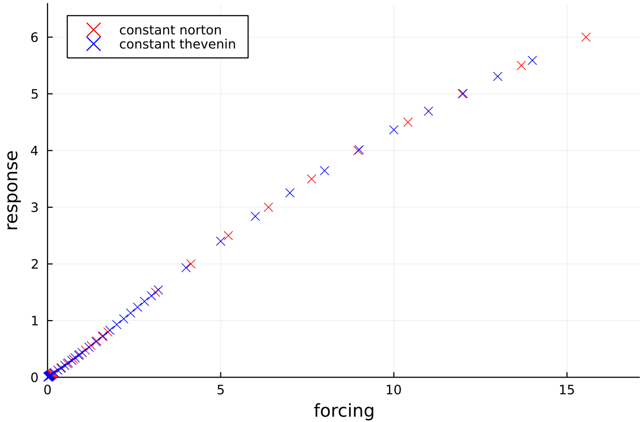
We apply the shear viscosity Norton method to a Lennard-Jones fluid, first using a sinusoidal forcing profile.



We observe convergence to the same thermodynamic limit, with agreement well before that point.

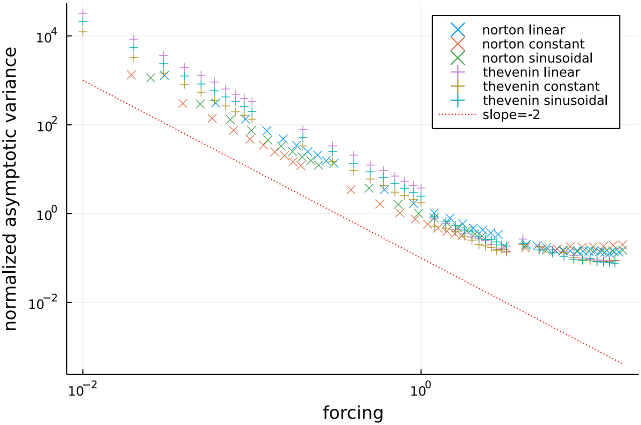
Numerical results: shear viscosity

Again, we observe agreement between Norton and Thévenin responses in the non-linear regime. Here, with a piecewise-constant forcing profile:



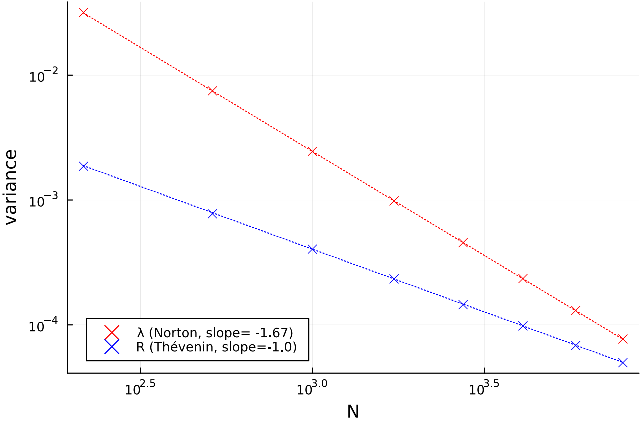
Numerical results: shear viscosity

However: we observe an improvement in the asymptotic variance for estimators coming from the Norton method.



Numerical results: shear viscosity

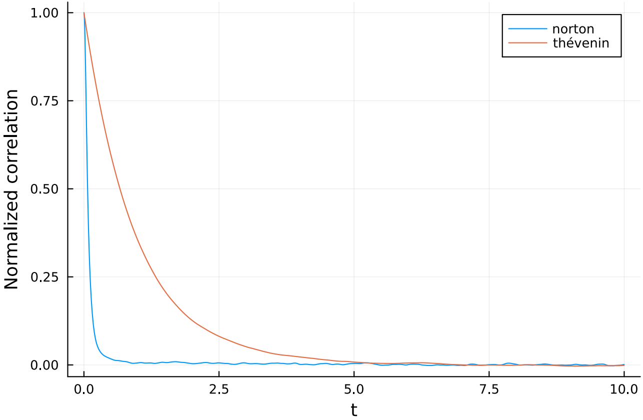
To explain this discrepancy, we compare the variance for λ in the Norton ensemble with the variance for R in the Thévenin ensemble.



Surprising and asymptotically better scaling for the Norton method, but higher variance: this suggest that the improvement comes from shorter correlations.

Numerical results: shear viscosity

Indeed, this is what we observe.



Here, we plot the (statistical) autocorrelations functions for two equivalent values of η and r in the Thévenin and Norton ensembles, at a fixed $N = 8000$.

Problems for future work

Many theoretical questions are left to tackle:

- Criteria for well-posedness, existence/uniqueness of the steady-state, ergodicity.
- Equivalence of ensemble results between the Thévenin and Norton ensembles.
- Providing an explanation for the variance and autocorrelation scaling of λ in the Norton ensemble.
- Linear response theory for the Norton method: derive Green-Kubo like expressions for the inverse transport coefficient.

Idea for linear response

Linear response results usually rely on a perturbative expansion of the non-equilibrium steady-state with respect to the equilibrium steady-state. However, there are issues to overcome in the Norton setting:

Idea for linear response

Linear response results usually rely on a perturbative expansion of the non-equilibrium steady-state with respect to the equilibrium steady-state. However, there are issues to overcome in the Norton setting:

- The equilibrium measure ν^0, supported on Σ_0, is not known.
- The perturbed measure ν^r, supported on Σ_r, is singular with respect to ν^0.
- The generator for the Norton dynamics on Σ_r cannot be expressed as a perturbation of the generator $\mathcal{L}^0$ on Σ_0: they have the same expression, but different domains.

Formal idea for the linear response

Idea: by a change of variables $\phi_{-r} : \Sigma_r \to \Sigma_0$, consider instead the generator $\mathcal{L}^r$ for the dynamics

$$\phi_{-r}(Y_t^r),$$

which lives on Σ_0. The map ϕ_{-r} can easily be found by considering ϕ to be the flow of the ODE

$$\dot{y} = \frac{N(y)}{\nabla R(y) \cdot N(y)}.$$

Natural choices include $N = \nabla R$ and $N = F$. Then,

$$\mathcal{L}^r \varphi(y) = \mathcal{L}^0 \left[\varphi \circ \phi_{-r}\right] \left(\phi_r(y)\right).$$

This is a non-linear perturbation of $\mathcal{L}^0$, but by a formal linearization, we can write the first-order term as

$$\nabla \left[\mathcal{L}^0 \varphi\right] \cdot \frac{N}{\nabla R \cdot N} - \mathcal{L}^0 \left[\nabla \varphi \cdot \frac{N}{\nabla R \cdot N}\right].$$