

# Extending the regime of linear response with synthetic forcings

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- **General setting**
  - ▶ (Non)equilibrium dynamics
  - ▶ Analytical framework
  - ▶ Linear response and transport coefficients
  
- **Optimizing the perturbation**
  - ▶ Notion of synthetic forcings
  - ▶ Examples
  
- **Numerical illustrations**

General setting

- The measure  $\mu$  has associated density  $\psi$
- $\mathcal{A}^\dagger$  denotes the  $L^2$ -adjoint of the operator  $\mathcal{A}$ , i.e.

$$\int (\mathcal{A}\varphi)\phi = \int \varphi(\mathcal{A}^\dagger\phi), \quad \forall \varphi, \phi \in C_0^\infty$$

- $\mathcal{A}^*$  denotes the  $L^2(\psi)$ -adjoint of the operator  $\mathcal{A}$ , i.e.

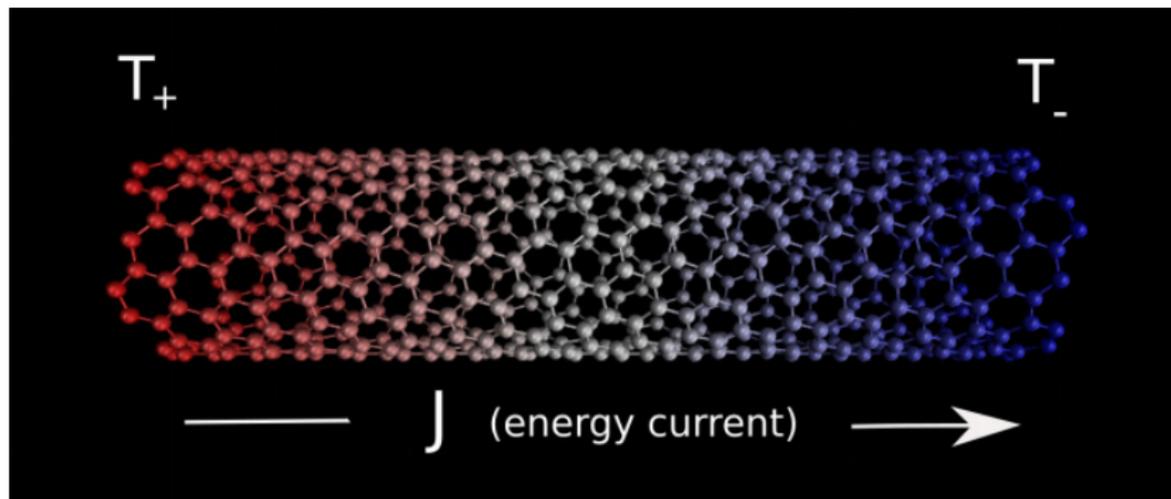
$$\int (\mathcal{A}\varphi)\phi\psi = \int \varphi(\mathcal{A}^*\phi)\psi, \quad \forall \varphi, \phi \in C_0^\infty$$

# Physical context and motivation

Transport coefficients are **quantitative** estimates.

**Example (thermal conductivity):** Fourier's law

$$J = -\kappa \nabla T$$



Long computational times to estimate  $\kappa$ ; can take up to weeks/months.

# Nonequilibrium framework

**Setting:**  $\mathcal{X} = \mathbb{T}^d$ , **nongradient** force  $F$ , periodic  $C^\infty$  potential  $V$

## Overdamped Langevin dynamics

$$dq_t = (-\nabla V(q_t) + \eta F(q_t)) dt + \sqrt{\frac{2}{\beta}} dW_t$$

Generator  $\mathcal{L}_\eta = \mathcal{L}_0 + \eta \tilde{\mathcal{L}}_{\text{phys}}$ , with

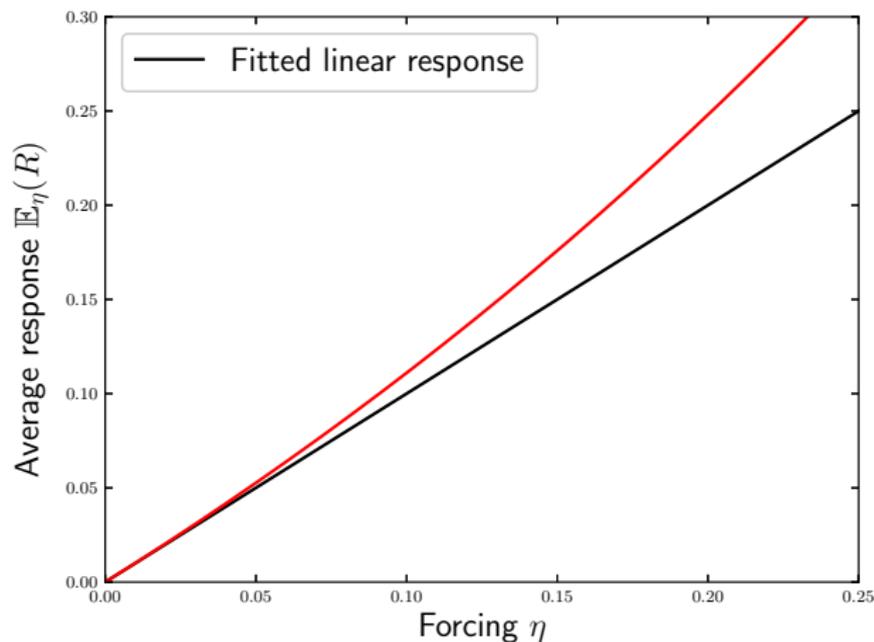
$$\mathcal{L}_0 = -\nabla V^T \nabla + \beta^{-1} \Delta, \quad \tilde{\mathcal{L}}_{\text{phys}} = F^T \nabla$$

Invariant probability measure  $\psi_\eta$  solves the Fokker–Planck

$$\mathcal{L}_\eta^\dagger \psi_\eta = 0, \quad \psi_0(q) = \frac{1}{Z} e^{-\beta V(q)}$$

The perturbation  $\eta F(q)$  induces a response  $\mathbb{E}_\eta(R)$  for some observable  $R(q)$ . For small  $\eta$ , the response is linear in  $\eta$  (linear response regime).

# Illustration - linear response



Linear response formally defined as

$$\rho_1 = \lim_{\eta \rightarrow 0} \frac{\mathbb{E}_\eta(R) - \mathbb{E}_0(R)}{\eta} = \lim_{\eta \rightarrow 0} \frac{\mathbb{E}_\eta(R)}{\eta} = \lim_{\eta \rightarrow 0} \frac{1}{\eta} \int_{\mathcal{X}} R \psi_\eta$$

- 1 Uniqueness of the invariant probability measure, trajectorial ergodicity.

$$\frac{1}{t} \int_0^t R(q_s^\eta) ds \xrightarrow[t \rightarrow +\infty]{\text{a.s.}} \mathbb{E}_\eta(R) := \int_{\mathcal{X}} R \psi_\eta$$

- 2 Lyapunov estimates
- 3 Stability of *regular* functions by inverse operators
- 4 Stability of *regular* functions by the perturbation operator

*Regular*: smooth functions that (and whose derivatives) grow at most polynomially

# Expansion of the invariant measure

Although unique,  $\psi_\eta$  has closed form unknown

**Perturbative regime:**<sup>1</sup> Write  $\psi_\eta$  as a perturbation of  $\psi_0$

$$\psi_\eta = f_\eta \psi_0,$$

with  $f_\eta$  a perturbation of the constant function **1**:

$$f_\eta = \mathbf{1} + \eta \mathbf{f}_1 + \eta^2 \mathbf{f}_2 + \dots$$

Formal asymptotics on the Fokker–Planck  $(\mathcal{L}_0 + \eta \tilde{\mathcal{L}}_{\text{phys}})^\dagger \psi_\eta = 0$  leads to

$$-\mathcal{L}_0^* \mathbf{f}_1 = \tilde{\mathcal{L}}_{\text{phys}}^* \mathbf{1}, \quad \mathbf{f}_{n+1} = (-\mathcal{L}_0^*)^{-1} \tilde{\mathcal{L}}_{\text{phys}}^* \mathbf{f}_n$$

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<sup>1</sup>T. Lelièvre and G. Stoltz, *Acta Numerica* **25**, (2016)

# (Non)linear response

Since  $\psi_\eta = f_\eta \psi_0$ , write  $\rho_1$  as

$$\rho_1 = \lim_{\eta \rightarrow 0} \frac{1}{\eta} \int_{\mathcal{X}} R \psi_\eta = \lim_{\eta \rightarrow 0} \frac{1}{\eta} \int_{\mathcal{X}} R f_\eta \psi_0 = \int_{\mathcal{X}} R f_1 \psi_0$$

More generally, the  $n$ -th order response is given by

$$\rho_n = \int_{\mathcal{X}} R f_n \psi_0$$

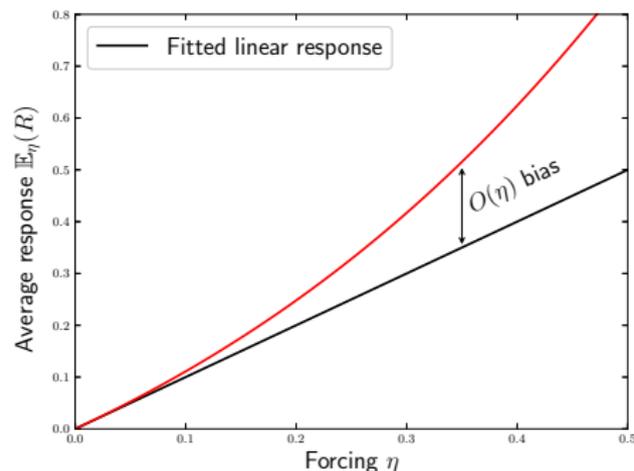
Full response can be written as a polynomial in  $\eta$

$$r(\eta) = \mathbb{E}_\eta(R) = \eta \rho_1 + \eta^2 \rho_2 + \eta^3 \rho_3 + \dots$$

# Estimating linear response - variance vs bias

## Estimator of linear response

$$\hat{\rho}_{\eta,t} = \frac{1}{\eta t} \int_0^t R(q_s) ds \xrightarrow[t \rightarrow +\infty]{\text{a.s.}} \frac{1}{\eta} \int_{\mathcal{X}} R f_{\eta} \psi_0 = \rho_1 + O(\eta)$$



**Main issue:** Statistical error with asymptotic variance  $O(\eta^{-2})$

**Idea:** Reduce variance by increasing  $\eta$ , but at which values of  $\eta$  does the nonlinear response develop?

**Goal:** Want to stay in the linear regime for  $\eta$  as large as possible.

# Optimizing the perturbation

## Synthetic forcings

# Optimizing the perturbation

**Idea:** Introduce perturbation with generator  $\tilde{\mathcal{L}}_{\text{extra}}$ , where

$$\tilde{\mathcal{L}}_{\text{extra}}^* \mathbf{1} = 0$$

Resulting dynamics has generator

$$\mathcal{L}_\eta = \mathcal{L}_0 + \eta(\tilde{\mathcal{L}}_{\text{phys}} + \alpha\tilde{\mathcal{L}}_{\text{extra}})$$

The resulting perturbation is called a **synthetic forcing**<sup>2</sup>.

With the addition of the extra forcing,  $f_1$  remains unchanged

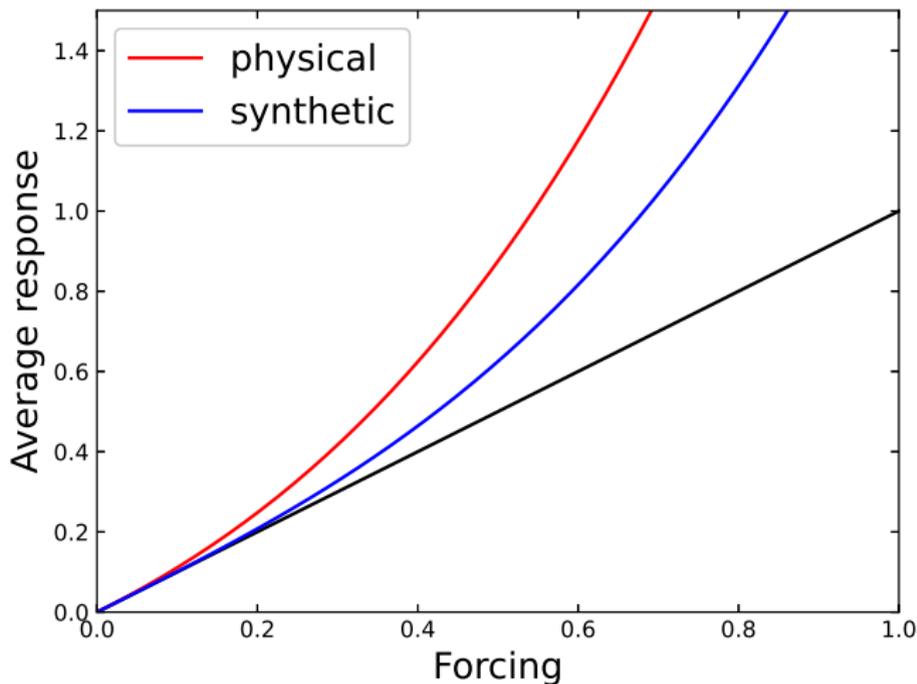
$$\begin{aligned} f_1 &= -\mathcal{L}_0^{-1}(\tilde{\mathcal{L}}_{\text{phys}} + \alpha\tilde{\mathcal{L}}_{\text{extra}})^* \mathbf{1} \\ &= -\mathcal{L}_0^{-1} \tilde{\mathcal{L}}_{\text{phys}}^* \mathbf{1} \end{aligned}$$

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<sup>2</sup>Evans, Morriss, (2008)

# Illustration - effect of synthetic forcing

In theory, we can find some  $\tilde{\mathcal{L}}_{\text{extra}}$  that extends the linear regime



# Classes of synthetic forcings

- 1 *First-order differential operators*  $\tilde{\mathcal{L}}_{\text{extra}} = G^T \nabla_x$ , with  $\text{div}(G\psi_0) = 0$ .
- 2 *Second-order differential operators* of the form  $\tilde{\mathcal{L}}_{\text{extra}} = -\partial_{x_i}^* \partial_{x_i}$ . In this case, the operator is self-adjoint, i.e.  $\tilde{\mathcal{L}}_{\text{extra}} = \tilde{\mathcal{L}}_{\text{extra}}^*$ .
- 3 *First-order differential operators with nontrivial zero order parts*, such as  $\tilde{\mathcal{L}}_{\text{extra}} = \partial_{x_i}^* = \partial_{x_i} U - \partial_{x_i}$  for  $\psi_0(x) = e^{-U(x)}$ .

# Examples of synthetic forcings (overdamped Langevin)

## Example 1: Divergence-free vector field

$$\begin{cases} \tilde{\mathcal{L}}_{\text{extra}} = G(q)^T \nabla, & \text{such that } \operatorname{div}(G e^{-\beta V}) = 0 \\ dq_t = -\nabla V(q_t) dt + \eta F(q_t) dt + \alpha \eta G(q_t) dt + \sigma dW \end{cases}$$

## Example 2: Modified fluctuation-dissipation

$$\begin{cases} \tilde{\mathcal{L}}_{\text{extra}} = -\beta^{-1} \nabla^* \nabla = -\nabla V^T \nabla + \beta^{-1} \Delta \\ dq_t = -(1 + \alpha \eta) \nabla V(q_t) dt + \eta F(q_t) dt + \sqrt{\frac{2(1 + \alpha \eta)}{\beta}} dW \end{cases}$$

## Example 3: Feynman–Kac forcing

$$\begin{cases} \tilde{\mathcal{L}}_{\text{extra}} = \xi^T \nabla^* = -\xi^T \nabla + \xi^T \nabla V \\ dq_t = -\nabla V(q_t) dt + \eta F(q_t) dt - \eta \alpha \xi dt + \sigma dW \\ \omega_t \propto \exp\left(\alpha \eta \int_0^t \xi^T V(q_s) ds\right) \end{cases}$$

# Examples of synthetic forcings (Langevin dynamics)

**Example 1:** Divergence-free vector field  $\tilde{\mathcal{L}}_{\text{extra}} = G_1^T \nabla_q + G_2^T \nabla_p$

$$\begin{cases} dq_t = M^{-1} p_t dt + \alpha \eta G_1(q_t, p_t) dt, \\ dp_t = -\nabla V(q_t) dt + \eta(F(q_t) + \alpha G_2(q_t, p_t)) dt - \gamma M^{-1} p_t dt + \sqrt{\frac{2\gamma}{\beta}} dW_t. \end{cases}$$

**Example 2:** Modified fluctuation-dissipation  $\tilde{\mathcal{L}}_{\text{extra}} = -\beta^{-1} \nabla_q^* \nabla_q - \beta^{-1} \nabla_p^* \nabla_p$

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

**Example 3:** Feynman–Kac forcing  $\tilde{\mathcal{L}}_{\text{extra}} = \xi_1(p)^T \nabla_q^* + \xi_2(q)^T \nabla_p^*$

$$\begin{cases} dq_t = M^{-1} p_t dt - \alpha \eta \xi_1(p_t) dt, \\ dp_t = -\nabla V(q_t) dt + \eta(F(q_t) - \alpha \xi_2(q_t)) dt - \gamma M^{-1} p_t dt + \sqrt{\frac{2\gamma}{\beta}} dW_t, \end{cases}$$

# Choosing magnitude of perturbation

**Recall:** Response as a polynomial in  $\eta$

$$r_\alpha(\eta) = \mathbb{E}_{\eta,\alpha}(R) = \eta\rho_1 + \eta^2\rho_2(\alpha) + \eta^3\rho_3(\alpha) + \dots$$

- **First approach:** Choose  $\alpha$  s.t. the second-order response is killed:

$$\rho_2(\alpha^*) = 0$$

- **Second approach:** Choose  $\alpha$  s.t.  $\delta_\alpha(\eta) < \varepsilon$  for as long as possible, namely  $\alpha_\star(\varepsilon)$ , where

$$\delta_\alpha(\eta) = \left| \frac{r_\alpha(\eta) - \rho_1\eta}{\rho_1\eta} \right|.$$

# Numerical illustration

# Choosing the observable

**Setting:** Overdamped Langevin dynamics in 1D, potential  $V(q) = \cos(2\pi q)$ . We consider the observable

$$R(q) = (a \cos(2\pi q) + b \sin(2\pi q)) e^{\beta V(q)}$$

where  $a, b \in \mathbb{R}$ .

- $b$  is chosen such that  $\rho_1 = 1$ , i.e.,

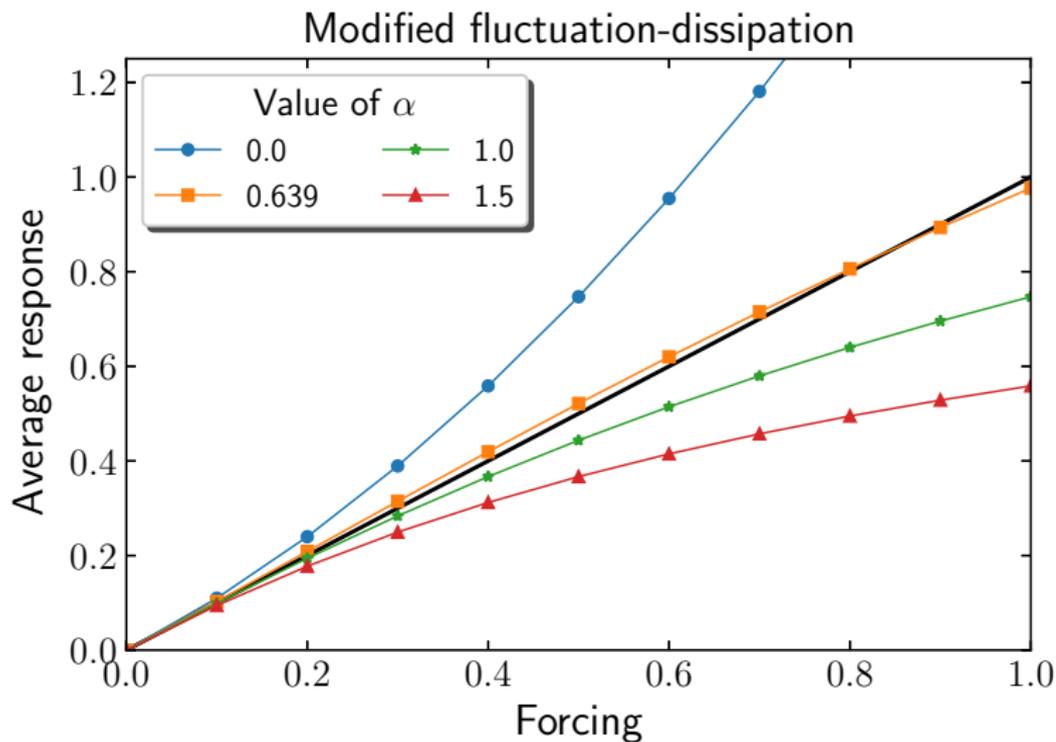
$$b = \left( Z^{-1} \int_{\mathcal{X}} \sin(2\pi q) f_1(q) dq \right)^{-1}, \quad Z = \int_{\mathcal{X}} e^{-\beta V(q)} dq$$

- Similarly,  $a$  can be chosen such that  $\rho_2$  is arbitrarily large.

For nonsymmetric potentials, the above still gives  $\rho_1, \rho_2 \sim O(1)$ .

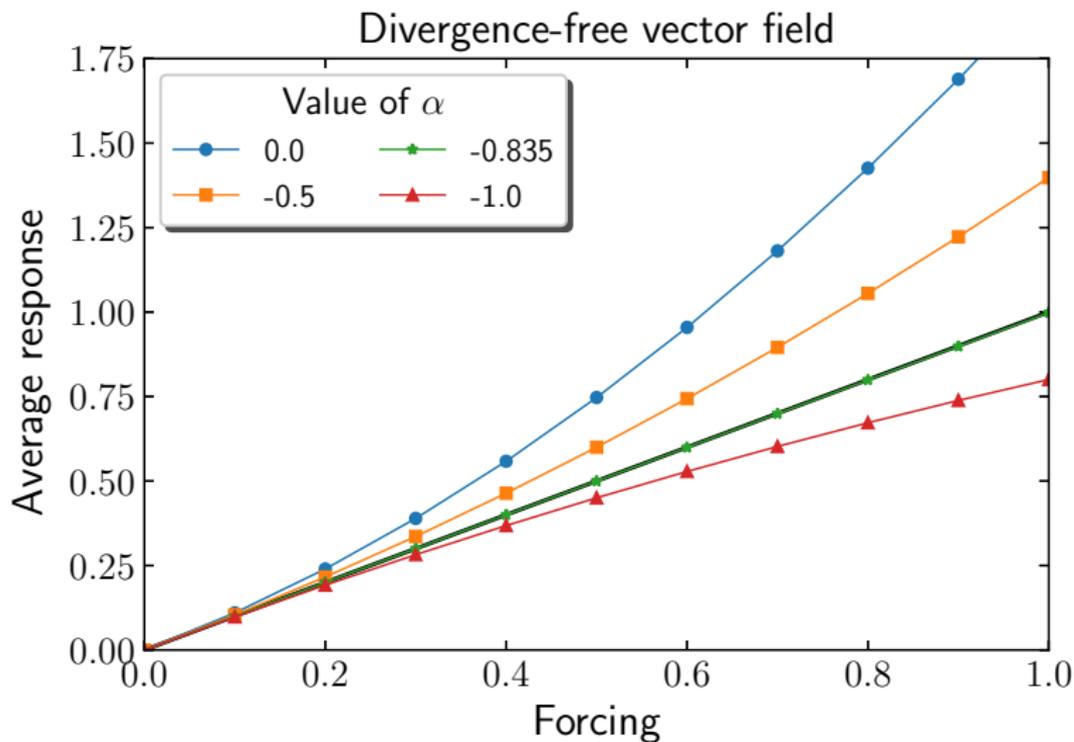
# Numerical illustration: modified FD

$$\alpha^* = 1.0, \quad \alpha_*(\varepsilon = 0.05) = 0.639$$



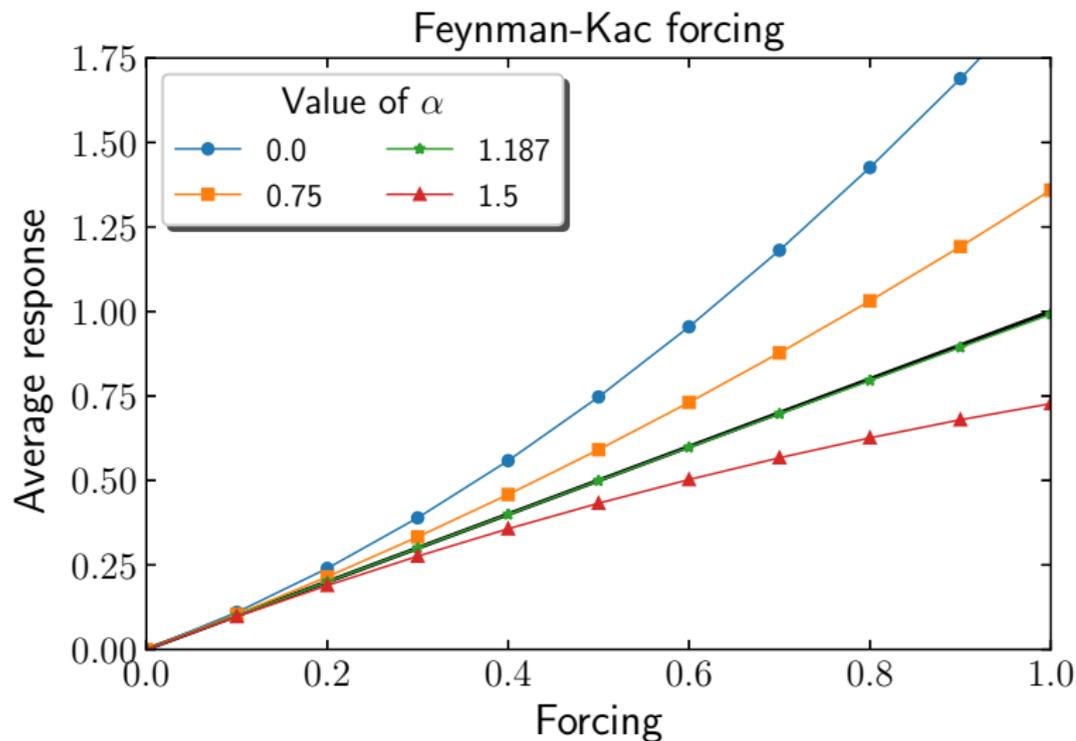
# Numerical illustration: div-free vector field

$$\alpha^* = -0.835$$

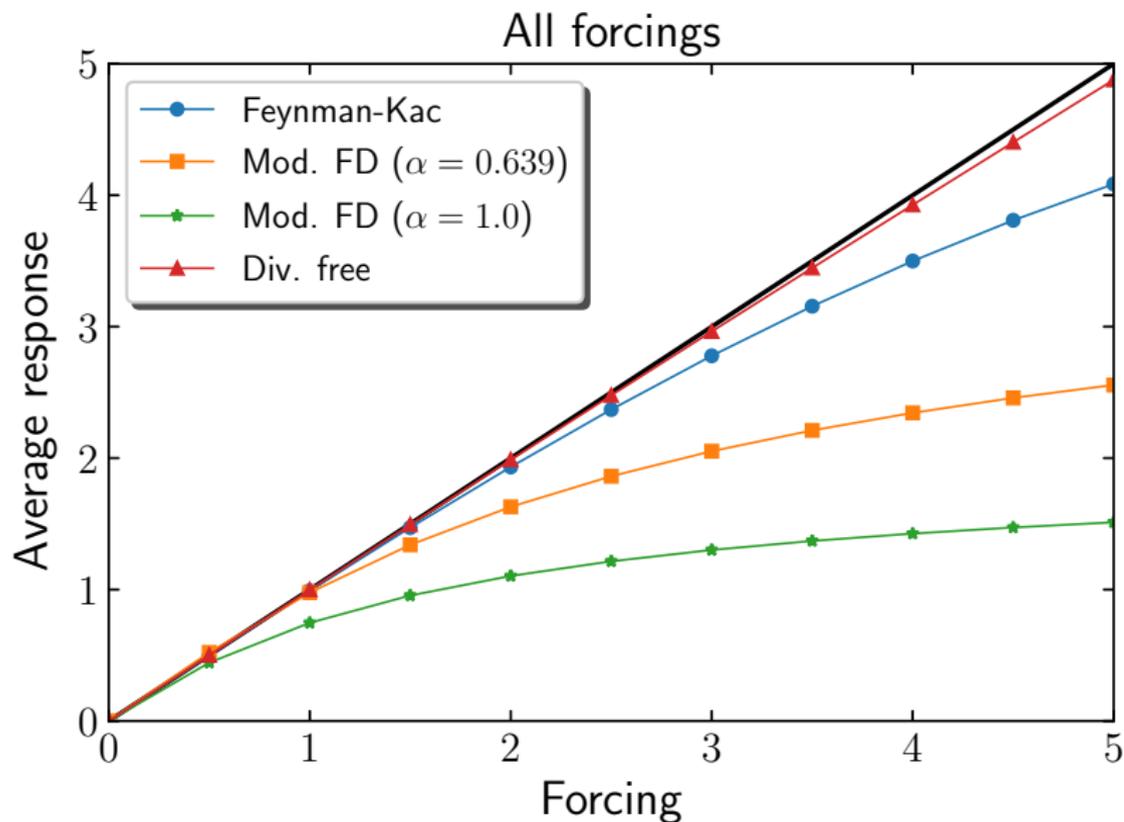


# Numerical illustration: Feynman–Kac forcing

$$\alpha^* = 1.187$$



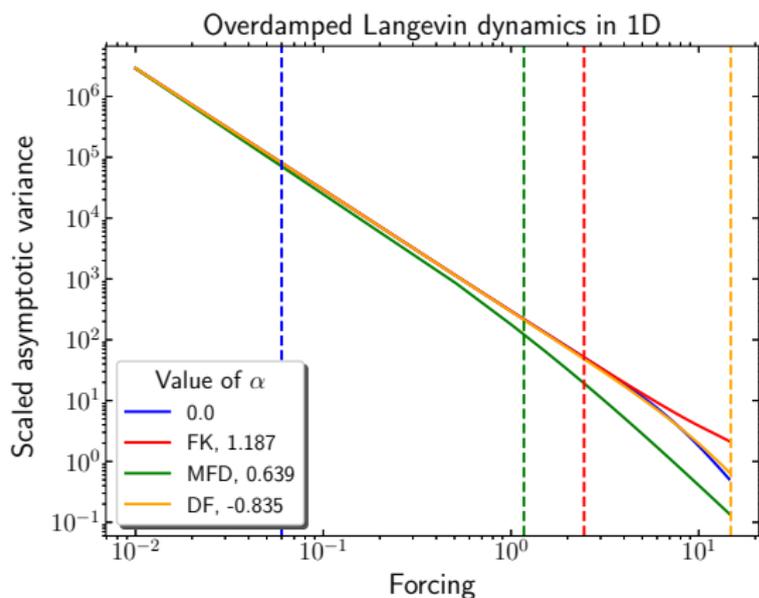
# Numerical illustration: all forcings



# Numerical illustration: variance reduction (1)

Asymptotic variance  $\sigma_{R,\eta}^2$  same order as  $\sigma_{R,0}^2$ , up to small bias  $O(\eta)$ :

$$\frac{\sigma_{R,\eta}^2}{\eta^2} = \frac{\sigma_{R,0}^2}{\eta^2} + O\left(\frac{1}{\eta}\right)$$



## Numerical illustration: variance reduction (2)

Define the gain as

$$\text{gain} = \left( \frac{\sigma_{R, \eta_0(\varepsilon)}^2}{\eta_0(\varepsilon)^2} \right) \left( \frac{\sigma_{R, \eta_\alpha(\varepsilon)}^2}{\eta_\alpha(\varepsilon)^2} \right)^{-1}.$$

*"ratio of the variances of physical system to the synthetic system"*

Dynamics	Extra forcing				
	none	MFD	FK	DF ( $e^V$ )	DF ( $A\nabla V$ )
Ovd. 1D	1	$6.56 \times 10^2$	$1.58 \times 10^3$	$1.28 \times 10^5$	-
Ovd. 2D	1	$7.65 \times 10^2$	$3.23 \times 10^4$	$3.33 \times 10^3$	$4.03 \times 10^0$
Lang. 1D	1	$2.18 \times 10^3$	$1.29 \times 10^3$	$1.42 \times 10^3$	-

# Future work and extensions

- **Promising method:** Can reduce variance by several orders of magnitude
- **Potential applications:** Lennard–Jones fluids (shear viscosity), systems of atom chains (thermal transport)
- **Extension to actual MD systems:** Transport coefficients are *intensive quantities*, i.e. not dependent on system size
  - ⇒ Notion of *prescreening*: two small simulations with  $\alpha_1 \neq \alpha_2$ , from which optimal  $\alpha$  can be extrapolated