Steady-State Solutions for Nonequilibrium Langevin Dynamics

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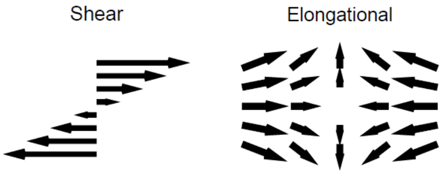
First Part

Deforming Periodic Boundary Conditions

NEMD

- Study molecular fluids under steady flow [Evans and Morriss(2007), Todd and Daivis(2017)]
- Motivation: simulation of micro-scale fluid motion with local strain rate $\nabla \mathbf{u} \in \mathbb{R}^{3\times 3}$
- Background flow matrix A



- Special challenges in formulating the PBCs for NEMD due to **deforming simulation cell**

Simulation Box

Three linearly independent vectors define our simulation box and PBCs:

$$L_t = \begin{bmatrix} \mathbf{v}_t^1 & \mathbf{v}_t^2 & \mathbf{v}_t^3 \end{bmatrix} \in \mathbb{R}^{3\times 3}, \qquad t \in [0, \infty).$$

Unit cell	Image cell
$(\mathbf{q}, \mathbf{p})$	$(\mathbf{q} + L_t\mathbf{n}, \mathbf{p} + AL_t\mathbf{n})$
$\frac{d}{dt}\mathbf{q} = \mathbf{p}$	$\frac{d}{dt}(\mathbf{q} + L_t\mathbf{n}) = \mathbf{p} + AL_t\mathbf{n}$

Simulation box deforms with the background flow

$$\frac{d}{dt}L_t = AL_t \implies L_t = e^{At}L_0$$

Warning: A particle can become arbitrarily close to its image depending on geometry.

Remapping PBCs

There is freedom in choosing a lattice basis. For any $M \in SL(3, \mathbb{Z})$, $L_t M$ and L_t generate the same lattice

Lattice Remapping Algorithms:

1. Carefully choose L_0, so that we can use automorphisms so that $L_t M_t$ stays bounded.
2. In fact, M will tell us how to choose L_0.
3. Minimum distance between a particle and its images

$$d = \inf_{\substack{\mathbf{n} \in \mathbb{Z}^3 \backslash 0 \\ t \in \mathbb{R} \geq 0}} ||L_t M \mathbf{n}||_2 > 0.$$

PBCs

Existing Algorithms:

- **Lees-Edwards** for Planar Shear Flows
- **Kraynik-Reinelt** for Planar Elongational Flows
- **Generalized KR** for (non-defective) Three-Dimensional Flows

Our analysis focuses on the two planar flow types.

(Appendix) Improving the Three-Dimensional Case

- Rotating Algorithm
- Comparison of the Three-Dimensional Flow Algorithms

Shear Flow: Lees-Edwards PBCs

Background flow

$$A = \begin{bmatrix} 0 & \epsilon & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

L_t is highly sheared as t becomes large

$$L_t = e^{tA} L_0 = \begin{bmatrix} 1 & t\epsilon & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} L_0, \text{ where } L_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Interparticle interaction computation becomes more difficult

Shear Flow: Lees-Edwards PBCs

$$M^n = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^n = \begin{bmatrix} 1 & -n & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad n \in \mathbb{Z}.$$

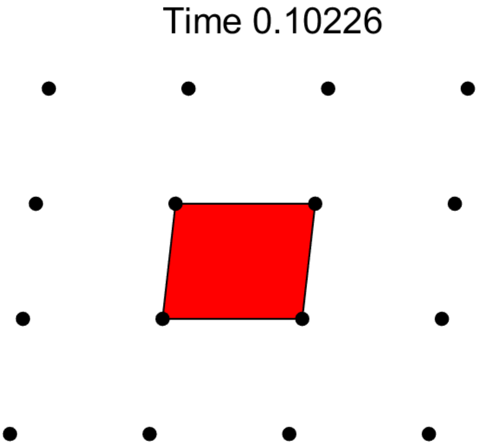
Remapped lattice

$$L_t M^n = \begin{bmatrix} 1 & t\epsilon - \lfloor t\epsilon \rceil & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = e^{[t]A} L_0, \quad \begin{cases} [t] \equiv t \mod T \\ n = -\lfloor \frac{t}{T} \rceil, \quad T = \frac{1}{\epsilon} \end{cases}$$

Periodic domain

$$\widehat{\mathcal{L}}_t = \{ e^{[t]A} L_0 \mathbf{x} \vert \mathbf{x} \in \mathbb{T}^3 \}, \text{ where } \mathbb{T}^3 = \mathbb{R}^3 \backslash \mathbb{Z}^3.$$

Shear Flow: Lees-Edwards PBCs



Planar Elongational Flow: Kraynik & Reinelt PBCs

Background flow

$$A = \begin{bmatrix} -\epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

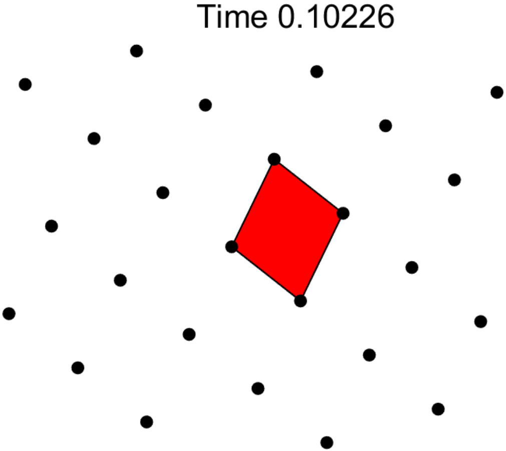
Simulation box shrinks in x direction and stretches y direction

$$M = V\Lambda V^{-1}, \quad \Lambda = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda^{-1} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad 0 < \lambda < 1$$

$$M = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad L_0 = V^{-1}$$

$$L_t M^n = e^{[t]A} L_0, \quad n = -\left\lfloor \frac{t}{T} \right\rfloor, \quad T = \frac{\log(\lambda)}{\epsilon}.$$

Planar Elongational Flow: Kraynik & Reinelt PBCs



General 3d Flow: GenKR PBCs Dobson & Hunt

Background flow

$$A = \begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & -\epsilon_1 - \epsilon_2 \end{bmatrix}.$$

$M_1, M_2 \in SL(3, \mathbb{Z})$ are commutative automorphism matrices which have positive eigenvalues

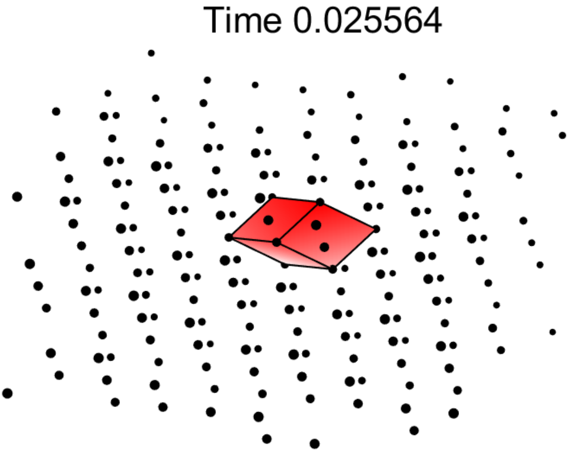
$$M_i = V \Lambda_i V^{-1}, \quad \hat{\omega}_i = \log \Lambda_i, \quad A = \delta_1 \hat{\omega}_1 + \delta_2 \hat{\omega}_2$$

$$L_0 = V^{-1}$$

$$L_t M_1^{n_1} M_2^{n_2} = e^{A_t} V^{-1},$$

$$A_t = tA + n_1 \hat{\omega}_1 + n_2 \hat{\omega}_2 = (t\delta_1 - \lfloor t\delta_1 \rceil)\hat{\omega}_1 + (t\delta_2 - \lfloor t\delta_2 \rceil)\hat{\omega}_2$$

General 3d Flow: GenKR PBCs D. & Hunt



Part Two

Convergence of NELD: Planar Flows

NELD

The Nonequilibrium Langevin Dynamics is derived in:
- [McPhie, Daivis, Ennis, Snook, Evans, Physica A 2001],
- [D., Legoll, Lelièvre, Stoltz, M2AN 2013]

$$\begin{cases} d\mathbf{q} &= \mathbf{p}dt, \\ d\mathbf{p} &= -\nabla V(\mathbf{q})dt - \gamma(\mathbf{p} - A\mathbf{q})dt + A\mathbf{p}dt + \sigma dW \end{cases},$$

NELD in terms of the relative momentum

$$\begin{cases} d\widehat{\mathbf{q}} &= (\widehat{\mathbf{p}} + A\widehat{\mathbf{q}})dt, \\ d\widehat{\mathbf{p}} &= -\nabla V(\widehat{\mathbf{q}})dt - \gamma\widehat{\mathbf{p}}dt + \sigma dW \end{cases}, \quad (\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) \in \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d},$$

- $\sigma^2 = \frac{2\gamma}{\beta}$ the fluctuation coefficient
- β the inverse temperature
- γ the dissipation coefficient
- $V \in C^\infty$ the potential

Equilibrium Langevin Dynamics Equation

Equilibrium Langevin Dynamics

$$\begin{cases} d\mathbf{q} &= \mathbf{p}dt, \\ d\mathbf{p} &= -\nabla V(\mathbf{q})dt - \gamma \mathbf{p}dt + \sigma dW \end{cases}, \quad (\mathbf{q},\mathbf{p}) \in \mathcal{L}_0^d \times \mathbb{R}^{3d}$$

Boltzmann-Gibbs distribution

$$\nu(\mathbf{q},\mathbf{p})d\mathbf{q}d\mathbf{p} = \frac{1}{Z}e^{-\beta H(\mathbf{q},\mathbf{p})}d\mathbf{q}d\mathbf{p}, \qquad \begin{array}{l} Z = \int_{\mathcal{L}_0^d \times \mathbb{R}^{3d}} e^{-\beta H(\mathbf{q},\mathbf{p})}d\mathbf{q}d\mathbf{p} \\ H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\langle \mathbf{p},\mathbf{p}\rangle + V(\mathbf{q}) \end{array}$$

Motivation: Can we establish the convergence of a limiting measure for the NELD in the moving domain?

Convergence of NELD to a Limit Cycle

We employ a technique similar to [Joubaud, Pavliotis, Stoltz, J. Stat. Phys. 2015] which examined time and space-periodic external forcing.

Steps of the proof:

1. Markov Chain Generator
2. Regularity
3. Invariant Measure of the Discrete Process
4. Convergence of the NELD

Key Intuitions:

1. Discrete time process between remapping times kT to $(k+1)T$ maps from $\mathcal{L}_0$ to $\mathcal{L}_0$.
2. Generator is smooth in between remappings.
3. Remapping is continuous function, while trajectories discontinuous.

Markov Chain Generator

Steps of the proof:

1. Markov Chain Generator
   - Transition Functions
   - Generator
2. Regularity
3. Invariant Measure of the Discrete Process
4. Convergence of the NELD

Markov Process Generator

NELD in vector form

$$\begin{cases} d\widehat{\mathbf{X}}_t = \widehat{\mathbf{b}}(\widehat{\mathbf{X}}_t)dt + \widehat{\Sigma}dW_t, & \widehat{\mathbf{X}}_t \in \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}, \qquad t \in [kT, (k+1)T), \\ \widehat{\mathbf{X}}_t = \begin{bmatrix} \widehat{\mathbf{q}} \\ \widehat{\mathbf{p}} \end{bmatrix}, \quad \widehat{\mathbf{b}}(\widehat{\mathbf{X}}_t) = \begin{bmatrix} \widehat{\mathbf{p}} + A\widehat{\mathbf{q}} \\ -\nabla V(\widehat{\mathbf{q}}) - \gamma\widehat{\mathbf{p}} \end{bmatrix}, & \widehat{\Sigma} = \begin{bmatrix} 0 & 0 \\ 0 & \sigma \end{bmatrix}, \end{cases}$$

Density transition function

$$\widehat{\mathcal{P}}_{t,s}(\widehat{\mathbf{y}}, \widehat{B}_t) = \mathbb{P}\left(\widehat{\mathbf{X}}_t \in \widehat{B}_t \middle| \widehat{\mathbf{X}}_s = \widehat{\mathbf{y}}\right) = \int_{\widehat{B}_t} \widehat{\psi}(t, \widehat{\mathbf{x}} | s, \widehat{\mathbf{y}}) d\widehat{\mathbf{x}},$$

$$\widehat{\psi}(t, \widehat{\mathbf{x}} | s, \widehat{\mathbf{y}})\Big|_{t=s} = \delta(\widehat{\mathbf{x}} - \widehat{\mathbf{y}}), \;\; \widehat{B}_t \in \mathcal{B}(\widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d})$$

$$\mathbb{E}^{s,\mathbf{y}}[\widehat{\mathbf{f}}_t(\widehat{\mathbf{X}}_t)] = \int_{\widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}} \widehat{\mathbf{f}}_t(\widehat{\mathbf{x}}) \widehat{\psi}(t, \widehat{\mathbf{x}} | s, \widehat{\mathbf{y}}) d\widehat{\mathbf{x}}$$

Regularity

Steps of the proof:

1. Markov Chain Generator
2. Regularity
   - Smoothness of the Transition Probability
   - Positivity of the Transition Probability
3. Invariant Measure of the Discrete Process
4. Convergence of the NELD

Regularity

Regularity proof:

- Smoothness of the Transition Probability
  - * Markov Process Generator in a Fixed Domain
  - * Infinitesimal Generator
  - * Hypoellipticity
  - * Kolmogorov Equation
- Positivity of the Transition Probability

Markov Process Generator in a Fixed Domain

Change of variables

$$\begin{cases} \widehat{\mathbf{q}}_t = e^{[t]A}\overline{\mathbf{q}}_t \\ \widehat{\mathbf{p}}_t = e^{[t]A}\overline{\mathbf{p}}_t \end{cases}, \ (\overline{\mathbf{q}}, \overline{\mathbf{p}}) \in \mathcal{L}_0^d \times \mathbb{R}^{3d}, \ (\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) \in \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}.$$

NELD in the fixed domain

$$\begin{cases} d\overline{\mathbf{q}}_t &= \overline{\mathbf{p}}_t dt, \\ d\overline{\mathbf{p}}_t &= -e^{-[t]A}\nabla V\left(e^{[t]A}\overline{\mathbf{q}}_t\right)dt - \Gamma\overline{\mathbf{p}}_t dt + \sigma e^{-[t]A} dW_t \end{cases}, \quad \frac{t}{T} \notin \mathbb{Z},$$

where $\Gamma = A + \gamma$.

$$\begin{cases} d\overline{\mathbf{X}}_t = \overline{\mathbf{b}}_t(\overline{\mathbf{X}}_t)dt + \overline{\Sigma}_t dW_t, \ \frac{t}{T} \notin \mathbb{Z}, \quad \overline{\mathbf{X}}_t \in \mathcal{L}_0^d \times \mathbb{R}^{3d} \\ \overline{\mathbf{X}}_t = \begin{bmatrix} \overline{\mathbf{q}} \\ \overline{\mathbf{p}} \end{bmatrix}, \overline{\mathbf{b}}_t(\overline{\mathbf{X}}_t) = \begin{bmatrix} \overline{\mathbf{p}} \\ -e^{-[t]A}\nabla V(e^{[t]A}\overline{\mathbf{q}}) - \Gamma\overline{\mathbf{p}} \end{bmatrix}, \overline{\Sigma}_t = \begin{bmatrix} 0 & 0 \\ 0 & \sigma e^{-[t]A} \end{bmatrix} \end{cases}$$

Markov Process Generator in a Fixed Domain

$$\Phi_t : \mathcal{L}_0^d \times \mathbb{R}^{3d} \to \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d} \quad \begin{bmatrix} \widehat{\mathbf{q}}_t \\ \widehat{\mathbf{p}}_t \end{bmatrix} = \begin{bmatrix} e^{[t]A} & 0 \\ 0 & e^{[t]A} \end{bmatrix} \begin{bmatrix} \overline{\mathbf{q}}_t \\ \overline{\mathbf{p}}_t \end{bmatrix}.$$

Generator in the fixed domain

$$\bar{\phi}_{t,s}(s, \overline{\mathbf{y}}) = \mathbb{E}^{s,\mathbf{y}}(\mathbf{f}_t \circ \Phi_t)(\overline{\mathbf{X}}_t) = \int_{\mathcal{L}_0^d \times \mathbb{R}^{3d}} (\mathbf{f}_t \circ \Phi_t)(\overline{\mathbf{x}}) \bar{\psi}(t, \overline{\mathbf{x}} \big| s, \overline{\mathbf{y}}) d\overline{\mathbf{x}}$$

Infinitesimal Generator

$$\overline{G} = \overline{\mathcal{X}}_0 + \frac{1}{2} \sum_{i=1}^{d} \overline{\mathcal{X}}_i, \text{ for } 1 \le i \le d,$$

$$\overline{\mathcal{X}}_0 = \langle \overline{\mathbf{p}}, \nabla_{\overline{\mathbf{q}}} \cdot \rangle - \left\langle e^{-[t]A} \nabla V(e^{[t]A} \overline{\mathbf{q}}), \nabla_{\overline{\mathbf{p}}} \cdot \right\rangle - \langle \Gamma \overline{\mathbf{p}}, \nabla_{\overline{\mathbf{p}}} \cdot \rangle$$

$$\overline{\mathcal{X}}_i = \sqrt{\sigma^2} s_{j,i} \partial_{\overline{\mathbf{p}}_i}, \quad (s_{j,i}) = e^{-[t]A} (e^{-[t]A})^T.$$

Smoothness

[Cass et al.(2021)Cass, Crisan, Dobson, and Ottobre]

Lemma 1

If $-\partial_t + \overline{G}_t^\dagger$ *is hypoelliptic and there exists* $\overline{\nu}_t(\cdot),\ t \in [kT, (k+1)T]$ *s.t.*

$$\big(-\partial_t \overline{\nu}_t + \overline{G}_t^\dagger \overline{\nu}_t\big)(\cdot) = 0,\ \textit{then } \overline{\nu}_t(\cdot) \in C^\infty$$

Lemma 2

The Markov process generator of $\overline{\mathbf{X}}_t$ *and* $\widehat{\mathbf{X}}_t$ *are smooth and we have:*

$$\mathbb{E}^{s,\mathbf{y}} \mathbf{f}_t(\widehat{\mathbf{X}}_t) = \mathbb{E}^{s,\mathbf{y}}[(\mathbf{f}_t \circ \Phi_t)(\overline{\mathbf{X}}_t)] \quad \frac{t}{T} \notin \mathbb{Z}.$$

$$\int_{\mathcal{L}_0^d \times \mathbb{R}^{3d}} (\mathbf{f} \circ \Phi_t)(\overline{\mathbf{x}}) \overline{\psi}(t, \overline{\mathbf{x}} | s, \overline{\mathbf{y}}) d\overline{\mathbf{x}} = \int_{\widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}} \mathbf{f}(\widehat{\mathbf{x}}) (\overline{\psi} \circ \Phi_t^{-1})(t, \widehat{\mathbf{x}} | s, \widehat{\mathbf{y}}) d\widehat{\mathbf{x}}$$

Hypoellipticity

Lemma 3

$\partial_t + \overline{G}_t, -\partial_t + \overline{G}_t^\dagger, \frac{t}{T} \notin \mathbb{Z}$ are hypoelliptic.

Lie bracket between two operators $\mathscr{C}$ and $\mathscr{D}$

$$[\mathscr{C}, \mathscr{D}] = \mathscr{C}\mathscr{D} - \mathscr{D}\mathscr{C}.$$

Since for every point $(\overline{\mathbf{q}}_{kT+\theta}, \overline{\mathbf{p}}_{kT+\theta}) \in \mathcal{L}_0^d \times \mathbb{R}^{3d}$

$$[\overline{\mathcal{X}}_i, \overline{\mathcal{X}}_0] = \sqrt{\sigma^2}(\partial_{\overline{\mathbf{q}}_i} + \gamma s_{i,j})\partial_{\overline{\mathbf{p}}_i}, \quad \forall i \in \{1 \dots d\},$$

evaluated at $(\overline{\mathbf{q}}_0, \overline{\mathbf{p}}_0)$ span $\mathcal{L}_0^d \times \mathbb{R}^{3d}$
$\overline{G}_t$ and $\overline{G}_t^\dagger$ are hypoelliptic using [Hörmander(1987), Theorem 1.1]

Kolmogorov Equation

Lemma 4

[Friedman(1975)] The backward Kolmogorov equation for the NELD is

$$\partial_s \overline{\phi}_{t,s}(\overline{\mathbf{y}}) + \big(\overline{G}_s \overline{\phi}_{t,s}\big)(\overline{\mathbf{y}}) = 0, \quad \textit{where} \quad \overline{\psi}(t, \overline{\mathbf{x}}\,|s, \overline{\mathbf{y}})\Big|_{t=s} = \delta(\overline{\mathbf{x}} - \overline{\mathbf{y}}).$$

Lemma 5

The forward Kolmogorov equation for the NELD is

$$\big(-\partial_t \overline{\psi} + \overline{G}_s^{\dagger} \overline{\psi}\big)(t, \overline{\mathbf{x}} \big| s, \overline{\mathbf{y}}) = 0.$$

$$\overline{\nu}(t, \overline{\mathbf{x}}) = \int_{\mathcal{L}_0^d \times \mathbb{R}^{3d}} \overline{\psi}(t, \overline{\mathbf{x}} \big| s, \overline{\mathbf{y}}) \overline{\nu}(s, \overline{\mathbf{y}}) d\overline{\mathbf{y}}$$

Regularity

Regularity proof:

- Smoothness of the Transition Probability
- Positivity of the Transition Probability

Positivity

- $\widehat{B}_t$ can be reached at any time with $\widehat{\mathcal{P}}_{t,0}(\widehat{\mathbf{y}}, \widehat{B}_t) > 0$
- Control problem

$$\frac{d\widetilde{\mathbf{X}}_t}{dt} = \mathbf{b}(\widetilde{\mathbf{X}}_t) + \widehat{\Sigma}\frac{d\mathcal{U}_t}{dt}, \quad \widetilde{\mathbf{X}}_t = \begin{bmatrix} \widetilde{\mathbf{q}} \\ \widetilde{\mathbf{p}} \end{bmatrix} \in \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d},$$

- $\mathcal{C}^2$ path $\varphi(t) \in \mathbb{R}^{3d}$ from $\mathcal{L}_0^d \times \mathbb{R}^{3d} \to \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}$

$$\begin{aligned} \varphi(0) &= \widetilde{\mathbf{q}}_0 & \varphi(t) &= \widetilde{\mathbf{q}}_t \\ \varphi'(0) &= \widetilde{\mathbf{p}}_0 & \varphi'(t) &= \widetilde{\mathbf{p}}_t + A\widetilde{\mathbf{q}}_t \end{aligned}$$

- Accessible points $\mathcal{A}_t(\widetilde{\mathbf{q}}_0, \widetilde{\mathbf{p}}_0) = \widehat{\mathcal{L}}_t^d \times \mathbb{R}^{3d}$
- [Rey-Bellet(2006), Corollary 6.2]: supp $\widehat{\mathcal{P}}_{t,0}(\widehat{\mathbf{y}}, \widehat{B}_t)$ is equal to the closure in the uniform topology of $\mathcal{A}_t(\widetilde{\mathbf{q}}_0, \widetilde{\mathbf{p}}_0)$

Invariant Measure of the Discrete Process

Steps of the proof:

1. Markov chain Generator
2. Regularity
3. Invariant Measure of the Discrete Process
    - Uniform Lyapunov Condition
    - Uniform Minorization Condition
4. Convergence of the NELD

The Invariant Measure of the Discrete Process

Discrete Markov chain

$$(Q_k = \widehat{\mathbf{q}}_{kT}, P_k = \widehat{\mathbf{p}}_{kT}) \in \mathcal{L}_0^d \times \mathbb{R}^{3d}$$

Discrete generator

$$(\mathcal{G}_T \mathbf{f})(Q_k, P_k) = \mathbb{E}\Big(\mathbf{f}(Q_{k+1}, P_{k+1}) | (Q_k, P_k)\Big),$$

Lyapunov function

$$\mathcal{K}_n(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) = 1 + \|\widehat{\mathbf{p}}\|^{2n}, n \geq 1$$

with the associated weighted L^∞ norms

$$\|\mathbf{h}\|_{L^\infty_{\mathcal{K}_n}} = \left\| \frac{\mathbf{h}}{\mathcal{K}_n} \right\|_{L^\infty}.$$

The Invariant Measure of the Discrete Process

[Hairer and Mattingly(2008)]

Theorem 6

If $\mathcal{G}_T$ satisfies the Lyapunov condition and the minorization condition, then $\exists \pi_0$ and $C_n, \lambda_n > 0$ for any $n \geq 1$ s.t.

$$\left\|\mathcal{G}_T^k \mathbf{f} - \overline{\mathbf{f}}\right\|_{L^\infty_{\mathcal{K}_n}} \leq C_n e^{-k\lambda_n T} \left\|\mathbf{f} - \overline{\mathbf{f}}\right\|_{L^\infty_{\mathcal{K}_n}}, \quad \forall k \geq 0,$$

$$\overline{\mathbf{f}} = \int_{\mathcal{L}_0^d \times \mathbb{R}^{3d}} \mathbf{f}(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) \pi_0(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) d\widehat{\mathbf{q}} d\widehat{\mathbf{p}}.$$

Uniform Lyapunov Condition

Lemma 7

There exists $a_n \in [0,1)$ and $b_n > 0$ such that

$$\mathcal{G}_T \mathcal{K}_n \leq a_n \mathcal{K}_n + b_n,$$

$$G = \left\langle \widehat{\mathbf{p}} + A\widehat{\mathbf{q}}, \nabla_{\widehat{\mathbf{q}}} \cdot \right\rangle + \left\langle -\nabla V(\widehat{\mathbf{q}}), \nabla_{\widehat{\mathbf{p}}} \cdot \right\rangle - \gamma \left\langle \widehat{\mathbf{p}}, \nabla_{\widehat{\mathbf{p}}} \cdot \right\rangle + \frac{1}{2}\sigma\sigma^T : \nabla^2.$$

$$G\mathcal{K}_n \leq -\widehat{a}_n \mathcal{K}_n + \widehat{b}_n, \quad \widehat{a}_n, \widehat{b}_n \geq 0$$

$$d\mathcal{K}_n(\widehat{\mathbf{X}}_t) \leq (-\widehat{a}_n \mathcal{K}_n + \widehat{b}_n)dt + \left\langle \nabla \mathcal{K}_n(\widehat{\mathbf{X}}_t), \widehat{\Sigma} dW \right\rangle.$$

$$\mathbb{E}[\mathcal{K}_n(Q_{k+1}, P_{k+1})] \leq e^{-\widehat{a}_n T} \mathcal{K}_n(Q_k, P_k) + \widehat{b}_n / \widehat{a}_n.$$

Uniform Minorization Condition

Lemma 8

Fix any $p_{max} > 0$, then $\exists$ prob. meas. $\vartheta : \mathcal{L}_0^d \times \mathbb{R}^{3d} \to \mathbb{R}$ and cst κ s.t.

$$\forall \overline{B} \in \mathcal{B}(\mathcal{L}_0^d \times \mathbb{R}^{3d}), \quad \mathbb{P}\Big((Q_{k+1}, P_{k+1}) \in \overline{B} \;\Big|\; \|P_k\|_2 \le p_{max}\Big) \ge \kappa\vartheta(\overline{B}).$$

[Mat(2002), Lemma 2.3]

Lemma 9

$C \in \mathcal{B}(\mathcal{L}_0^d \times \mathbb{R}^{3d})$ a fixed compact set. There is a choice of $t_k = kT$, $\kappa \ge 0$, a prob. meas. ϑ, with $\vartheta(C^c) = 0$ and $\vartheta(C) = 1$ s.t.

$$\overline{\mathcal{P}}_{t_k,0}(\mathbf{y}, \overline{B}) \ge \kappa\vartheta(\overline{B}), \quad \forall \overline{B} \in \mathcal{B}(\mathcal{L}_0^d \times \mathbb{R}^{3d}),\ \mathbf{y} \in C.$$

Convergence of the NELD

Steps of the proof:

1. Markov chain Generator
2. Regularity
3. Invariant Measure of the Discrete Process
4. Convergence of the NELD
   - Convergence to a limit cycle
   - Convergence in Law of Large Numbers

Convergence of the Continuous Process

Proposition 10

The Markov process $(\widehat{\mathbf{q}}_t, \widehat{\mathbf{p}}_t)$ *converges exponentially to the limit cycle* π_θ*:*

$$\left|\mathbb{E}^{s,\mathbf{y}}[\mathbf{f}(\widehat{\mathbf{X}}_t)] - \overline{\mathbf{f}}([t])\right| \leq C_n e^{-\lambda_n t} \left\|\mathbf{f} - \overline{\mathbf{f}}([t])\right\|_{L^\infty_{\mathcal{K}_n}} \left(1 + \mathcal{K}_n(\mathbf{y})\right), \quad \mathbf{y} = \widehat{\mathbf{X}}_0,$$

$$\overline{\mathbf{f}}(\theta) = \int_{\widehat{\mathcal{L}}^d_\theta \times \mathbb{R}^{3d}} \mathbf{f}_\theta(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) \pi_\theta(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) d\widehat{\mathbf{q}} d\widehat{\mathbf{p}}.$$

[Meyn and Tweedie(1993), Mat(2002)]

$$\left|\mathbb{E}^{0,\mathbf{y}}[\mathbf{f}(\widehat{\mathbf{X}}_{kT+\theta})] - \overline{\mathbf{f}}(\theta)\right| \leq C_n e^{-\lambda_n kT} \left\|\mathbf{f} - \overline{\mathbf{f}}(\theta)\right\|_{L^\infty_{\mathcal{K}_n}} \mathbb{E}^{0,\mathbf{y}}[\mathcal{K}_n(\widehat{\mathbf{X}}_\theta)]$$

$$\mathbb{E}^{0,\mathbf{y}}[\mathcal{K}_n(\widehat{\mathbf{X}}_\theta)] \leq e^{-\widehat{a}_n \theta} \mathcal{K}_n(\mathbf{y}) + \frac{\widehat{b}_n}{\widehat{a}_n} \quad \text{and } C_n \to \left(1 + \frac{\widehat{b}_n}{\widehat{a}_n} e^{\lambda_n T}\right)$$

Convergence in Law of Large Numbers

Proposition 11

[Meyn et al.(2009)Meyn, Tweedie, and Glynn]

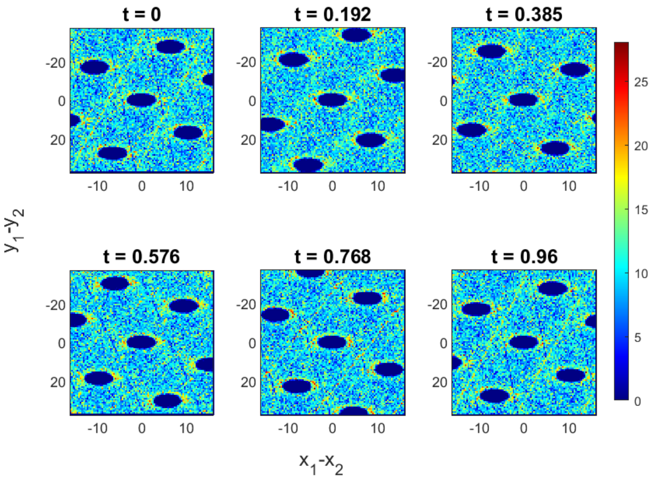
$$\frac{1}{N}\sum_{k=1}^{N}\mathbf{f}(\widehat{\mathbf{q}}_{kT+\theta},\widehat{\mathbf{p}}_{kT+\theta}) \xrightarrow[N\to+\infty]{} \int_{\mathcal{L}_\theta^d\times\mathbb{R}^{3d}}\mathbf{f}(\widehat{\mathbf{q}},\widehat{\mathbf{p}})\nu(\widehat{\mathbf{q}},\widehat{\mathbf{p}})d\widehat{\mathbf{q}}d\widehat{\mathbf{p}} \quad a,s. \ ,$$

for all the initial conditions (Q_0, P_0) *and any* $\mathbf{f} \in L^\infty_{\mathcal{K}_n}$.

$(\widehat{\mathbf{q}}_{kT+\theta},\widehat{\mathbf{p}}_{kT+\theta})$ is a positive Harris recurrent simple chain

- (Q_k, P_k) is irreducible w.r.t to the Lebesgue measure
- Every set in the domain is Harris recurrent [Tierney(1994), Cor 1]
  1. (Q_k, P_k) is positive recurrent
  2. (Q_k, P_k) is absolutely continuous w.r.t Lebesgue meas. $\forall (Q_k, P_k)$

Sample for Two Particle Elongational Flow



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