Convergence of Nonequilibrium Langevin Dynamics for Planar Flows

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Abstract
We prove that incompressible two-dimensional nonequilibrium Langevin dynamics (NELD) converges exponentially fast to a steady-state limit cycle. We use automorphism remapping periodic boundary conditions (PBCs) such as Lees–Edwards PBCs and Kraynik–Reinelt PBCs to treat respectively shear flow and planar elongational flow. The convergence is shown using a technique similar to (Joubaud et al. in J Stat Phys 158:1–36, 2015).

Keywords Nonequilibrium · Langevin dynamics · Stochastic convergence · Planar flows

1 Introduction

A wide range of nonequilibrium molecular dynamics (NEMD) techniques [1, 2] are used in the study of molecular fluids under steady flow, and some recent applications can be found in [3–17]. Here we study the exponential convergence of the probability density of nonequilibrium Langevin dynamics under incompressible two-dimensional flows such as shear flow and planar elongational flow with spatial periodic boundary conditions (PBCs).

We consider a molecular system corresponding to the micro-scale motion of a fluid with local strain rate \( \nabla u \) and denote the constant steady background flow matrix of the molecular system by \( A = \nabla u \in \mathbb{R}^{3 \times 3} \). The coordinates of the simulation box are given by three linearly independent column vectors coming from the origin, and we write them in a matrix

\[
L_t = \begin{bmatrix} v^1_t & v^2_t & v^3_t \end{bmatrix} \in \mathbb{R}^{3 \times 3}, \quad t \geq 0.
\]

The initial simulation box is given by \( L_0 \) and the lattice deforms with the background flow according to the equation

\[
L_t = e^{tA}L_0.
\]

If \( L_0 \) is not chosen appropriately, the simulation box can become extremely stretched with degenerate geometry. For example, in the elongational flow case, if the compression is

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parallel to one of the edges of the simulation box, then the box will become degenerate to
the point where a particle and its image become arbitrarily close. Thus, to perform a long
simulation, we consider specialized PBCs consisting of a lattice automorphism represented
as a $3 \times 3$ integer matrix with a determinant one to remap the simulation box at various
times during the simulation. These types of PBCs were first used in the shear flow case by
Lees and Edwards (LE) [18] and were then later extended to the planar elongational flow
case by Kraynik and Reinelt (KR) [19]. The analog of these types of PBCs that treats three
dimensional flows such as uniaxial flow, biaxial flow, and generalized three-dimensional
diagonalizable flow can be found in [20–22].

The NELD equation is written in terms of the relative momentum as
\[
\begin{align*}
    dq &= (p + Aq)dt, \\
    dp &= -\nabla V(q)dt - \gamma pdt + \sigma dW,
\end{align*}
\]
where $V$ is the potential and $\sigma^2 = 2\gamma / \beta$ is the fluctuation coefficient with $\beta$ being the inverse
temperature. The position and the momentum of the particles are denoted by $(q, p) \in \mathbb{L}^d \times \mathbb{R}^{3d}$. Under the planar PBCs, the simulation box is represented by
\[
\begin{align*}
    \mathcal{L}_t &= \{ \hat{L}_t x \mid x \in T^3 \}, \quad \text{where } T^3 = \mathbb{R}^3 \setminus \mathbb{Z}^3, \\
    \hat{L}_t &= e^{[t]A}L_0, \quad \text{where } [t] \equiv t \mod T,
\end{align*}
\]
where $L_t$ defines a remapped periodic lattice with a period of $T$. Although these remappings
introduce a discontinuity in the simulation, the system as a whole remains homogeneous in
space just as in [13, 23]. This is due to the fact that during the remapping, a particle within
the simulation box is replaced by its image whose coordinates are denoted by $(q + Ln, p)$
whose position satisfies (1):
\[
d(q + Ltn) = (p + Aq + ALtn)dt \implies dq = (p + Aq)dt,
\]
as
\[
\frac{d}{dt} L_t = AL_t.
\]
Throughout this paper, we assume that the potential is smooth $V \in C^\infty$, which results in a
finite gradient $\|\nabla V(q)\|_2 < \infty$ because the position space is compact. An example of an
observable computed using the NELD is the bulk pressure tensor in a Lennard–Jones liquid [2]
\[
f(t, q, p) = \frac{1}{\det L_t} \sum_{i=1}^{d} \left( \|p_i\|_2^2 - \frac{1}{2} \sum_{j \neq i}^{d} r_{ij} \cdot \frac{\partial V}{\partial r_{ij}}(r_{ij}) \right),
\]
where $r_{ij} = \|q_i - q_j\|_2$.

In the absence of a background flow, the domain of the simulation is stationary, and (1)
becomes equilibrium Langevin Dynamics. It has been shown (see for instance [24–29]) that
under suitable conditions, the equilibrium Langevin Dynamics is ergodic with respect to the
Boltzmann-Gibbs distribution
\[
v(q, p)dqd\!p = \frac{1}{Z}e^{-\beta H(q, p)}dqd\!p, \quad Z = \int_{\mathbb{L}^d_0 \times \mathbb{R}^{3d}} e^{-\beta H(q, p)}dqd\!p,
\]
where $Z$ is the normalization constant, and $H$ is the Hamiltonian of the system given by

$$H(q, p) = \frac{1}{2} \langle p, p \rangle + V(q).$$

However, convergence to a limiting measure has not been established for NELD under moving domains.

In this paper, we show the existence, uniqueness, and exponential convergence of the planar flow case of NELD to a time-periodic invariant measure referred to as a limit cycle, following the work done in [30]. To accomplish this, it will be necessary to reformulate the NELD within a fixed domain in order to show the regularity of the probability distribution. In addition, we will construct a Markov chain at integer multiples of the remapping time, established when the particles are in the initial box $L_0$. This Markov chain can be utilized to show both the existence and uniqueness of an invariant measure at the remapping times. In Sect. 2, we present the derivation of the particle remapping function. The main result of the paper is then established in Sect. 3, where we prove the convergence of the NELD to a probability density function, as shown in Proposition 1.

2 Time-Periodic Remapping

First, we derive the remapping of the simulation box under LE and KR PBCs. Next, we proceed to define the remapping function of the particle coordinates while the simulation box is being remapped.

2.1 Remapping the Unit Cell

We start by defining the remapped Eulerian domain in the shear flow case, followed by the planar elongational flow case.

2.1.1 Shear Case

We denote the background matrix of the shear flow by

$$A = \begin{bmatrix} 0 & \varepsilon & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \varepsilon \in \mathbb{R}^*.$$

At a time $t$, the basis vectors for the simulation box are the columns of the matrix

$$L_t = \begin{bmatrix} 1 & t & \varepsilon \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} L_0 \quad \text{where} \quad L_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}.$$

Since $L_t$ is highly sheared as $t$ becomes large, the interparticle interaction computation becomes more difficult. We can prevent this anomaly by applying the LE PBCs which consists in multiplying $L_t$ by the lattice automorphism matrix

$$M^k = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}^k = \begin{bmatrix} 1 & -k & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad k \in \mathbb{Z},$$
to get the remapped simulation box lattice

\[ L_t M^k = \begin{bmatrix} 1 & t\epsilon - k \frac{1}{\epsilon} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad k \in \mathbb{Z}. \]

Since \( M \) is an integer matrix with determinant equal to one (\( M \in SL(3, \mathbb{Z}) \)), the lattice basis vectors in \( L_t \) and \( L_t M^k \) generate the same lattice. By choosing \( k = -\lfloor t\epsilon \rfloor \), where \( \lfloor x \rfloor \) denotes \( x \) rounded to the nearest integer, we ensure that the stretch is at most half of the simulation box. Then we observe that the stretch matrix is time-periodic with the period \( T = \frac{1}{\epsilon} \), and discontinuous at time multiple of \( T \):

\[
\begin{bmatrix}
0 & t\epsilon - \lfloor t\epsilon \rfloor & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} = [t]\epsilon D, \quad \text{where } D = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [t] = \theta \equiv t \mod T. \tag{5}
\]

This implies that the particle position belongs to remapped Eulerian domain

\[ L_t = \{e^{[t]A}L_0x | x \in \mathbb{T}^3\}, \quad \text{where } \mathbb{T}^3 = \mathbb{R}^3 \setminus \mathbb{Z}^3. \tag{6} \]

In the Sect. 2.2, we analyse the particles remapped position in \( L_t \) and in the unit cell.

### 2.1.2 Planar Elongational Flow Case

We consider the planar elongational flow (PEF) case with background flow matrix given by

\[
A = \begin{bmatrix} \epsilon & 0 & 0 \\ 0 & -\epsilon & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \epsilon \in \mathbb{R}^*,
\]

which means that the simulation box elongates in the \( x \) direction and shrinks in the \( y \) direction of the standard coordinate plane. As \( t \) goes to infinity, a particle and its image can become arbitrarily close if an edge of the simulation box is aligned with the \( y \) coordinate. This would lead to a breakdown in the simulation. We prevent this issue by applying the KR PBCs, which consists in carefully choosing the alignment of the initial simulation box and remapping the simulation box with a matrix \( M \in SL(3, \mathbb{Z}) \). We choose \( M \) such that it is diagonalizable with eigenvalues of the form

\[
MS = S\Lambda, \quad \Lambda = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda^{-1} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda > 0, \quad \lambda \neq 1.
\]

We choose the initial lattice \( L_0 = S^{-1} \) rather than the standard coordinate directions, and this will prevent particle images from becoming too close. If we remap the lattice basis vectors by applying \( M^k \), we get

\[
L_t M^k = e^{J^A}L_0M^k = e^{t\epsilon D}\Lambda^nS^{-1} = e^{(t\epsilon+k\eta)D}S^{-1}, \quad \text{where } D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \eta = \log(\lambda).
\]

Letting \( T = \frac{\eta}{\epsilon} \), the stretched matrix \( [t]A \) and the position domain of the particles are also respectively expressed in the periodic form as in (5) and (6).
2.2 Remapping of the Particle Coordinates

We will formulate the dynamics with remappings of the particle positions. While this does lead to discontinuities of the particle paths in real space, it is not a true discontinuity of the system. When the particles are remapped, we are choosing a different image particle to track, but the set of all periodic images of the tracked particle is unchanged when considered in $\mathbb{R}^3$. This is the same effect of applying spatial periodic boundary conditions whenever a particle in the simulation would move outside the simulation box.

Now, we define the function which remaps the particle positions when the unit cell is remapped at multiples of the period $kT$. This function chooses the image particle that lives within the unit cell for the remapped lattice. We start by defining the modulus operation applied to each vector component

$$g(x) \equiv x \mod 1, \text{ where } x \in \mathbb{R}^3.$$  

At time $T$, we denote the simulation box before remapping by $L_T^{-}$ and after remapping by $L_T$, where we note that by definition, $L_T = L_0$. Let us define by $\tilde{g} : L_T^{-} \rightarrow L_0$:

$$q_{kT} = \tilde{g}(q_{kT}^{-}) = L_0 g \left( L_0^{-1} q_{kT}^{-} \right),$$  

which maps the particle positions after the simulation box is remapped. Since the momentum is not affected by the remapping, the function

$$\mathcal{R}_T : L_T^d \times \mathbb{R}^{3d} \rightarrow L_0^d \times \mathbb{R}^{3d} \quad (q_{kT}, p_{kT}) = (\tilde{g}(q_{kT}^{-}), p_{kT}^{-}),$$

describes the remapping of particle coordinates.

3 Ergodicity of NELD under Planar Flow

We start this section by deriving the forward and backward Kolmogorov equation of the NELD and show the regularity property of the NELD in Sect. 3.1, then build on the latter result to prove the main result of the paper, the convergence of the NELD to a measure in Sect.3.4.

3.1 Markov Process Generator

We derive the generator of the NELD and use it to find the forward and backward Kolmogorov equations. Then, we establish the regularity of the NELD by showing that its transition kernel is smooth and positive using respectively [31, Lemma A.5] and [29, Corollary 6.2].

3.1.1 Fokker–Planck Equation

The NELD dynamics (1) can be written in vector form as

$$\begin{cases}
    dX_t = b(X_t)dt + \Sigma dW_t, & X_t \in \mathbb{L}_t^d \times \mathbb{R}^{3d}, \\
    X_t = \begin{bmatrix} q \\ p \end{bmatrix}, & b(X_t) = \begin{bmatrix} p + Aq \\ -\nabla V(q) - \gamma p \end{bmatrix}, & \Sigma = \begin{bmatrix} 0 & 0 \\ 0 & \sigma \end{bmatrix}.
\end{cases}$$  

(8)
Lemma 1 [32, Theorem 6.1] The backward Kolmogorov equation for the NELD is
\[ \partial_s \phi_{t,s}(y) + (G\phi_{t,s})(y) = 0, \] where \( \psi(t, x \mid s, y) \big|_{t=s} = \delta(x - y). \) \( \tag{10} \)

The forward Kolmogorov equation of the NELD is given in the following lemma:

Lemma 2 The forward Kolmogorov equation of the NELD is
\[ (- \partial_t \psi + G^\dagger \psi)(t, x \mid s, y) = 0. \] \( \tag{11} \)

The proof of this Lemma is obtained by using the adjoint property to have
\[ \int_{\mathcal{L}_t^d \times \mathbb{R}^{3d}} (\partial_t f_t + G f_t)(x) \psi(t, x \mid s, y) dx \]
\[ = \int_{\mathcal{L}_t^d \times \mathbb{R}^{3d}} f_t(x)(- \partial_t \psi + G^\dagger \psi)(t, x \mid s, y) dx. \]

and by applying (11). Note that the probability density of \( X_t \), denoted by
\[ \nu(t, x) = \int_{\mathcal{L}_t^d \times \mathbb{R}^{3d}} \psi(t, x \mid s, \bar{y}) \nu(s, \bar{y}) d\bar{y} \]
satisfies the forward Kolmogorov equation, and the backward evolution from \( \phi_{t', s}(t, x) \) to \( \phi_{t, s}(s, y) \), \( s \leq t \leq t' \) satisfies
\[ \phi_{t, s}(s, y) = \int_{\mathcal{L}_t^d \times \mathbb{R}^{3d}} \phi_{t', s}(t, x) \psi(t, x \mid s, y) dx. \]
3.2 Markov Process Generator in a Fixed Domain

We derive the NELD equation and its Markov process generator in a fixed domain to show the transition kernel’s regularity in the moving domain in the next section.

3.2.1 NELD with LE and KR PBCs in Fixed Coordinates

We write the NELD equation in a fixed domain by considering the change of variables

\[
\begin{align*}
q_t &= e^{[t]A} \tilde{q}_t, \quad (\tilde{q}, \tilde{p}) \in L^d_0 \times \mathbb{R}^{3d}, \\
\rho_t &= e^{[t]A} \tilde{p}_t, \\
(\tilde{q}, \tilde{p}) &\in L^d_t \times \mathbb{R}^{3d}.
\end{align*}
\]

Next, we compute the time derivative of the position when \( \frac{t}{T} \not\in \mathbb{Z} \) to have:

\[
dq_t = e^{[t]A} (dq_t + Aq_t dt) = (p + Aq_t) dt,
\]
which implies that

\[
d\tilde{q} = \tilde{p} dt.
\]

Computing the time derivative of the momentum when \( \frac{t}{T} \not\in \mathbb{Z} \) gives

\[
\begin{align*}
d\tilde{p} &= - Ae^{[-t]A} (p - Ap) dt \\
&= - e^{[-t]A} \nabla V (e^{[t]A} \tilde{q}_t) dt - (A + \gamma) \tilde{p}_t dt + \sigma e^{[-t]A} dW_t.
\end{align*}
\]

This leads to the NELD equation written in the fixed domain:

\[
\begin{align*}
\begin{cases}
d\tilde{q}_t &= \tilde{p}_t dt, \\
d\tilde{p}_t &= - e^{[-t]A} \nabla V (e^{[t]A} \tilde{q}_t) dt - \Gamma \tilde{p}_t dt + \sigma e^{[-t]A} dW_t, \quad \frac{t}{T} \not\in \mathbb{Z},
\end{cases}
\end{align*}
\]

where \( \Gamma = A + \gamma \).

3.2.2 Markov Process Generator

Let us rewrite (13) as,

\[
\begin{align*}
\begin{cases}
d\overline{X}_t &= \overline{b}_t(\overline{X}_t) dt + \Sigma_t dW_t, \quad \frac{t}{T} \not\in \mathbb{Z}, \\
\overline{X}_t &\in L^d_0 \times \mathbb{R}^{3d}
\end{cases}
\end{align*}
\]

and express the strong solution of the latter equation as

\[
\overline{X}_t - \overline{X}_s = \int_s^t \overline{b}_u(\overline{X}_u) du + \Sigma_u dW_u, \quad s \leq u < t, \quad s, t \in [kT, (k+1)T).
\]

Then, we define the density transition function from one state to another in the continuous-time Markov chain \( \overline{X}_t \) by

\[
P(\overline{X}_t \in \overline{B} | \overline{X}_s = \overline{y}) = \int_{\overline{B}} \overline{\psi}(t, \overline{x} | s, \overline{y}) d\overline{x}, \quad \text{where} \ \overline{\psi}(t, \overline{x} | t, \overline{y}) = \delta(\overline{x} - \overline{y}),
\]
The forward Kolmogorov equation of the NELD is given in the following lemma:

**Lemma 4** The probability density of \( \mathbf{X}_t \), denoted by,

\[
\overline{\psi}(t, \mathbf{x}) = \int_{L_0^d \times \mathbb{R}^d} \overline{\psi}(t, \mathbf{x}|s, \mathbf{y}) \overline{\psi}(s, \mathbf{y}) d\mathbf{y}
\]

satisfies the forward Kolmogorov equation and the backward evolution from \( \overline{\phi}_{t^{'}, t}(t, \mathbf{x}) \) to \( \overline{\phi}_{t-s}(s, \mathbf{y}) \), \( s \leq t \leq t^{'} \) satisfies

\[
\overline{\phi}_{t-s}(s, \mathbf{y}) = \int_{L_0^d \times \mathbb{R}^d} \overline{\phi}_{t^{'}, t}(t, \mathbf{x}) \overline{\psi}(t, \mathbf{x}|s, \mathbf{y}) d\mathbf{x}.
\]

**3.3 Regularity of the NELD**

The smoothness of the transition kernel of \( \mathbf{X} \) on an interval \([kT, (k + 1)T]\) is obtained by using the result from [31, Lemma A.5], and the positivity is obtained using a standard control theory argument.
3.3.1 Smoothness

First, we show that $\overline{G}_t$, $t/T \notin \mathbb{Z}$ is hypoelliptic in the following Lemma:

**Lemma 5** $\partial_t + \overline{G}_t$, $-\partial_t + \overline{G}_t^\dagger$, $t/T \notin \mathbb{Z}$ are hypoelliptic.

**Proof** We define $\mathcal{L}(\overline{X}_0, \ldots, \overline{X}_d)$, the Lie algebra of the family of the vectorial space operators $(\overline{X}_0, \ldots, \overline{X}_d) \in \text{Span}(\overline{X}_0, \ldots, \overline{X}_d)$ satisfying the stability property:

$$B \in \mathcal{L}(\overline{X}_0, \ldots, \overline{X}_d) \implies [B, \overline{X}_i] \in \mathcal{L}(\overline{X}_0, \ldots, \overline{X}_d), \quad i = 0, \ldots, d,$$

where the Lie bracket between two operators $\mathcal{C}$ and $\mathcal{D}$ is

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

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

$$[\overline{X}_i, \overline{X}_0] = \sqrt{\frac{\gamma}{2\beta}} (\partial_{\overline{q}_i} + \gamma s_{i,j}) \partial_{\overline{p}_i}, \quad \forall i \in \{1 \ldots d\},$$

evaluated at $(\overline{q}_0, \overline{p}_0)$ span $\mathcal{L}_0^d \times \mathbb{R}^{3d}$, it follows that $\overline{G}_t$ and $\overline{G}_t^\dagger$ are hypoelliptic using [33, Theorem 1.1].

**Lemma 6** [31, Lemma A.5] If $-\partial_t + \overline{G}_t^\dagger$ is hypoelliptic and there exists $\overline{\nu}_t(\cdot)$, $t \in [kT, (k + 1)T]$ such that

$$(- \partial_t \overline{\nu}_t + \overline{G}_t^\dagger \overline{\nu}_t)(\cdot) = 0,$$

then $\overline{\nu}_t(\cdot) \in C^\infty$, $t/T \notin \mathbb{Z}$.

Now, we derive the smoothness of the Markov process generator of $\overline{X}_t$ and $X_t$ in the following Lemma:

**Lemma 7** The Markov process generator of $\overline{X}_t$ and $X_t$ are smooth and we have:

$$\mathbb{E}^{x,y} f_t(X_t) = \mathbb{E}^{x,y}[(f_t \circ \Phi_t)(\overline{X}_t)], \quad \frac{t}{T} \notin \mathbb{Z}.$$

**Proof** Using Lemma 6, we have the transition map $\overline{\psi}$ for $\overline{X}_t$ is smooth. Next, we have

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

where $\psi = \overline{\psi} \circ \Phi_t^{-1}$. Therefore, $\psi(t, x|\cdot)$ is smooth. \qed
3.3.2 Positivity

Now, we will show that the bounded periodic domain $B_t \in \mathcal{B}(\mathcal{L}_t \times \mathbb{R}^{3d})$ can be reached at any time with a positive transition kernel $\mathcal{P}_{t,0}(y, B_t) > 0$, using a method similar to the control theory technique developed in [29, Section 6] and [25]. Intuitively, the control approach replaces the noise term with a control, showing the accessible configurations of the stochastic system. We first establish that the control has a positive kernel, and then prove that it approximates the NELD.

Lemma 8 \textit{G}_t \text{ has a positive transition kernel.}

\begin{proof}
Let us consider the following associated control problem, derived from (8):
\begin{equation}
\frac{d\tilde{X}_t}{dt} = b(\tilde{X}_t) + \Sigma_{\delta} dU_t, \quad \tilde{X}_t = \begin{bmatrix} \tilde{q} \\ \tilde{p} \end{bmatrix} \in \mathcal{L}_t^d \times \mathbb{R}^{3d},
\end{equation}
where \( \tilde{X}_{kt} = \mathcal{R}(\tilde{X}_{kt}) \) at the remapping time $t_k = kT$. For $t > 0$ and two points $\tilde{(q_0, p_0)}$ and $\tilde{(q_1, p_1)}$, we can find smooth $U_t \in C^\infty([0, t], \mathbb{R}^{3d})$ such that (16) is satisfied. In addition, there is $C^2$ path denoted by $\varphi(t)$ in $\mathbb{R}^{3d}$, defined from $\mathcal{L}_t^d \times \mathbb{R}^{3d}$ to $\mathcal{L}_t^d \times \mathbb{R}^{3d}$, and satisfies $\varphi(0) = \tilde{q}_0, \varphi(t) = \tilde{q}_t, \varphi'(0) = \tilde{p}_0$, and $\varphi'(t) = \tilde{p}_t + A\tilde{q}_t$. This can be shown by setting
\begin{equation}
\tilde{X}_t = \begin{bmatrix} \varphi(t) \\ \varphi'(t) \end{bmatrix}, \quad \text{then} \quad V_t = \frac{dU_t}{dt} = \sqrt{\frac{2\beta}{\gamma}} \left( \tilde{\psi}_t + \nabla V(\varphi_t) - A\varphi_t + \gamma \tilde{\psi}_t \right),
\end{equation}
where $V_t$ is a smooth control. Thus $(\varphi_t, \tilde{\psi}_t)$ is a solution of the control system so that, $V_t$ drives the system from $(\tilde{q}_0, \tilde{p}_0)$ to $(\tilde{q}_t, \tilde{p}_t)$. We let $A_t(\tilde{q}_0, \tilde{p}_0)$ denote the set of accessible points starting from $(\tilde{q}_0, \tilde{p}_0)$ at time $t$, and using the control above we have $A_t(\tilde{q}_0, \tilde{p}_0) = \mathcal{L}_t^d \times \mathbb{R}^{3d}$. Since, by [29, Corollary 6.2], the support of the transition kernel is equal to the closure in the uniform topology of $A_t(\tilde{q}_0, \tilde{p}_0)$, it follows that the transition kernel is positive. \hfill \Box
\end{proof}

Now, let us denote $B_\delta(x)$ the open ball of radius $\delta$ centered at $x$. We fix the domain at the initial position $\mathcal{L}_0$, and summarize the results of this section in the following Corollary:

Corollary 1 \textit{At time $t_k = kT$, the transition kernel}
\begin{equation*}
\mathcal{P}_{t_k,0}(y, \mathcal{B}), \quad \mathcal{B} \in \mathcal{B}(\mathcal{L}_0^d \times \mathbb{R}^{3d}), \quad y = x_0,
\end{equation*}
satisfies, for some fixed compact set $C \in \mathcal{B}(\mathcal{L}_0^d \times \mathbb{R}^{3d})$, the following:
\begin{itemize}
  \item for some $z^* \in \text{int}(C)$ there exists $\delta > 0$, such that
  \begin{equation*}
  \mathcal{P}_{t_k,0}(y, B_\delta(z^*)) > 0, \quad \forall x \in C
  \end{equation*}
  \item for $t_k$, the transition kernel possesses a density $\psi(x, y)$ precisely
  \begin{equation*}
  \mathcal{P}_{t_k,0}(y, \mathcal{B}) = \int_{\mathcal{B}} \psi(x, y)dy, \quad \forall x \in C, \quad \mathcal{B} = \mathcal{B}(\mathcal{L}_t^d \times \mathbb{R}^{3d}) \cap \mathcal{B}(C),
  \end{equation*}
  and $\psi(x, y)$ is jointly continuous in $(x, y) \in C \times C$.
\end{itemize}

\begin{proof}
The proof of the first argument relies on the positivity of the transition kernel as proven in Lemma 8, while the second argument is based on the smoothness of the density demonstrated in Lemma 7. \hfill \Box
\end{proof}

We use Corollary 1 in the next section to show that the Lyapunov function satisfies the minorization condition.
3.4 Markov Process Convergence

We show in this section that the Markov process $X_t$ converges to a measure on $\mathcal{L}_t^d \times \mathbb{R}^{3d}$.

Let us denote by $(Q_k = q_{kT}, P_k = p_{kT}) \in \mathcal{L}_0^d \times \mathbb{R}^{3d}$, a discrete Markov chain constructed from the particle coordinates at the start of each period, where $X_0 = (Q_0, P_0)$ is the initial coordinate of the time-inhomogeneous process $(q_t, p_t)$. Then, we define

$$(G_T f)(Q_k, P_k) = \mathbb{E} \left( f(Q_{k+1}, P_{k+1}) | (Q_k, P_k) \right),$$

the discrete generator of the Markov chain. In addition, we consider the Lyapunov function

$$K_n(q, p) = 1 + \|p\|^{2n}, \quad n \geq 1 \quad (17)$$

with the associated weighted $L^\infty$ norms defined by

$$\|h\|_{L^\infty_{K_n}} = \frac{\|h\|_{L^\infty}}{K_n}.$$

We begin by demonstrating that the discrete process converges exponentially to an invariant measure, and then we use this result to prove that the continuous process also converges to a measure.

3.4.1 The Invariant Measure of the Discrete Process

The convergence of the Markov chain $(Q_{k+1}, P_{k+1})$ is based on the uniform Lyapunov condition [34, Assumption 1] and the uniform minorization condition [34, Assumption 2] that we prove in the following two Lemmas.

**Lemma 9** (Uniform Lyapunov condition) There exists $a_n \in [0, 1)$ and $b_n > 0$ such that

$$G_T K_n \leq a_n K_n + b_n,$$

for $K_n$ defined in (17).

**Proof** Using the Itô’s lemma, we get

$$df(X_t) = (Gf)(X_t)dt + \langle \nabla f(X_t), \Sigma dW \rangle,$$

where

$$G = \langle p + Aq, \nabla q \rangle + \langle -\nabla V(q), \nabla p \rangle - \gamma \langle p, \nabla p \rangle + \frac{1}{2} \sigma \sigma^T : \nabla^2.$$

Then, it follows that

$$GK_n(q, p) = -n \|p\|^{n-2} \langle \nabla V(q), p \rangle - n\gamma \left( \langle p, p \rangle - \frac{n + d - 2}{\beta} \right) \|p\|^{n-2}$$

$$\leq -n\gamma \|p\|^{n-2} + n \|\nabla V(q)\|_2 \|p\|^{n-1} + n\gamma \frac{n + d - 2}{\beta} \|p\|^{n-2}.$$

Thus, there exists $a_n, b_n \geq 0$ such that

$$GK_n \leq -a_n K_n + b_n, \quad a_n = n\gamma / 2, \quad \text{as} \quad \lim_{[q, p] \to \infty} \frac{GK_n}{K_n} \leq -a_n,$$

and it follows that

$$dK_n(X_t) \leq (-a_n K_n + b_n)dt + \langle \nabla K_n(X_t), \Sigma dW \rangle.$$
Using Grönwall’s inequality, we have the desired result
\[
\mathbb{E}[\mathcal{K}_n(Q_{k+1}, P_{k+1})] \leq e^{-anT} \mathcal{K}_n(Q_k, P_k) + \frac{b_n}{a_n} (1 - e^{-an\theta}) \leq e^{-anT} \mathcal{K}_n(Q_k, P_k) + \frac{b_n}{a_n}.
\]

**Lemma 10** (Uniform minorization condition) Fix any \( p_{\text{max}} > 0 \), then there exists a probability measure \( \vartheta : \mathfrak{L}^d_0 \times \mathbb{R}^{3d} \to \mathbb{R} \) and a constant \( \kappa \) such that,
\[
\forall \overline{B} \in \mathcal{B}(\mathfrak{L}^d_0 \times \mathbb{R}^{3d}), \quad \mathbb{P}\left((Q_{k+1}, P_{k+1}) \in \overline{B} \mid \|P_k\|_2 \leq p_{\text{max}}\right) \geq \kappa \vartheta(\overline{B}).
\]

The proof is essentially based on the arguments from [25, 29] which uses the continuity property of the Markov process, the regularity of the transition kernel. Before we start the proof, we consider the following Lemma:

**Lemma 11** [25, Lemma 2.3] If the Markov chain \((Q_k, P_k)\) satisfies the assumption in Corollary 1, then there is a choice of time \( t_k = kT, \kappa \geq 0 \), a probability measure \( \vartheta \), with \( \vartheta(C^c) = 0 \) and \( \vartheta(C) = 1 \), such that
\[
\overline{P}_{k,0}(y, \overline{B}) \geq \kappa \vartheta(\overline{B}), \quad \forall \overline{B} \in \mathcal{B}(\mathfrak{L}^d_0 \times \mathbb{R}^{3d}), \, y \in C.
\]

The proof of Lemma 10 follows from the fact that the discrete chain \((Q_{k+1}, P_{k+1}) \in \overline{B}\) satisfies the assumption in Corollary 1. By using the above Lemma, we can deduce the desired result.

Using the previous Lemmas, we state the following uniform convergence result for the sampled chain \((Q_k, P_k)\) from [34]:

**Theorem 1** [34, Theorem 1.2] If \( G_T \) satisfies the Lyapunov condition as in Lemma 9 and the minorization condition as in Lemma 10, then there exists an invariant measure \( \pi_0 \) and constants \( C_n, \lambda_n > 0 \) for any \( n \geq 1 \) such that
\[
\left\| G^k_T f - \overline{f} \right\|_{L^\infty_{\mathcal{K}_n}} \leq C_n e^{-k\lambda_n T} \left\| f - \overline{f} \right\|_{L^\infty_{\mathcal{K}_n}}, \quad \forall k \geq 0,
\]
where
\[
\overline{f} = \int_{\mathfrak{L}^d_0 \times \mathbb{R}^{3d}} f(q, p) \pi_0(q, p) dq dp.
\]

Then, we derive the convergence of the continuous process \((q_t, p_t)\) in the following Lemma:

**Proposition 1** The Markov process \((q_t, p_t)\) converges exponentially to the limit cycle \( \pi_\theta \):
\[
\left| \mathbb{E}^{0, \mathcal{Y}}[f(X_t)] - \overline{f}(\mathcal{I}) \right| \leq C_n e^{-\lambda_n t} \left\| f - \overline{f}(\mathcal{I}) \right\|_{L^\infty_{\mathcal{K}_n}} \left(1 + \mathcal{K}_n(y)\right), \quad y = X_0,
\]
where \( \overline{f}(\mathcal{I}) \) is defined as
\[
\overline{f}(\theta) = \int_{\mathfrak{L}^d_0 \times \mathbb{R}^{3d}} f_\theta(q, p) \pi_0(q, p) dq dp.
\]

**Proof** We use an argument from [25, 35] and the result from Theorem 1 to show that the Markov process \((q_t, p_t) \in \mathfrak{L}^d_0 \times \mathbb{R}^{3d}\) converges exponentially to the limit cycle \( \pi_\theta \). We start by using the result from Lemmas 9 and 10, and derive from Theorem 1 that
\[
\left| \mathbb{E}^{0, \mathcal{Y}}[f(X_{kT})] - \overline{f} \right| \leq C_n e^{-\lambda_n kT} \left\| f - \overline{f} \right\|_{L^\infty_{\mathcal{K}_n}} \mathcal{K}_n(y), \quad \overline{f} = \int_{\mathfrak{L}^d_0 \times \mathbb{R}^{3d}} f(q, p) \pi_0(q, p) dq dp.
\]
Further, we have
\[ \| E^{0,y} [f(X_{kT+\theta})] - \tilde{f}(\theta) \| \leq C_n e^{-\lambda_{n}kT} \| f - \tilde{f}(\theta) \|_{L_{K_n}^{\infty}} E^{0,y} [K_n(X_{\theta})]. \] (22)

We compute an upper bound on \( E^{0,y}[K_n(X_{\theta})] \) as follows: Then, we get an upper bound on \( E^{0,y}[K_n(x_{\theta})] \) by using Grönwall’s inequality:
\[ E^{0,y}[K_n(x_{\theta})] \leq e^{-\alpha_{n}\theta} K_n(y) + \frac{b_{n}}{a_{n}} \left( 1 - e^{-\alpha_{n}\theta} \right) K_n(y) + \frac{b_{n}}{a_{n}}. \]

Plugging the latter result in (22), we have
\[ \| E^{0,y} [f(X_{kT+\theta})] - \tilde{f}(\theta) \| \leq C_n e^{-\lambda_{n}kT} \| f - \tilde{f}(\theta) \|_{L_{K_n}^{\infty}} \left( e^{-\alpha_{n}\theta} K_n(y) + \frac{b_{n}}{a_{n}} \right). \]

Defining \( \lambda_{n} \) by \( e^{-\lambda_{n}} = \frac{1}{a_{n}} \), we obtain the expected result by redefining \( C_n \to \left( 1 + \frac{b_{n}}{a_{n}} e^{\lambda_{n}T} \right): \)
\[ \| E^{0,y} [f(X_{kT+\theta})] - \tilde{f}(\theta) \| \leq C_n e^{-\lambda_{n}(kT+\theta)} \| f - \tilde{f}(\theta) \|_{L_{K_n}^{\infty}} \left( 1 + K_n(y) \right). \]
\[ \square \]

3.4.2 Convergence in Law of Large Numbers for \( (q_{kT+\theta}, p_{kT+\theta}) \)

We use Lemmas from the previous section and mainly [36] to show that \( (q_{kT+\theta}, p_{kT+\theta}) \) is a positive Harris recurrent chain. Thus, the Law of Large Numbers holds:

**Proposition 2** (Law of Large Numbers for the sampled chain) For any \( f \in L_{K_n}^{\infty}, \)
\[ \frac{1}{N} \sum_{k=1}^{N} f(q_{kT+\theta}, p_{kT+\theta}) \xrightarrow{N \to +\infty} \int_{L_{0}^{d} \times \mathbb{R}^{3d}} f(q, p) \nu(q, p) dqd \text{d}p \quad a.s., \] (23)
for all the initial conditions \((Q_0, P_0)\).

**Proof** Since \( (q_{kT+\theta}, p_{kT+\theta}) \) is regularized for all \( \theta \in T\mathbb{T} \), showing that the Law of Large Numbers converges for the Markov chain \((Q_k, P_k) \in L_{0}^{d} \times \mathbb{R}^{3d}\) when \( \theta = 0 \) is sufficient to establish the validity of (23) for all \( \theta \in T\mathbb{T}\). Corollary 1 from the previous Section shows that the chain \((Q_k, P_k)\) is irreducible with respect to the Lebesgue measure. Thus, the result from [37, Corollary 1] based on [36, p. 199] provides that the chain \((Q_k, P_k)\) is Harris recurrent. In addition as \( \nu(t, q, p) \) is positive using Lemma 8, it follows from [36, Theorem 17.0.1] that the Law of Large Numbers holds.
\[ \square \]

4 Conclusion

In this paper, we study the ergodicity of NELD under shear flow and planar elongational flow using respectively LE and KR Periodic boundary conditions. This is essentially formulated in Proposition 1 where, after showing existence and uniqueness of the limit cycle using a Lyapunov function and a minorization condition, we established the exponential convergence of the Markov chain generated by the NELD equation given all the initial conditions. It will be interesting to establish the convergence analysis for the three dimensional diagonalizable
incompressible flow cases using the R–KR [20] algorithm or the GenKR [21, 22] algorithm. However additional analysis will be needed since these PBCs have geometry that is not as simple as the current case studied.

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Declarations

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