PDMP characterisation of event-chain Monte Carlo algorithms for particle systems

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Abstract

Monte Carlo simulations of systems of particles such as hard spheres or soft spheres with singular kernels can display around a phase transition prohibitively long convergence times when using traditional Hasting-Metropolis reversible schemes. Efficient algorithms known as event-chain Monte Carlo were then developed to reach necessary accelerations. They are based on non-reversible continuous-time Markov processes. Proving invariance and ergodicity for such schemes cannot be done as for discrete-time schemes and a theoretical framework to do so was lacking, impeding the generalisation of ECMC algorithms to more sophisticated systems or processes. In this work, we characterize the Markov processes generated in ECMC as piecewise deterministic Markov processes. It first allows us to propose more general schemes, for instance regarding the direction refreshment. We then prove the invariance of the correct stationary distribution. Finally, we show the ergodicity of the processes in soft- and hard-sphere systems, with a density condition for the latter.

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I. INTRODUCTION

Since the introduction of the Markov-chain Monte Carlo method (MCMC) [1], continuous particle systems evolving according to pairwise and central interactions have filled the part of both an important scientific motivation in itself and a formidable testbed and accelerator for MCMC development. Indeed, despite the simplicity of the interactions (e.g. hardcore, Lennard-Jones or powerlaw-decaying repulsions), the behaviours displayed by these systems are rich. They are however described by high-dimensional integrals, whose analytical resolution remains ouf of reach. Their MCMC numerical evaluation by a discrete sum over a large collection of system configurations has thus been an important focus of the computational physics [2–4] as well as of the probability community [5] for example. MCMC methods rely on Markov processes to produce system configurations in a random sequence. Such sequence should preferrably exhibit the least correlations possible between two succeeding states, in order to minimise the asymptotic error on the integral estimation [6]. Typically, reversible Markov processes rely on move rejections for correctness and display a diffusive dynamics [7]. They then show important correlations, which can furthermore be greatly increased in presence of critical slowing down phenoma at phase transitions [8]. The development of MCMC methods which can break free from any diffusive behavior and slow physical time scales has thus been instrumental to reach system sizes big enough to control finite-size effects, as achieved by the rejection-free cluster algorithms in lattice-spin sytems [9, 10].

In continuous particle systems, the lack of a natural involution symmetry, necessary to ensure the reversibility and correctness of cluster methods, has led to the development of non-reversible MCMC methods[11, 12], among which Event-Chain Monte Carlo (ECMC) [13, 14]. By producing persistent global moves forming up a sequence of ballistic trajectories of single particles, the accelerations brought by ECMC allowed to resolve the heavily-debated question of the scenario for the melting of bidimensional hard disks [4, 15] and to investigate the same phenomenon with power-law decaying interactions [16]. These successes have thus motivated the application of ECMC algorithms to other classic systems in statistical physics (polymers [17], continuous spins [18, 19]) and started the development of generalized and accelerated ECMC variant (e.g. generalisation to n-body interactions [20], Forward ECMC [21], Newtonian ECMC [22, 23]). Stemming from this research line in statistical physics, similar

non-reversible Markov processes as the ones used in ECMC were applied to sampling problems in statistical Bayesian inference [24, 25] and were mathematically framed as Piecewise Deterministic Markov Processes (PDMP) [26, 27], leading to the general name of Piecewise Deterministic Monte Carlo (PDMC). Piecewise deterministic Markov processes have already been studied in queuing theory [27], biology [28, 29] and physics, see for example [30] for a review of a variety of PDMP applications. Now under focus in Bayesian statistics, efforts have been made towards a rigorous analysis of the properties of invariance, ergodicity and convergence of the processes found in PDMC [25, 31, 32].

In this work, we push this analytical effort and characterize the PDMP generated by ECMC in bidimensional disk systems. This allows to prove the invariance of the commonly-used schemes and gives a framework to do so for future algorithmic upgrades or applications. In particular, we show how the refreshment of the direction of the ballistic trajectories can be described by a boundary effect instead of a Poisson process, as commonly found in PDMC in the statistics literature. Doing so reflects better the algorithmic implementations as done in physics, as fixed-time refreshment schemes can greatly ease the computations. Furthermore, this allows us to give conditions on valid refreshment schemes, opening up to a larger choices of strategies than the exponential refreshment generated by a Poisson process or the uniform one as obtained by a fixed-time scheme. Finally, we study the ergodicity property of those processes for soft and hard disks. We use the Harris recurrence theory [33–35] starting from the uniform continuity property of the process [36, 37] and adapting the proof done in [38]. In presence of hardcore repulsions, even at low densities and for reversible Markov chains, proving ergodicity is a hard problem, first starting with a usually simple task such as showing irreducibility. Here, we follow the approach used in [5] for a reversible Markov chain, so as to show connectivity of the state space, but obtain ergodicity for higher densities.

In the present paper, we start by introducing the ECMC method and its implementation in disk systems in Section II. We then present the PDMP characterisation of ECMC and in particular of its refreshment strategy in Section III. This allows us to derive the invariance in Section IV through a generator characterization and the ergodicity in Section V.

II. EVENT-CHAIN MONTE CARLO FOR SOFT- AND HARD-SPHERE SYSTEMS

A. Soft- and hard-sphere systems

Event-chain Monte Carlo algorithms were first developed for hard- and soft-sphere systems in a periodic bidimensional box [13, 14]. Both systems share a common description, and henceforth we will only use subscripts S or H when making statements restricted to respectively the soft- or hard-sphere systems.

For both systems, a configuration of the $N \in \mathbb{N}$ spheres of radius $\sigma \in \mathbb{R}_+^*$ in a periodic box of length $L \in \mathbb{R}_+^*$ is completely characterized by the sphere positions $x = (x_i = (x_{i,0}, x_{i,1}))_{i\in[\![1,N]\!]} \in \Omega(N) \subset (\mathbb{R}/L\mathbb{Z})^{2N}$. The configuration set $\Omega(N)$ of valid configurations is an open set, completely defined according to the excluded minimal pairwise distance $d_{\text{pair}} \in \mathbb{R}_+$, as,

$$\Omega(N) = \{x \in (\mathbb{R}/L\mathbb{Z})^{2N}; \forall (i,j) \in [\![1,N]\!]^2, i \neq j, (x_i, x_j) \in \Omega_{\text{pair}}\}, \tag{1}$$

with Ω_{pair} the open set of valid pair of positions,

$$\Omega_{\text{pair}} = \{(x, x') \in (\mathbb{R}/L\mathbb{Z})^4; d(x, x') > d_{\text{pair}}\} \tag{2}$$

where d is the L-periodic distance $d : (\mathbb{R}/L\mathbb{Z})^4 \to \left[0, \frac{L}{\sqrt{2}}\right]$, which corresponds for any pair of positions $(x = (x_0, x_1), x' = (x'_0, x'_1)) \in (\mathbb{R}/L\mathbb{Z})^4$ to the minimal distance between all their periodic copies,

$$d(x, x') = \sqrt{\sum_{k=0}^{1} \min(|x_k - x'_k|, L - |x_k - x'_k|)^2}. \tag{3}$$

The configuration set $\Omega(N)$ presents the boundary,

$$\partial\Omega(N) = \{x \in (\mathbb{R}/L\mathbb{Z})^{2N}; \forall (i,j) \in [\![1,N]\!]^2, i \neq j, (x_i, x_j) \in \Omega_{\text{pair}} \cup \partial\Omega_{\text{pair}}\} \setminus \Omega,$$

with

$$\partial\Omega_{\text{pair}} = \{(x, x') \in (\mathbb{R}/L\mathbb{Z})^4; d(x, x') = d_{\text{pair}}\}.$$

Form now on, we will drop the dependence in N of $\Omega(N)$ for simplicity, when there is no possible confusion on the number N of spheres involved.

Sphere configurations then follow at equilibrium a Boltzmann distribution,

$$\forall x \in \Omega, \pi(x) \propto \prod_{1 \leq i < j \leq N} \exp[-\beta u(d(x_i, x_j))], \tag{4}$$

with β the inverse temperature, set to 1 in the following, and $u :]d_{\text{pair}}, +\infty[\to \mathbb{R}_+$ a continuous and piecewise differentiable function, which codes for the potential energy arising from the pairwise interactions and depending only on the pairwise periodic distance. We define by continuity the extended distribution $\tilde{\pi}$,

$$\begin{aligned} \forall x \in \Omega \cup \partial\Omega, \tilde{\pi}(x) \propto & \lim_{r \to d_{\text{pair}}^+} \exp\left[-\beta u(r) \textstyle\sum_{1 \leq i < j \leq N} \mathbb{1}_{\partial\Omega_{\text{pair}}}((x_i, x_j))\right] \\ & \times \exp\left(-\beta \textstyle\sum_{1 \leq i < j \leq N} u(d(x_i, x_j))(1 - \mathbb{1}_{\partial\Omega_{\text{pair}}}((x_i, x_j)))\right] \end{aligned} \tag{5}$$

Explicitely, for soft spheres,

$$\begin{cases} \Omega_S = (\mathbb{R}/L\mathbb{Z})^{2N} \setminus \{x \in (\mathbb{R}/L\mathbb{Z})^{2N} \, ; \exists (i,j) \in [\![1, N]\!]^2, i \neq j, d(x_i, x_j) = 0\} \\ d_{S,\text{pair}} = 0 \\ \Omega_{S,\text{pair}} = \{(x, x') \in (\mathbb{R}/L\mathbb{Z})^2; d(x, x') > 0\}, \end{cases} \tag{6}$$

and the interactions are ruled for any pair interdistance $r \in \mathbb{R}_+^*$,by

$$u_S(r) = \begin{cases} \left(\frac{\sigma}{r}\right)^\gamma - \left(\frac{\sigma}{r_c}\right)^\gamma & \text{for } r \leq r_c \\ 0 & \text{otherwise} \end{cases}, \tag{7}$$

with $r_c \in \left]0, \frac{L}{2}\right]$ a cut-off length. It leads to the soft-sphere equilibrium distribution π_S and corresponding extended one $\tilde{\pi}_S$,

$$\begin{cases} \forall x \in \Omega_S, & \pi_S(x) \propto \prod_{1 \leq i < j \leq N} \exp[-\beta u_S(d(x_i, x_j))] \\ \forall x \in \Omega_S \cup \partial\Omega_S, & \tilde{\pi}_S(x) = \mathbb{1}_\Omega(x)\pi(x). \end{cases} \tag{8}$$

Now, for hard spheres,

$$\begin{cases} \Omega_H = (\mathbb{R}/L\mathbb{Z})^{2N} \setminus \{x \in (\mathbb{R}/L\mathbb{Z})^{2N}; \exists (i,j) \in [\![1, N]\!]^2, i \neq j, d(x_i, x_j) \leq 2\sigma\} \\ d_{H,\text{pair}} = 2\sigma \\ \Omega_{H,\text{pair}} = \{(x, x') \in (\mathbb{R}/L\mathbb{Z})^2; d(x, x') > 2\sigma\}. \end{cases} \tag{9}$$

For hard-sphere systems, there is no interaction apart from the hard-core repulsions which are already encoded in the non-zero $d_{H,\text{pair}}$, so that we have for any $r \in]2\sigma, +\infty[$,

$$u_H(r) = 0, \tag{10}$$

and the hard-sphere equilibrium distribution π_H (resp. the extended distribution $\tilde{\pi}_H$) is then the uniform one on Ω_H (resp. on $\Omega_H \cup \partial\Omega_H$),

$$\begin{cases} \forall x \in \Omega_H, & \pi_H(x) \propto \mathbb{1}_{\Omega_H}(x) \\ \forall x \in \Omega_H \cup \partial\Omega_H, & \tilde{\pi}_H(x) \propto \mathbb{1}_{\Omega_H \cup \partial\Omega_H}(x). \end{cases} \tag{11}$$

B. Event-chain Monte Carlo

Sampling configurations in a set Ω according to a target probability distribution π is achieved in a MCMC method through the recursive application of a Markov kernel, denoted as K, such that π is left invariant, equivalently, such that the global balance condition $\pi K = \pi$ is satisfied, i.e.,

$$\int_{x' \in \Omega} \pi(\mathrm{d}x') K(x', \mathrm{d}x) = \int_{x' \in \Omega} \pi(\mathrm{d}x) K(x, \mathrm{d}x') = \pi(dx). \tag{12}$$

The seminal Metropolis algorithm [1], was first developed for sampling from sphere systems by enforcing a sufficient condition to the global balance, the detailed balance, i.e. $\pi(\mathrm{d}x')K(x', \mathrm{d}x) = \pi(\mathrm{d}x)K(x, \mathrm{d}x')$ for every pair of configurations $(x, x') \in \Omega$, through the following choice for K,

$$K(x, \mathrm{d}x') = q(x'|x)a(x'|x)\mathrm{d}x' + \left(1 - \int_{y \in \Omega} q(y|x)a(y|x)\mathrm{d}y\right) \delta_{x=x'}, \tag{13}$$

where q identifies with the proposal distribution, a common choice (e.g. as studied in [5]) verifying $\int_\Omega q(x'|x)\mathrm{d}x' = 1$ being,

$$q(x'|x) = \frac{1}{h^2 \mathrm{vol}(B_1)} \mathbb{1}_{B_1}\left(\frac{x - x'}{h}\right), \tag{14}$$

with $h \in]0, 1]$ and B_1 the unit ball of $\mathbb{R}^2$, and where a identifies with the acceptance rate,

$$a(x'|x) = \min\left(1, \frac{\pi(x')}{\pi(x)}\right), \tag{15}$$

generalized in [39] to,

$$a(x'|x) = \min\left(1, \frac{q(x|x')}{q(x'|x)} \frac{\pi(x')}{\pi(x)}\right), \tag{16}$$

for an asymmetric proposal distribution q.

Event-chain Monte Carlo algorithms [13, 14] were developed so that only the necessary condition of global balance is satisfied, while the detailed-balance one is broken. This is achieved by generating a non-reversible Markov process through the exploitation of the pairwise translational invariance or mirror symmetry for any pair of spheres $(i,j) \in [\![1,N]\!]^2$, i.e. $\nabla \cdot u(d(x_i,x_j)) = 0$ (resp. $\nabla \cdot H(d(x_i,x_j)) = 0$ in the limit of hard spheres systems, H being the Heaviside function). ECMC schemes are now also generalized to systems presenting general n-body interactions by exploiting the global translational invariance ($\nabla \cdot u = 0$), see [20].

The initial introduction of these methods relied on taking an infinitesimal limit and using continuous-time Markov processes, while extending the state x to (x,v), with v an auxiliary variable, commonly referred to as the *lifting* variable, following [40]. The purpose of such variable is to introduce persistence into the proposal distribution while ensuring the process remains Markovian. In bidimeniosal sphere systems, the state space Ω is thus extended to $\Omega \times \mathcal{V}$ with $\mathcal{V} = \{(1,0),(0,1)\} \times [\![1,N]\!]$, associated with the measure $\mu_{\mathcal{V}} = \mu_{\mathcal{D}} \otimes \mu_N$ where $\mu_{\mathcal{D}}$ and μ_N are the counting measures over $\mathcal{D} = \{(1,0),(0,1)\}$ and $[\![1,N]\!]$ respectively. The Markov process should then be targetting as stationary distribution $\pi \otimes \mu_{\mathcal{V}}$. For any pair of configurations $(x, v = (e,i)), (x', v' = (e',i')) \in (\Omega \times \mathcal{V})^2$ the acceptance is set to 1 (i.e. $a((x',v')|(x,v)) = 1$). The auxiliary variable $v = (e,i)$ codes for proposing moves of the i-th sphere along the direction e, setting,

$$
\begin{aligned}
&q_\epsilon((x',(e',i')))|(x,(e,i))) \\
&= (1-r)\delta(e-e')\delta(i-i')\delta(x_i+\epsilon e - x_i')\prod_{j\neq i}\delta(x_j-x_j')\prod_{j\neq i}p_\epsilon(x_i,x_j,e) && \text{(physical move)} \\
&+ (1-r)\delta(e-e')(1-\delta(i-i'))\delta(x-x')(1-p_\epsilon(x_i,x_{i'},e))\prod_{j\neq i,i'}p_\epsilon(x_i,x_j,e) && \text{(lifting move)} \\
&+ r\delta(x-x')\mu_{\mathcal{V}}(\mathrm{d}e',\mathrm{d}i') && \text{(refreshment)}
\end{aligned}
\tag{17}
$$

with $\epsilon \in \mathbb{R}_+^*$ the step magnitude, $0 < r < 1$, the refreshment probability and p_ϵ the *factor* probability [14] for $(x_i,x_j) \in \Omega_{\text{pair}}$,

$$
p_\epsilon(x_i,x_j,e) = \min\left(1, \mathbb{1}_{\Omega_{\text{pair}}}((x_i+\epsilon e, x_j))\frac{\exp(-u(x_i+\epsilon e, x_j))}{\exp(-u(x_i,x_j))}\right), \tag{18}
$$

which builds up a factorized variant of the usual Metropolis probability (15) and which also satisfies detailed balance in a *skewed* form, as

$$\exp(-u(x_i,x_j))\prod_{j\neq i}p_\epsilon(x_i,x_j,e)=\exp(-u(x_i+\epsilon e,x_j))\prod_{j\neq i}p_\epsilon(x_i+\epsilon e,x_j,-e). \tag{19}$$

The idea behind this choice for the proposal distribution q_ϵ is to propose *physical* moves (i.e. updates of x) by moving the i-th sphere by $+\epsilon e$ until a *rejection* triggered by another sphere i' through its pairwise interaction with i occurs. Then, the physical move is replaced by a *lifting* one (i.e update of v from $v=(e,i)$ to $v'=(e,i')$) and the i'-th sphere is now the one being updated by $+\epsilon e$ increment. Eventually, the proposal distribution includes a *refreshment* term in order to ensure irreducibility, which can also halt the persistent physical moves to update v.

Nonetheless, in spite of the property (19) of the factor probabiliy p_ϵ, the proposal distribution (17) does not define a valid MCMC scheme for finite ϵ since *rejections* of the physical move from multiple pairs at once are not accounted for, i.e.,

$$\int \mathrm{d}x'\mathrm{d}e'\mathrm{d}i' q_\epsilon((x',(e',i'))|(x,(e,i)))=1-(1-r)\Big[1-\sum_{i'\neq i}\Big(1-\frac{N-2}{N-1}p_\epsilon(x_i,x_{i'},e)\Big)\prod_{j\neq i,i'}p_\epsilon(x_i,x_j,e)\Big] < 1. \tag{20}$$

A solution is to add the following lifting move,

$$(1-r)\delta(e+e')\delta(i-i')\delta(x-x')\sum_{k=2}^{N-1}\sum_{1\leq j_1<\cdots<j_k\leq N}\prod_{m=1}^{k}(1-p_\epsilon(x_i,x_{j_m},e))\prod_{j\notin(i,j_1,\ldots,j_k)}p_\epsilon(x_i,x_j,e),$$

which replaces the *rejected* physical move by a flip of e. This however comes at the cost of extending the set $\mathcal{D}$ to include backward moves, i.e. $\{(-1,0),(0,-1)\}$. Fortunately, in the infinitesimal limit $\epsilon\to 0$ corresponding to the continuous-time limit, this multiple rejection term is of order $O(\epsilon^2)$, as $p_\epsilon(x_i,x_j,e)\overset{\epsilon\to 0}{\sim}1-\epsilon\langle\nabla u(x_i,x_j),e\rangle_+$[48], whereas the other terms in the proposal distribution q_ϵ are at least of order $O(\epsilon)$,

$$\begin{aligned}
&q_\epsilon((x',(e',i')))|(x,(e,i)))\\
&=(1-r)\delta(e-e')\delta(i-i')\delta(x_i'+\epsilon e-x_i)\left(\prod_{j\neq i}\delta(x_j'-x_j)\right)\left(1-\epsilon\sum_{j\neq i}\langle\nabla u(x_i,x_j),e\rangle_+\right)\quad,\\
&+(1-r)\delta(e-e')(1-\delta(i-i'))\delta(x-x')\epsilon\langle\nabla u(x_i,x_{i'},e\rangle_+ + r\delta(x-x')\mu_{\mathcal{V}}(\mathrm{d}e',\mathrm{d}i')+O(\epsilon^2)
\end{aligned} \tag{21}$$

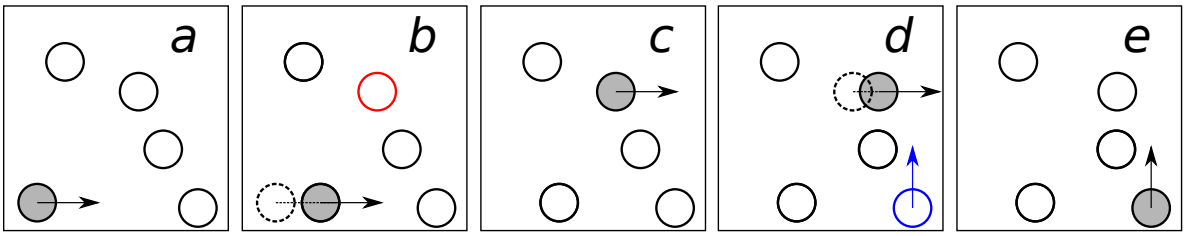

FIG. 1: Illustration of moves produced from an ECMC algorithm in a system of soft spheres. The grey sphere, set by the label i, is updated along the direction $e = (1, 0)$ (physical move, a) until a first event occurs, here with the j-th sphere (in red, b). The label then is updated from i to j (lifting move, c) and it is the j-th sphere which is now being updated along e before being stopped at a refreshment time (d), where a new label and direction (in blue, d) is resampled and from which a new chain of physical and lifting moves is produced (e).

leading in this infinitesimal limit to

$$\int_{\Omega\times\mathcal{V}} q_\epsilon((x',v')|(x,v))\mathrm{d}x'\mathrm{d}v' = \int_{\Omega\times\mathcal{V}} q_\epsilon((x,v)|(x',v'))\mathrm{d}x'\mathrm{d}v' = 1 - O(\epsilon^2).$$

Thus, Markov processes generated by ECMC are composed of chains of ballistic trajectories following the direction e of spheres successively set by the label i, updated at *events* ruled by Poisson clocks stemming from the continuous-time limit and of total rate $\sum_{j\neq i}\langle\nabla u(x_i, x_j)\cdot e\rangle_+$. An illustration can be found in Figure 1. As the acceptance function a is always returning 1, these schemes have been referred to as rejection-free. A pseudocode implementation is exhibited in Algorithm 1 and shows how to sample the sequence of ballistic trajectories separated by the Poisson events.

As can be seen from the above informal derivation, the description of ECMC schemes in term of an infinitesimal limit of some finite schemes may appear cumbersome. In the next section, after introducing piecewise deterministic Markov processes (PDMP), we show how they offer a robust analytical framework for the analytical description of such scheme, making the derivation of some properties, e.g. invariance of a given distribution, more straightforward and allowing to properly describe schemes relying on a fixed-time refreshment.

Algorithm 1 ECMC implementation for soft disks outputting a set S of n samples

Set $S = \{\}$
Set $x \in \Omega$
for $k = 1$ to $k = n$ **do**
  Sample uniformly $(e, i) \in \{(1,0),(0,1)\} \times [\![1, N]\!]$
  Set E_R an exponential random variable with parameter 1
  Set $\Delta_R = -\frac{1}{r}\ln E_R$
  while $\Delta_R > 0$ **do**
    for $j = 1$ to $j = N$, $j \neq i$ **do**
      Set E_j an exponential random variable with parameter 1
      Compute Δ_j such that $\int_0^{\Delta_j} \langle \nabla u(x_i + se, x_j), e\rangle_+ \mathrm{d}s = -\ln(E_j)$
    end for
    Set $\Delta_{\mathrm{Ev}}, j_{\mathrm{Ev}} = \min_{j\neq i}(\Delta_j), \mathrm{argmin}_{j\neq i}(\Delta_j)$, $x_i \leftarrow x_i + e\min(\Delta_R, \Delta_{\mathrm{Ev}})$
    if $\Delta_R > \Delta_{\mathrm{Ev}}$ **then**
      Set $(e, i) \leftarrow (e, j_{\mathrm{Ev}})$
      Set $\Delta_R \leftarrow \Delta_R - \Delta_{\mathrm{Ev}}$
    end if
  end while
  Add x to S
end for
  return S

III. PIECEWISE DETERMINISTIC MARKOV PROCESSES IN ECMC ALGORITHMS FOR MULTIPARTICLE SYSTEMS

A. Definition of a PDMP

Piecewise Deterministic Markov Processes have been formalized by Davis in his seminal paper [26] and book [27]. Briefly, and to fit to our setting, a PDMP $\{X_t, V_t\}_{t\geq 0}$, defined on a space $\Omega \times \mathcal{V}$, refers to a Markov process composed of ballistic trajectories whose succession is ruled by a Poisson process. In more details, once an initial state $(X_0, V_0) \in \Omega \times \mathcal{V}$ is set, the process evolves ballistically according to a deterministic differential flow $(\phi_t)_{t\geq 0}$, until an event occurs or the process reaches the domain boundary. Events are characterized by their rate $\lambda : \Omega \times \mathcal{V} \to \mathbb{R}_+$ and a Markov kernel Q, defined on $(\Omega \times \mathcal{V}, \mathcal{B}(\Omega \times \mathcal{V}))$, which updates

$\{X_t, V_t\}$. At the boundary, for $(x, v) \in \partial\Omega \times \mathcal{V}$, the differential flow would cause an exit from $\Omega \times \mathcal{V}$ for the subset $\Gamma^* = \{(z, v') \in \partial\Omega \times \mathcal{V}; \exists (t, (x, v)) \in \mathbb{R}_+ \times \Omega \times \mathcal{V}, \phi_t(x, v) = (z, v')\}$, referred in the following as the exit boundary. On this exit boundary, it is then another Markov kernel Q^b, called the boundary kernel and defined on $(\Gamma^*, \mathcal{B}(\Omega \times \mathcal{V}))$, which updates the process.

For $(x, v) \in (\Omega \times \mathcal{V})$ and f in a suitable functional space, say continuously differentiable function as an example [49], on $(\Omega \cup \partial\Omega) \times \mathcal{V}$, the infinitesimal generator (or strong generator [27]). associated with a PDMP is,

$$\mathcal{A}f(x, v) = D_\phi f(x, v) + \lambda(x, v) \left(\int_{\Omega \times \mathcal{V}} f(x', v') Q((x, v), \mathrm{d}x' \mathrm{d}v') - f(x, v) \right) \tag{22}$$

with D_φ defined as,

$$D_\phi f(x, v) = \begin{cases} \lim_{t \to 0^+} \frac{f(\phi_t(x,v)) - f(x,v)}{t} & \text{if this limit exists.} \\ 0 & \text{otherwise.} \end{cases} \tag{23}$$

Now, on the exit boundary $(x, v) \in \Gamma^*$, we have the boundary condition,

$$f(x, v) = \int_{\mathcal{V}} f(x', v') Q^b((x, v), \mathrm{d}x' \mathrm{d}v'). \tag{24}$$

Note that it is actually not necessary to specify Q^b for boundary points which the process never actually hits and in the following we will note this set of reachable exit boundary points $\Gamma = \{(z, v') \in \Gamma^*; \exists (x, v) \in \Omega \times \mathcal{V}, P(\text{No event occured before reaching } (z, v') \text{ starting from } (x, v)) > 0\}$, as in [26].

B. Generator characterisation of PDMP in ECMC algorithms for multiparticle systems

We now characterize the stochastic processes produced by ECMC algorithms as PDMP, in the first and most common forms of ECMC schemes, as introduced in [13, 14]. A PDMP characterisation can be done either algorithmically, as done up until now in statistical physics and as presented in section II B, or by its generator as presented in the previous section and as done more recently in the context of Bayesian inference [24, 38]. In this section, we exhibit a generator characterisation of PDMP in ECMC, which is particularly helpful to prove the invariance of a given probability distribution.

We first present a generator description common to previous PDMP characterisation of sampling algorithms and which is only valid for refreshment relying on a Poisson process. We then introduce another valid writing, which deals with the refreshment part as a boundary effect. In that way, it allows for more freedom in its choice, while better reflecting the algorithmic implementation based on fixed-time refreshment schemes as popularly used in statistical physics.

1. Standard exponential refreshment strategy

Differential flow ϕ. After extension of the state space from $x \in \Omega \sim \pi$ to $(x, v) \in \Omega \times \mathcal{V} \sim \pi \otimes \mu_{\mathcal{V}}$, the process (X_t, V_t) generated through ECMC is first characterized by the following differential flow ϕ_t for all $(x, v) \in \Omega \times \mathcal{V}$ and $t \geq 0$,

$$\phi_t(x = (x_k)_{k\in[\![1,N]\!]}, v = (e, i)) = ((x_1, \dots, x_{i-1}, x_i + te, x_{i+1}, \dots, x_N), v = (e, i)). \tag{25}$$

This differential flow, translating the i-th sphere along e is interrupted at events, ruled by the pairwise interactions and refreshment, and where only the lifting variable is updated through the Markov kernel Q.

Markov kernel Q. For all $(x = (x_k)_{k\in[\![1,N]\!]}, v = (e, i)) \in \Omega \times \mathcal{V}$ and $A \in \mathcal{B}(\Omega \times \mathcal{V})$,

$$Q((x, (e, i)), A) = \sum_{\substack{k=1 \\ k\neq i}}^{N} \frac{\lambda_k(x, (e, i))}{\lambda(x, (e, i))} \int_{\mathcal{V}} \mathbb{1}_A((x, (e', i')))Q_k((e, i), (\mathrm{d}e', \mathrm{d}i')) + \frac{\lambda_r}{\lambda(x, (e, i))}\mu_{\mathcal{V}}(A), \tag{26}$$

where, for all $k \in [\![1, N]\!]$,$k \neq i$,

$$\lambda_k(x, (e, i)) = \langle \nabla_{x_i} u(x_i, x_k), e\rangle_+ \tag{27}$$

is the (ik)-pairwise event rate, $\lambda_r \in \mathbb{R}_+$ is a homogeneous refreshment rate, making the total event rate now $\lambda = \sum_{\substack{k=1 \\ k\neq i}}^{N} \lambda_k + \lambda_r$, and $(Q_k)_{k\in[\![1,N]\!]}$ are Markov kernels defined on $\mathcal{V} \times \mathcal{B}(\mathcal{V})$, so that, for all $e \in \{(1, 0), (0, 1)\}$ and $(i, i') \in [\![1, N]\!]^2$,

$$Q_k((e, i), (\mathrm{d}e', \mathrm{d}i')) = \delta(e - e')\delta(k - i')\mathrm{d}e'\mathrm{d}i', \tag{28}$$

thus coding for the k-th sphere being the one translated along e after an (ik)-pairwise event occured.

Boundary Markov kernel Q^b. For sphere systems, the exit boundary is

$$\Gamma^* = \{(x,(e,i)) \in \partial\Omega \times \mathcal{V}; \exists j \in [\![1,N]\!], (x_i,x_j) \in \Gamma^e_{\text{pair}}\}, \tag{29}$$

with,

$$\Gamma^e_{\text{pair}} = \{(x,x') \in \partial\Omega_{\text{pair}}; \langle \nabla_x d(x,x'), e\rangle \leq 0\}. \tag{30}$$

and, given (25), (26), (27) and (28), the corresponding set of reachable exit boundary points Γ can be determined. For $(x,v) \in \Gamma$, the boundary Markov kernel Q^b is then of the following form, with $A \in \mathcal{B}(\Omega \times \mathcal{V})$,

$$Q^b((x,(e,i)),A) = \sum_{\substack{k=1\\k\neq i}}^{N} \frac{\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)}{\sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)} \int_{\mathcal{V}} \mathbb{1}_A((x,(e',i')))Q_k((e,i),(\mathrm{d}e',\mathrm{d}i')), \tag{31}$$

with the $\{Q_k\}_{k\in[\![1,N]\!]}$ the Markov kernels defined on $(\mathcal{V},\mathcal{B}(\mathcal{V}))$ as in (28). Note that this choice of Q^b can be applied in case of tangential ($\langle \nabla_{x_i} d(x_i,x_k), e\rangle = 0$) or multiple collisions, but we could have excluded these points from the definition of Q^b as the set they form is small and does not impact the invariant stationary distribution. Thus, for $(x,(e,i))$ not at a tangential collision, we could also have proposed the following choice,

$$\tilde{Q}^b((x,(e,i)),A) = \sum_{\substack{k=1\\k\neq i}}^{N} \frac{n_-(x_i,x_k,e)}{\sum_{\substack{k=1\\k\neq i}}^{N} n_-(x_i,x_k,e)} \int_{\mathcal{V}} \mathbb{1}_A((x,(e',i')))Q_k((e,i),(\mathrm{d}e',\mathrm{d}i')),$$

with $n_-(\cdot)$ the unnormalized negative pairwise normal component,

$$\begin{aligned} n_-(x_i,x_k,e) &= 1_{\Gamma^e_{\text{pair}}}(x_i,x_k)\langle -\nabla_{x_i} d(x_i,x_k), e\rangle \\ &= \mathbb{1}_{\partial\Omega_{\text{pair}}}(x_i,x_k)\langle \nabla_{x_i} d(x_i,x_k), e\rangle_-, \end{aligned} \tag{32}$$

which differs only from (31) in a multiple collision situation, where it is handled as when dealing with $n-$body interactions as done in [20]. We expect these different choices to have an impact while studying out-of-equilibrium processes though, but such consideration is delayed for future work. We also refer the reader to the recent work of [41] for a more general consideration into PDMP samplers for piecewise continuous densities.

Eventually, it leads to the following condition on the boundary, for $(x,(e,i)) \in \Gamma$ and f a continuous and continuously differentiable function on $(\Omega \cup \partial\Omega) \times \mathcal{V}$,

$$f(x,(e,i)) = \sum_{\substack{k=1\\k\neq i}}^{N} f(x,(e,k)) \frac{\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)}{\sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)}. \tag{33}$$

Soft-sphere systems. All in all, the following infinitesimal generator associated with PDMP generated by ECMC for soft-sphere systems comes down to, with f a continuous and continuously differentiable function on $(\Omega_S \cup \partial\Omega_S) \times \mathcal{V}$ and $(x,(e,i)) \in \Omega_S \times \mathcal{V}$,

$$\begin{aligned}\mathcal{A}_S f(x,(e,i)) = \langle \nabla_{x_i} f(x,(e,i)), e\rangle + \sum_{k=1}^{N} \langle \nabla_{x_i} u_S(x_i,x_k), e\rangle_+ \{f(x,(e,k)) - f(x,(e,i))\} \\ + \lambda_r \left(\int_{\mathcal{V}} f(x,(e',i')) \mathrm{d}\mu_{\mathcal{V}}((e',i')) - f(x,(e,i)) \right).\end{aligned} \tag{34}$$

For soft-sphere systems, Γ_S is empty, as the event rate diverges as a pair distance goes to $d_{\text{pair}} = 0$ (27), and the boundary Markov kernel is without any object.

Hard-sphere systems. For hard-sphere systems, the infinitesimal generator associated, with f a continuous and continuously differentiable function on $(\Omega_H \cup \partial\Omega_H) \times \mathcal{V}$ and $(x,(e,i)) \in \Omega_H \times \mathcal{V}$,

$$\mathcal{A}_H f(x,(e,i)) = \langle \nabla_{x_i} f(x,(e,i)), e\rangle + \lambda_r \left(\int_{\mathcal{V}} f(x,(e',i')) \mathrm{d}\mu_{\mathcal{V}}((e',i')) - f(x,(e,i)) \right). \tag{35}$$

For hard-sphere systems, $\Gamma_H = \Gamma_H^*$, as the events can only be triggered by refreshments and they do not impact a point reachability. Then, for $(x,v) \in \Gamma_H$, the boundary Markov kernel is the one defined in (31) and eventually leading to the condition (33) on the reachable exit boundary Γ_H. Thus the hardcore repulsions are only appearing as boundary effects.

2. Boundary refreshment strategy

The PDMP description where the refreshment part is treated as part of the jump process is the most common one. It can however not be used to study ECMC implementations where the refreshment process is not an exponential process. For instance, the fixed-time refreshment is a common and useful practice in statistical physics, all the more while dealing with periodic boundaries. It can also alleviate some difficulties in the computation of the event times set by the pairwise rates $(\lambda_k)_{k\in[\![1,N]\!]}$.

Therefore we now explain how to treat the refreshment as a boundary effect by adding an additional variable $l \in \mathcal{L}$, with $\mathcal{L} =]0,+\infty[$, $\partial\mathcal{L} = \{0\}$, associated with the measure μ_L, extended by continuity to $\tilde{\mu}_L$ on $\mathcal{L} \cup \partial\mathcal{L}$. The state space Ω is now extended to $\Omega \times \mathcal{L} \times \mathcal{V}$ and the process (X_t, L_t, V_t) now targets as a stationary distribution $\pi \times \mu_L \times \mu_{\mathcal{V}}$. We then discuss a broader range of possible refreshment strategies.

Differential flow. The differential flow φ_t for all $(x, l, (e, i)) \in \Omega \times \mathcal{L} \times \mathcal{V}$ and $t \geq 0$ is now

$$\varphi_t(x, l, (e, i)) = ((x_1, \dots, x_i + te, \dots, x_N), l - t, (e, i)). \tag{36}$$

Markov kernel Q. The Markov kernel Q is, for all $(x, l, (e, i)) \in \Omega \times \mathcal{L} \times \mathcal{V}$ and $A \in \mathcal{B}(\Omega \times \mathcal{L} \times \mathcal{V})$,

$$Q((x, l, (e, i)), A) = \sum_{\substack{k=1 \\ k \neq i}}^{N} \frac{\lambda_k(x, (e, i))}{\lambda(x, (e, i))} \int_{\mathcal{V}} \mathbb{1}_A((x, l, (e', i'))) Q_k((e, i), (\mathrm{d}e', \mathrm{d}i')), \tag{37}$$

where $\{\lambda_k(x, (e, i))\}_{k \neq i}$ are the pairwise rates defined in (27), the total event rate being now $\lambda = \sum_{k=1; k \neq i}^{N} \lambda_k$ and $(Q_k)_{k \in [\![1, N]\!]}$ are the Markov kernels defined on $\mathcal{V} \times \mathcal{B}(\mathcal{V})$ in (28).

Boundary kernel Q^b. We first define the set of exit boundary points,

$$\Gamma^* = \{(x, l, (e, i)) \in \partial(\Omega \times \mathcal{L}) \times \mathcal{V}; \exists j \in [\![1, N]\!], (x_i, x_j) \in \Gamma^e_{\text{pair}} \text{ or } l = 0\}$$

and Γ^e_{pair} is defined as in (30). The corresponding set Γ of reachable exit boundary points is included in Γ^*, and, for $(x, l, v) \in \Gamma \times \mathcal{V}$, the boundary Markov kernel Q^b is, with $A \in \mathcal{B}(\Omega \times \mathcal{L} \times \mathcal{V})$,

$$\begin{aligned} Q^b((x, l, (e, i)), A) &= \mathbb{1}_{\partial\mathcal{L}}(l) \int_{\mathcal{L}} 1_A((x, l', (e', i'))) R(l, \mathrm{d}l') \mathrm{d}\mu_{\mathcal{V}}((e', i')) \\ &+ (1 - \mathbb{1}_{\partial\mathcal{L}}(l)) \sum_{\substack{k=1 \\ k \neq i}}^{N} \frac{\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i, x_k)}{\sum_{\substack{k=1 \\ k \neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i, x_k)} \int_{\mathcal{V}} \mathbb{1}_A((x, l, (e', i'))) Q_k((e, i), \mathrm{d}(e', i')) \end{aligned} \tag{38}$$

with R a Markov kernel defined on $\mathcal{L} \times \mathcal{B}(\mathcal{L})$ and the $\{Q_k\}_{k \in [\![1, N]\!]}$ the Markov kernels defined on $(\mathcal{V}, \mathcal{B}(\mathcal{V}))$ as in (28). One could naturally consider more general choice for R than just a kernel acting on the refreshment time l. Also, as previously mentioned, we could have given an explicit definition of the boundary kernel on only points forming a non-small set, excluding tangential, multiple collisions or coincidental collision and refreshment.

Eventually, the infinitesimal generator comes down to, with f a continuous and continuously differentiable function on $((\Omega \times \mathcal{L}) \cup \partial(\Omega \times \mathcal{L})) \times \mathcal{V}$ and $(x, l, (e, i)) \in \Omega \times \mathcal{L} \times \mathcal{V}$,

$$\begin{aligned} \mathcal{A}f(x, l, (e, i)) =& \langle \nabla_{x_i} f(x, l, (e, i)), e \rangle - \partial_l f(x, l, (e, i)) \\ &+ \sum_{k=1}^{N} \lambda_k(x, l, (e, i)) \left\{ f(x, l, (e, k)) - f(x, l, (e, i)) \right\}, \end{aligned} \tag{39}$$

And, we have the condition on the boundary for $(x, l, (e, i)) \in \Gamma \times \mathcal{V}$ and for f a continuous and continuously differentiable function on $((\Omega \times \mathcal{L}) \cup \partial(\Omega \times \mathcal{L})) \times \mathcal{V}$,

$$\begin{aligned} f(x, l, (e, i)) =& \mathbb{1}_{\partial\mathcal{L}}(l) \int_{\mathcal{L}} f(x, l', (e', i')) R(l, \mathrm{d}l') \mathrm{d}\mu_{\mathcal{V}}((e', i')) \\ &+ (1 - \mathbb{1}_{\partial\mathcal{L}}(l)) \sum_{\substack{k=1 \\ k \neq i}}^{N} \frac{\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i, x_k)}{\sum_{\substack{k=1 \\ k \neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i, x_k)} f(x, l, (e, k)). \end{aligned} \tag{40}$$

This shift in description from an exponential jump process to a boundary effect could also be carried on regarding the events stemming from the pairwise interactions and ruled by the rates $(\lambda_k)_{k \in [\![1,N]\!]}$ (27). It nicely reflects the picture of an energy reservoir emptied along the differential flow from the positive energy increment, as described in the first works introducing these algorithmic methods [14, 18]. We will present conditions on R to ensure the correct invariance towards our target measure $\pi \times \mu_L \times \mu_{\mathcal{V}}$ in the next section.

IV. INVARIANCE OF THE EQUILIBRIUM DISTRIBUTION

The generator is an efficient tool to prove invariance of a measure w.r.t. a given process (e.g. [27, Prop. 34.7]). It will be normally required to do the formal effort to characterize the core of its generator (e.g. [31, Cor. 22]). As it is not the heart of our problematic, we will not detail the approximation procedure, as described via [31, Prop. 23, Cor.24] or [42], so that $\pi \otimes \mu_{\mathcal{V}}$ is shown to be left invariant by the PDMP by means of its infinitesimal generator (34) applied to continuously differentiable functions. Note that as we consider the torus, f is also bounded so that we have no problem defining the condition on the boundary and thus requires no additional condition on Q_b.

A. Standard exponential refreshment strategy

This comes down to show, with f a continuous and continuously differentiable function on $(\Omega \cup \partial\Omega) \times \mathcal{V}$, that,

$$\int_{\Omega \times \mathcal{V}} \mathcal{A} f(x, (e, i)) \pi(x) \mathrm{d}x \mathrm{d}\mu_{\mathcal{V}}(e, i) = 0 \tag{41}$$

Remark here that, from a dynamical point of view, starting from a measure with a nonzero density with regards to π is important, so as not to charge overlapping configurations in the

soft-sphere case or spheres in contact in the hard-sphere one.

Expliciting $\mathcal{A}$ from (34) for soft spheres or (35) for hard ones, we obtain

$$\begin{aligned}\int_{\Omega\times\mathcal{V}} \mathcal{A}f(x,(e,i))\mathrm{d}\pi(x)\mathrm{d}\mu_{\mathcal{V}}(e,i) = &\int_{\Omega\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}\mu_{\mathcal{V}}(e,i)\langle\nabla_{x_i} f(x,(e,i)),e\rangle \\ &+ \int_{\Omega\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}\mu_{\mathcal{V}}(e,i)\sum_{\substack{k=1\\k\neq i}}^{N}\langle e,\nabla_{x_i}u(x_i,x_k)\rangle_+\left\{f(x,(e,k))-f(x,(e,i))\right\} \\ &+ \lambda_r\int_{\Omega}\mathrm{d}\pi(x)\left(\int_{\mathcal{V}}\mathrm{d}\mu_{\mathcal{V}}(e',i')f(x,(e',i'))-\int_{\mathcal{V}}\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\right)\end{aligned} \tag{42}$$

The refreshment term cancels itself. Now, by integration by parts,

$$\begin{aligned}&= \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,(e,i))\pi(x)e) - \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\langle\nabla_{x_i}\pi(x),e\rangle \\ &+ \int_{\Omega\times\mathcal{D}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{D}}(e)\frac{1}{N}\sum_{i=1}^{N}\sum_{\substack{k=1\\k\neq i}}^{N}\pi(x)\langle e,\nabla_{x_i}u(x_i,x_k)\rangle_+\left\{f(x,(e,k))-f(x,(e,i))\right\}.\end{aligned} \tag{43}$$

Key point of these schemes, we make use of the pairwise mirror symmetry $\nabla_{x_i}u(x_i,x_k) = -\nabla_{x_k}u(x_i,x_k)$ to show the compensation of the transport by the events,

$$\begin{aligned}&= \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,(e,i))\pi(x)e) - \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\langle\nabla_{x_i}\pi(x),e\rangle \\ &+ \int_{\Omega\times\mathcal{D}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{D}}(e)\frac{1}{2N}\sum_{i=1}^{N}\sum_{\substack{k=1\\k\neq i}}^{N}\pi(x)\langle\nabla_{x_i}u(x_i,x_k),e\rangle\left\{f(x,(e,k))-f(x,(e,i))\right\} \\ &= \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,(e,i))\pi(x)e) - \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\langle\nabla_{x_i}\pi(x),e\rangle \\ &+ \int_{\Omega\times\mathcal{D}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{D}}(e)\frac{1}{2N}\left(\sum_{i=1}^{N}\langle\nabla_{x_i}\pi(x),e\rangle f(x,(e,i))+\sum_{k=1}^{N}\langle\nabla_{x_k}\pi(x),e\rangle f(x,(e,k))\right) \\ &= \int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,(e,i))\pi(x)e).\end{aligned} \tag{44}$$

By the divergence theorem, the first term encodes for the effects on the boundary $\partial\Omega\times\mathcal{V}$,

$$\begin{aligned}\int_{\Omega\times\mathcal{V}}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,(e,i))\pi(x)e) = &\int_{(\partial\Omega\times\mathcal{V})\setminus\Gamma^*}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\tilde{\pi}(x)\left\langle n_i(x,(e,i)),e\right\rangle. \\ &+\int_{\Gamma}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\tilde{\pi}(x)\left\langle n_i(x,(e,i)),e\right\rangle \\ &+\int_{\Gamma^*\setminus\Gamma}\mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i)f(x,(e,i))\tilde{\pi}(x)\left\langle n_i(x,(e,i)),e\right\rangle,\end{aligned} \tag{45}$$

with n_i the i-th component of the local outward normal,

$$n_i(x,(e,i)) = -\sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Omega_{\text{pair}}}(x_i,x_k)\nabla_{x_i} d(x_i,x_k)$$

which can be rewritten as,

$$n_i(x,(e,i)) = \sum_{\substack{k=1\\k\neq i}}^{N} (\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\nabla_{x_k} d(x_i,x_k) - \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)\nabla_{x_i} d(x_i,x_k)). \tag{46}$$

For soft-sphere systems, $\tilde{\pi}(x)$ is 0 for $x \in \partial\Omega$ (8), yielding (45) to sum up to 0 and the invariance of $\pi_S \times \mu_V$. The situation is different for hard-sphere ones where $\Gamma_H = \Gamma_H^*$. Using the relation on the boundaries (33), the relation (46) and the definition of Γ_H, we get

$$\begin{aligned}
&= \int_{(\partial\Omega\times\mathcal{V})\setminus\Gamma_H} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,(e,i)) \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\langle\nabla_{x_k} d(x_i,x_k), e\rangle \\
&+ \int_{\Gamma_H} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,(e,i)) \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\langle\nabla_{x_k} d(x_i,x_k),, e\rangle \\
&- \int_{\Gamma_H} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) \sum_{\substack{j=1\\j\neq i}}^{N} f(x,(e,j)) \frac{\mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_j)}{\sum_{\substack{j=1\\j\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_j)} \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_i,x_k)\langle\nabla_{x_i} d(x_i,x_k), e\rangle.
\end{aligned} \tag{47}$$

Merging the first two terms and simplyfing the third as multicollisions form a small set,

$$\begin{aligned}
&= \int_{\partial\Omega\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,(e,i)) \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\langle\nabla_{x_k} d(x_i,x_k), e\rangle \\
&- \int_{\Gamma_H} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) \sum_{\substack{j=1\\j\neq i}}^{N} f(x,(e,j)) \mathbb{1}_{\Gamma^e_{pair}(x_i,x_j)}\langle\nabla_{x_i} d(x_i,x_j), e\rangle.
\end{aligned} \tag{48}$$

As $\Gamma_H \subset \partial\Omega \times \mathcal{V}$,

$$\begin{aligned}
&= \int_{\partial\Omega\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,(e,i)) \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\langle\nabla_{x_k} d(x_i,x_k), e\rangle \\
&- \int_{\partial\Omega\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_{\mathcal{D}}(e) \frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{j=1\\j\neq i}}^{N} \mathbb{1}_{\Gamma_H}(x,(e,i)) f(x,(e,j)) \mathbb{1}_{\Gamma^e_{pair}(x_i,x_j)}\langle\nabla_{x_i} d(x_i,x_j), e\rangle,
\end{aligned} \tag{49}$$

which identifies with,

$$
\begin{aligned}
&= \int_{\partial\Omega\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,(e,i)) \sum_{\substack{k=1\\k\neq i}}^{N} \mathbb{1}_{\Gamma^e_{\text{pair}}}(x_k,x_i)\langle \nabla_{x_k} d(x_i,x_k), e\rangle \\
&\quad - \int_{\partial\Omega\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_{\mathcal{V}}(e,j) f(x,(e,j)) \sum_{\substack{i=1\\i\neq j}}^{N} \mathbb{1}_{\Gamma^e_{pair}(x_i,x_j)}\langle \nabla_{x_i} d(x_i,x_j), e\rangle \\
&= 0,
\end{aligned}
\tag{50}
$$

leading to the invariance of $\pi_H \times \mu_{\mathcal{V}}$ in the hard-sphere case. The invariance can be obtained in the same manner when using $\tilde{Q}^b$ by noting the relation,

$$
\langle n_i(x,(e,i)), e\rangle = \sum_{\substack{k=1\\k\neq i}}^{N} (n_-(x_i,x_k,e) - n_-(x_k,x_i,e)). \tag{51}
$$

B. Refreshment as a boundary effect

We show the invariance of the target distribution $\pi \times \mu_L \times \mu_{\mathcal{V}}$ by verifying the invariance condition on (39). With f a continuous and continuously differentiable function on $((\Omega\times\mathcal{L})\cup \partial(\Omega\times\mathcal{L}))\times\mathcal{V}$ and $(x,l,(e,i)) \in \Omega\times\mathcal{L}\times\mathcal{V}$, we get by integration by part and running similar computations as done in (43) and (44),

$$
\begin{aligned}
\int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathcal{A}f(x,l,(e,i))\mathrm{d}\pi(x)\mathrm{d}\mu_L(l)\mathrm{d}\mu_{\mathcal{V}}(e,i) &= \int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_L(l)\mathrm{d}\mu_{\mathcal{V}}(e,i)\nabla_{x_i}\cdot(f(x,l,(e,i))\pi(x)e) \\
&\quad - \int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}\mu_L(l)\mathrm{d}\mu_{\mathcal{V}}(e,i)\partial_l f(x,l,(e,i))).
\end{aligned}
\tag{52}
$$

And, by the divergence theorem and integration by parts, we obtain,

$$
\begin{aligned}
&= \int_{\partial\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}x\mathrm{d}\mu_L(l)\mathrm{d}\mu_{\mathcal{V}}(e,i) f(x,l,(e,i))\tilde{\pi}(x)\langle n_i(x,(e,i)),e\rangle \\
&+ \int_{\Omega\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}\mu_{\mathcal{V}}(e,i)\tilde{\mu}_L(0) f(x,0,(e,i)) - \int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}l\mathrm{d}\mu_{\mathcal{V}}(e,i)(-\partial_l\mu_L(l)) f(x,l,(e,i))
\end{aligned}
\tag{53}
$$

Using condition (40), we obtain the following general condition on the boundary refreshment kernel R in order to set (53) to 0,

$$
\int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}\mu_{\mathcal{V}}(e,i)\tilde{\mu}_L(0) f(x,l,(e,i)) R(0,dl) = \int_{\Omega\times\mathcal{L}\times\mathcal{V}} \mathrm{d}\pi(x)\mathrm{d}l\mathrm{d}\mu_{\mathcal{V}}(e,i)(-\partial_l\mu_L(l)) f(x,l,(e,i)),
\tag{54}
$$

Note that here the kernel R has to compensate the transport term and strongly depends on μ_L, contrary to the boundary kernel Q^b which can only depend on local information as the local normal. This condition simplifies to, for $l \in \mathcal{L}$,

$$\tilde{\mu}_L(0)R(0, dl) = (-\partial_l \mu_L(l))\mathrm{d}l. \tag{55}$$

It is equivalent to requiring μ_L to be of the form,

$$\mu_L(l) = h(l)\mathbb{1}_D. \tag{56}$$

where $D \subset \mathcal{L}$ and h a decreasing function on D so that $\lim_{l\to 0^+} h(l) > 0$ and $\int_{\mathcal{L}} \frac{-\partial_l \mu_L(l)}{\tilde{\mu}_L(0)}\mathrm{d}l = 1$.

Naturally we directly recover processes currently used in most algorithms, i.e. the fixed-time refreshment or the exponential one, giving, for $l \in \mathcal{L}$,

$$\begin{cases} \text{fixed-time } T\text{:} & \mu_L(l) = \frac{1}{T}\mathbb{1}_{]0,T[} & \text{and } R(l, \mathrm{d}l') = \delta(l' - T)\mathrm{d}l', & \text{with } T > 0, D =]0, T] \\ \text{exponential of rate } \lambda_r\text{:} & \mu_L(l) = \lambda_r e^{-\lambda_r l}\mathbb{1}_{l>0} & \text{and } R(l, \mathrm{d}l') = \lambda_r e^{-\lambda_r l'}\mathbb{1}_{l'>0}\mathrm{d}l', & \text{with } \lambda_r > 0, D = \mathcal{L} \end{cases}.$$

But also, building on the flexibility of the boundary description, new refreshment strategies are possible

- $\mu_L(l) = A(T - l)^k \mathbb{1}_{0<l\leq T}$, and refreshment $R(0, \mathrm{d}l) = \frac{k}{T^k}(T - l)^{k-1}\mathbb{1}_{0<l\leq T}$,
- $\mu_L(l) = \frac{A}{(T+l)^k}\mathbb{1}_{0<l}$, and refreshment $R(0, \mathrm{d}l) = \frac{kT^k}{(T+l)^{k+1}}\mathbb{1}_{0<l}$,
- $\mu_L(l) = Ae^{-Tl^k}\mathbb{1}_{0<l}$, and refreshment $R(0, \mathrm{d}l) = kTl^{k-1}e^{-Tl^k}\mathbb{1}_{0<l}$,
- ...

where $(T, k) \in \mathbb{R}_+^{*2}$, $l \in \mathcal{L}$ and A is a suitable normalization constant.

We have thus provided a general framework, setting refreshment as boundary type conditions, in order to allow new algorithms with different refreshment strategies. It would be interesting to look at the effect on the speed of convergence towards the equilibrium, or equilibration of different observables of these algorithms. Remark that we may also combine the usual Poisson refreshment with other refreshment conditions coming from the boundary (at the expense of adding other variables) to enrich refreshment strategies.

V. ERGODICITY OF ECMC

Contrary to the random-walk Metropolis-Hasting algorithm addressed in [5], which generates a reversible Markov chain where each sphere is allowed to move uniformly in a neighborhood of its current position (if no collision occurs), the continuity of the underlying topological state space imposes to take care of the existence, not simply of a single path, but of a density of paths connecting any two states. We can gain such a density by the randomness of the jump times, and it can be achieved using events or refreshments. Out of simplicity, we will consider here only refreshments. It is a difficult and technical task to prove ergodicity for this very ballistic process. We refer to the recent [38, 43] for such a study for the Zig-Zag process and the Bouncy Particle Sampler.

It would be of course very interesting to get explicit exponential speed of convergence towards equilibrium, suitably scaled with respect to the number of spheres. However, our estimates are definitely too crude to provide such an evaluation and we thus stay at a qualitative level. We also provide an alternative reachability strategy, opening new perspectives into getting coupling or uniform ergodicity results. Note that, even for (kinetic) Langevin process in the soft-sphere case, the only results at our disposal are based on Lyapunov-type techniques [44], only asserting exponential convergence but no rates. We refer to [4, 13, 14] for numerical evidence of the efficiency of the ECMC for soft- and hard-sphere cases.

A. Results and schemes of proofs

We focus here on the usual case where the refreshment is not seen as a boundary effect. Following [33, Th. 6.1], and a recent application in a similar context [38], we show that the PDMP is positive Harris recurrent and that some skeleton chain is irreducible through the control of distances and probability minorization to obtain a density of path connecting the initial and final states. To this end, we define different paths depending on the starting and final configurations, e.g. if the spheres are well separated or not, which impacts how easy it is to define a connecting path which moves each sphere sequentially. In the case of spheres being not separated enough, we thus adapt the strategy of [5] for proving the connectivity of their reversible algorithm, while improving to some extent the density condition. We then

use the nice tools of [37] to gain density of paths from connectivity.

More precisely, the process $(X_t, V_t)_{t\geq 0}$ considered here is non-evanescent due to the periodic boundary conditions of Ω_S. It is Harris recurrent if it is in addition a ϕ-irreducible T-process ([33], Theorem 3.2) and the positivity comes from the existence of an invariant probability distribution ([45, 46]). Finally, a positive Harris recurrent process with an invariant probability distribution is ergodic if some skeleton chain is irreducible ([33], Theorem 6.1). This leads to

Theorem 1 *If the density condition*

$$\exists \epsilon > 0, 3N \leq \left\lfloor \frac{L}{2d_{pair}+\epsilon} \right\rfloor \left\lfloor \frac{L}{d_{pair}+\epsilon} \frac{\sqrt{3}}{3} \right\rfloor \tag{57}$$

is satisfied, the PDMP $(X_t, V_t)_{t\geq 0}$ with the differential flow (25), the Markov kernel (26), the event rates (27) and described by the generator (34) or (35), is ergodic.

The density condition (57) simply ensures the possibility to pack without contact $3N$ spheres of radius d_{pair} in the considered torus, via a hexagonal packing.

The distribution $\pi \otimes \mu_{\mathcal{V}}$ is invariant for the PDMP. Following [37], to prove the irreducibility of the process, we define the set of trajectories composed of $m \in \mathbb{N}^*$ jumps,

$$\mathbb{T}_m = \left\{ (\mathbf{t}, \mathbf{v});\ \mathbf{t} = (t_1, \dots, t_m) \in \mathbb{R}_+^m,\ \mathbf{v} = ((e_0, i_0), (e_1, i_1), \dots, (e_m, i_m)) \in \mathcal{V}^{m+1} \right\}, \tag{58}$$

and the composite flow $\phi_{\mathbf{t}}^{\mathbf{v}} = \phi_{t_m}^{(e_{m-1}, i_{m-1})} \circ \cdots \circ \phi_{t_1}^{(e_0, i_0)}$ for $(\mathbf{t}, \mathbf{v}) \in \mathbb{R}_+^m \times \mathcal{V}^{m'}, m' \geq m$, with $\phi_t^{(e,i)} : \Omega \to \Omega$ defined so that $\phi_t(x, (e, i)) = (\phi_t^{(e,i)}(x), (e, i))$. Our crucial tool will be

Lemma 1 *If there exists $\epsilon > 0$, $3N \leq \left\lfloor \frac{L}{2d_{pair}+\epsilon} \right\rfloor \left\lfloor \frac{L}{d_{pair}+\epsilon} \frac{\sqrt{3}}{3} \right\rfloor$, for any pair $((x^{(0)}, v^{(0)}), (x^{(f)}, v^{(f)})) \in (\Omega \times \mathcal{V})^2$, there exists a trajectory $(\mathbf{t}, \mathbf{v}) \in \mathbb{T}_m, m \in \mathbb{N}^*$, such that $v_0 = v^{(0)}$, $v_m = v^{(f)}$ and $\phi_{\mathbf{t}}^{\mathbf{v}}(x_0) = x_f$ and the application $\boldsymbol{\tau} = (\tau_k)_{k=1}^m \to \phi_{(t' - \sum_{k=1}^m \tau_k)}^{v_m} \left(\phi_{\boldsymbol{\tau}}^{\mathbf{v}}(x^{(0)}) \right)$ is a submersion at $\mathbf{t}$ for some $t' > \sum_{i=1}^m t_i$.*

Proving Lemma 1 comes down to designing a trajectory $(\mathbf{t}, \mathbf{v}) \in \mathbb{T}_m, m \in \mathbb{N}^*$, connecting $(x^{(0)}, v^{(0)})$ and $(x^{(f)}, v^{(f)})$ in which all the possible pairs $v = (e, i) \in \mathcal{V}$ appear at least once, i.e. $\mathcal{V} \subset \{v_k\}_{k=0}^m$. Furthermore, the resulting path on Ω can be deformed by using another sequence of times $\boldsymbol{\tau} \in \mathbb{R}_+^m$ while reaching the same endpoint x_f given some additional time $t' \in \mathbb{R}_+^*$.

Lemma 1 then ensures that the process can reach a neighborhood of the endpoint x_f. As a consequence, the theorem 4.2 of [37] applies. One may remark that they impose bounded jump rates, but it is only for the construction of their process, and it does not intervene in their proof of Theorem 4.2. Thus for all $t' > \sum_{i=1}^{m} t_i$, there exist neighborhoods $\mathcal{X}_0$ of x_0, $\mathcal{X}_f$ of x_f, and constants $c, \epsilon > 0$ such that

$$\forall x \in \mathcal{X}_0,\ \forall (v, v') \in \mathcal{V}^2,\ \forall t \in [t', t' + \epsilon],\ \mathbb{P}_{(x,v)}\left((X_t, V_t) \in \cdot \times \{v'\}\right) \geq c\mathrm{Leb}(\cdot \cap \mathcal{X}_f), \tag{59}$$

Such lower bound has the following consequences ([38, Lem 8, Th. 5]): there exist a locally finite family of open sets $(\omega_n)_{n\in\mathbb{N}}$, which forms a cover of $\Omega \times \mathcal{V}$ so that every (x, v) is at least in one and in at most a finite number of ω_n, a family of open sets $(\mathcal{X}_n)_{n\in\mathbb{N}}$ in $\mathcal{B}(\Omega)$, a sequence $(v_n)_{n\in\mathbb{N}}$ in $\mathcal{V}$ and constants $c_n, t_n, \epsilon_n > 0$, such that for $A \in \mathcal{B}(\Omega)$,

$$\forall (x, v) \in \omega_n, \forall t \in [t_n, t_n + \epsilon_n], \mathbb{P}_{(x,v)}\left((X_t, V_t) \in A \times \{v'\}\right) \geq c_n 1_{v_n = v'} \mathrm{Leb}(A \cap \mathcal{X}_n) \tag{60}$$

which leads to bounding by below the resolvent by the following kernel K defined for $(x, v) \in \omega_n$ and $A \in \mathcal{B}(\Omega)$ as,

$$K((x, v), A \times \{v'\}) = \int \mathbb{1}_A(y) \max_{n:(x,v)\in\omega_n} \left(c_n \mathbb{1}_{\mathcal{X}_n \times \{v_n\}}((y, v')) \int_{t_n}^{t_n+\epsilon_n} e^{-t} \mathrm{d}t \right) \mathrm{d}y, \tag{61}$$

and which satisfies,

$$K((x, v), \mathcal{X}_n \times \{v'\}) \geq c_n \mathrm{Leb}(\mathcal{X}_n) \int_{t_n}^{t_n+\epsilon_n} e^{-t} \mathrm{d}t > 0. \tag{62}$$

Thus, the kernel K is a nontrivial lower semi-continuous kernel, as shown by considering a sequence $(x_l)_l$ converging to x satisfying $K((x_l, v)), A \times \{v'\}) \geq K((x, v), A \times \{v'\})$ for l large enough. The process then is a T-process [47]. As more detailed in [38], another application of (59) implies that the process is open set irreducible so that the process is a ϕ-process ([34], Theorem 3.2). Finally, we use also (59) to obtain the irreducibility of the Δ-skeleton chain ending the proof.

Finally, by considering a particular path, see Figure 2, we aim at getting closer to a uniform ergodicity property, at least for soft spheres or for a more stringent density condition for hard spheres.

B. Proof of ergodicity

The following two subsections correspond to the two main steps of the proof showing the ergodicity of ECMC: first we prove Lemma 1, and then the irreducibility of a skeleton chain.

1. *Proof of Lemma 1*

Let us explain briefly our strategy. First our density condition (57) implies roughly that we may pack $3N$ spheres in our torus. We show that we can find a path between a starting and final configurations of N spheres, furthermore proving that we gain *density* during this path. For that, we will first exhibit a valid path depending on the initial and final configurations, starting in the situation of well-separated spheres and then working our way to more packed case thanks to an expansion procedure. We take profit of the works of [5] to construct such a procedure for a correct path and [37] to get densities for such path by the notion of submersion. In other words, we show how to construct a composite flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ from $(x^{(0)}, v^{(0)}) \in \Omega \times \mathcal{V}$, an initial configuration, to $(x^{(f)}, v^{(f)}) \in \Omega \times \mathcal{V}$, a final configuration, where the control sequence $(\mathbf{t}, \mathbf{v}) \in \mathbb{T}_m, m \in \mathbb{N}^*$, admits every pair $v = (e, i) \in \mathcal{V}$.

(i) Flows and paths. We first define for any flow $\phi^{\mathbf{v}}_{\mathbf{t}}(x)$, with $\mathbf{t} = (t_i)_{i=1}^m$ and $\mathbf{v} = (v_i)_{i=0}^m$, its corresponding cumulative time sequences $(T_k = \sum_{i=1}^k t_i)_{k=1}^m$ and *flow path*, i.e. a path $\gamma : [0,1] \to \Omega \times \bar{\mathcal{V}}$ so that

$$\gamma(s) = \left(x^{(0)} + \sum_{i=1}^{i_s} t_i \bar{v}_{i-1} + (sT_m - T_{i_s})\, \bar{v}_{i_s}, \bar{v}_{i_s}\right) \quad \text{for } T_{i_s} \leq sT_m < T_{i_s+1} \tag{63}$$

with $\bar{v}_k$ defined by the mapping $v_k = (e = (e_0, e_1), i) \in \mathcal{V} \to \bar{v}_k = (0, \dots, e_0, e_1, \dots, 0) \in \bar{\mathcal{V}}$, with $\bar{\mathcal{V}}$ the canonical basis of $\mathbb{R}^{2N}$ and e_0 (resp. e_1) placed at the $2i$-th (resp. $(2i+1)$-th) position. Conversely, for any path $\gamma : [0,1] \to \Omega \times \bar{\mathcal{V}}$ so that we can define sequences $\mathbf{t} = (t_i)_{i=1}^m \in \mathbb{R}_+^m$ and $\mathbf{v} = (v_i)_{i=0}^m \in \mathcal{V}^{m+1}$ leading to a specification of γ as in (63), there is a corresponding flow $\phi^{\mathbf{v}}_{\mathbf{t}}$.

Now, we consider a more general path $\gamma : [0,1] \to \Omega \times \mathbb{R}^{2N}$ so that

$$\gamma(s) = \left(x^{(0)} + \sum_{i=1}^{i_s} t_i n_{i-1} \bar{v}_{i-1} + (sT_m - T_{i_s})\, n_{i_s} \bar{v}_{i_s}, n_{i_s} \bar{v}_{i_s}\right) \quad \text{for } T_{i_s} < sT_m < T_{i_s+1} \tag{64}$$

with $(t_i)_{i=1}^m \in \mathbb{R}_+^m$, $(v_i)_{i=0}^m \in \mathcal{V}^{m+1}$, $(n_i)_{i=0}^m \in \{1\} \times \{-1, +1\}^{m-2} \times \{1\}$, then yielding $\gamma(0), \gamma(1) \in \Omega \times \mathcal{V}$. We can define a corresponding *positive* path $\gamma_+ : [0,1] \to \Omega \times \mathcal{V}$ so

that for $(sT_m) \in [T_{i_s}, T_{i_s+1}[$ with $n_{i_s} = 1$, $\gamma_+(s) = \gamma(s)$ and for $(sT_m) \in [T_{i_s}, T_{i_s+1}[$ with $n_{i_s} = -1$ and $v_i = (e_i, k_i)$, we replace γ by a continuous path γ_+ connecting the sphere configuration reached at $\gamma(T_{i_s}/T_m)$ to the one reached at $\gamma(T_{i_s+1}/T_m)$ by repeating sequential updates by at most $\epsilon > 0$ increment along $+e_i$ of all spheres but the k_i-th, until, by periodicity, this will amount to an effective translation of $-t_{i+1}e_i$ of the k_i-th sphere. As $\gamma(t_i) \in \Omega \times \mathbb{R}^{2N}$ is a valid configuration with spheres separated by a pairwise distance greater than $d_{\text{pair}} + \epsilon'$, $\epsilon' > 0$, one can always consider an increment $\epsilon = \epsilon'/2$ so that a translation of any sphere by $+\epsilon e_i$ does not lead to any pairwise distance being smaller than $d_{\text{pair}} + \epsilon'/2$, making the positive path a valid one, i.e. $\gamma_+ : [0,1] \to \Omega \times \bar{\mathcal{V}}$. We then can define the flow $\phi^{\mathbf{v}_+}_{\mathbf{t}_+}$ corresponding to the positive path γ_+.

Thus, finding a composite flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ from $(x^{(0)}, v^{(0)})$ to $(x^{(f)}, v^{(f)})$ amounts to finding a path $\gamma : [0,1] \to \Omega \times \mathbb{R}^{2N}$ so that $\gamma(0) = (x^{(0)}, v^{(0)})$ and $\gamma(1) = (x^{(f)}, v^{(f)})$. We introduce $u_{\mathsf{x}} = (1,0)$ and $u_{\mathsf{y}} = (0,1)$, the unitary vectors aligned with the x-axis and y-axis respectively. Without loss of generality and out of simplicity, we set $v^{(0)} = (u_{\mathsf{x}}, 1)$ and $v^{(f)} \neq (u_{\mathsf{y}}, N)$, as a different setting only impacts the construction order of $\mathbf{t}$ and $\mathbf{v}$.

(ii) Connectivity in the fully-expanded case. For $(x, x') \in \Omega^2$, we define,

$$I(x, x') = \min_{i \neq j} d(x_i, x'_j), \tag{65}$$

the minimal distance between any two spheres respectively picked in x and x'.

We first consider the case where $(x^{(0)}, x^{(f)}) \in \Omega^2$ is such that

$$I(x^{(0)}, x^{(0)}) > 2d_{\text{pair}}, I(x^{(f)}, x^{(f)}) > 2d_{\text{pair}} \text{ and } I(x^{(0)}, x^{(f)}) > 2d_{\text{pair}}. \tag{66}$$

Considering the first sphere initially positioned in $x^{(0)}_1$, we consider the continuous flow $\phi^{\tilde{\mathbf{v}}_1}_{\tilde{\mathbf{t}}_1}$ set by

$$\tilde{\mathbf{t}}_1 = \{t_{u_{\mathsf{x}}}, t_{u_{\mathsf{y}}}(x^{(f)}_{1,0} - x^{(0)}_{1,0}) \mod L, (x^{(f)}_{1,1} - x^{(0)}_{1,1}) \mod L\} \text{ and } \tilde{\mathbf{v}}_1 = \{u_{\mathsf{x}}, u_{\mathsf{y}}\}$$

with

$$t_{u_{\mathsf{x}}} = \begin{cases} (x^{(f)}_{1,0} - x^{(0)}_{1,0}) \mod L \text{ if } |x^{(f)}_{1,0} - x^{(0)}_{1,0}| > 0 \\ L \text{ otherwise} \end{cases} \qquad t_{u_{\mathsf{y}}} = \begin{cases} (x^{(f)}_{1,1} - x^{(0)}_{1,1}) \mod L \text{ if } |x^{(f)}_{1,1} - x^{(0)}_{1,1}| > 0 \\ L \text{ otherwise} \end{cases}$$

The flow $\phi^{\tilde{\mathbf{v}}_1}_{\tilde{\mathbf{t}}_1}$ pushes $x^{(0)}$ to $(x_1^{(f)}, x_2^{(0)}, \dots, x_N^{(0)})$ and admits $(u_{\mathsf{x},1})$ and $(u_{\mathsf{y}}, 1)$ in $\tilde{\mathbf{v}}_\mathbf{1}$ over strictly positive times. We now need to modify the sequences $\tilde{\mathbf{t}}_1$ and $\tilde{\mathbf{v}}_1$ into sequences $\mathbf{t}_1$ and $\mathbf{v}_1$ so that the minimal pairwise distance along $\phi^{\mathbf{v}_1}_{\mathbf{t}_1}$ is strictly greater than d_{pair}.

To do so, we consider the corresponding path $\tilde{\gamma}_1 : [0,1] \to \Omega \times \bar{\mathcal{V}}$ to the flow $\phi^{\tilde{\mathbf{v}}_1}_{\tilde{\mathbf{t}}_1}$ and we modify it into a path $\gamma_1 : [0,1] \to \Omega \times \mathbb{R}^{2N}$. As the path $\tilde{\gamma}_1$ is continuous and using condition (66), the collection of times $s \in [0,1]$ at which the distance constraint is not satisfied along $\tilde{\gamma}_1$ can be written down as a disjoint union of intervals $S = \cup_{k=1}^{K} [a_k, b_k]$ and so that there is only one sphere i_k verifying $d(\tilde{x}_1 - x_{i_k}^{(0)}) \leq d_{\text{pair}}$ for $s \in [a_k, b_k]$ and $\tilde{\gamma}(s) = (\tilde{x}, \tilde{v})$, $\tilde{v}$ updating the first sphere. Now, for $s \notin S$, we set $\gamma_1(s) = \tilde{\gamma}_1(s)$ and for $s \in [a_k, b_k]$, we modify $\tilde{\gamma}_1$ into a continuous path γ_1 connecting $\tilde{\gamma}_1(a_k)$ and $\tilde{\gamma}_1(b_k)$ so that it is composed of moves of the first sphere along $\pm u_{\mathsf{x}}$ and $\pm u_{\mathsf{y}}$ and verifies $d_{\text{pair}} + \epsilon_1/2 < d(x_1, x_{i_k}^{(0)}) < d_{\text{pair}} + \epsilon_1, \epsilon_1 > 0$ for $s \in [a_k, b_k]$ and $\gamma_1(s) = (x, v)$. As $I(x^{(0)}, x^{(0)}) > 2d_{\text{pair}}$, we can choose $\epsilon_1 > 0$ so that $I(x, x^{(0)}) > d_{\text{pair}} + \epsilon_1/2$ for any $x \in \Omega$ reached by $\gamma_1(s)$ with $s \in [a_k, b_k]$ and $k \in \{1, \dots, K\}$.

Eventually, the modified path γ_1 is continuous, connects $(x^{(0)}, v^{(0)})$ and $((x_1^{(f)}, x_2^{(0)}, \dots, x_N^{(0)}), u_{\mathsf{y}})$ and respects a minimal pairwise distance of $d_{\text{pair}} + \epsilon_1/2$. Up to the definition of a corresponding positive path, it yields a flow $\phi^{\mathbf{v}_1}_{\mathbf{t}_1}$ updating the sphere 1 to its final position while respecting a minimal pairwise distance greater than $d_{\text{pair}} + \epsilon_1/4$. The complete flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ is then obtained by iteration of this procedure for each sphere and the composition of the respective flow $\phi^{\mathbf{v}_i}_{\mathbf{t}_i}$, which keeps a minimal pairwise distance of $d_{\text{pair}} + \min_{i \in [\![1,N]\!]} \epsilon_i/4$. Thus, the flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ connects $(x^{(0)}, v^{(0)})$ to $(x^{(f)}, v^{(f)})$, admits every $(e, i) \in \mathcal{V}$ in $\mathbf{v}$ and keeps a minimal pairwise distance strictly greater than d_{pair}.

(iii) Connectivity in the individually-expanded case. We now consider the case where $(x^{(0)}, x^{(f)}) \in \Omega^2$ is such that

$$I(x^{(0)}, x^{(0)}) > 2d_{\text{pair}}, I(x^{(f)}, x^{(f)}) > 2d_{\text{pair}} \text{ and } I(x^{(0)}, x^{(f)}) \leq 2d_{\text{pair}}.$$

Finding a path connecting such configurations is immediate through the procedure **(ii)** if we can consider an intermediate configuration $x^{(I)} \in \Omega$ so that,

$$I(x^{(I)}, x^{(I)}) > 2d_{\text{pair}}, I(x^{(0)}, x^{(I)}) > 2d_{\text{pair}} \text{ and } I(x^{(I)}, x^{(f)}) > 2d_{\text{pair}}.$$

As noted in [5] for a more stringent density constraint, such a configuration $x^{(I)}$ is easily constructed by induction given the density constraint in lemma 1, since, for any $(x^{(0)}, x^{(f)}, x^{(I)}) \in$

Ω^3, we have $\mathrm{Vol}(\cup_{i=1}^N B(x_i^{(0)}, d_{\mathrm{pair}}) \cup_{i=1}^N B(x_i^{(f)}, d_{\mathrm{pair}}) \cup_{i=1}^N B(x_i^{(0)}, d_{\mathrm{pair}})) \leq 3N\pi d_{\mathrm{pair}}^2 < \frac{\pi L^2\sqrt{3}}{6}$, where $\frac{\pi\sqrt{3}}{6}$ is the highest achievable density of a disk packing into a periodic square box.

(iv) Connectivity in the collapsed case (expansion/collapse procedure). We now consider the case where $(x^{(0)}, x^{(f)}) \in \Omega^2$ is such that

$$d_{\mathrm{pair}} < I(x^{(0)}, x^{(0)}) \leq 2d_{\mathrm{pair}} \text{ or } d_{\mathrm{pair}} < I(x^{(f)}, x^{(f)}) \leq 2d_{\mathrm{pair}}.$$

Building on the procedures **(ii)** and **(iii)**, we only need to show how to find a path connecting $x^{(0)}$ to a configuration $x^{(I)}$ so that $I(x^{(I)}, x^{(I)}) > 2d_{\mathrm{pair}}$. The case where $I(x^{(f)}, x^{(f)}) \leq 2d_{\mathrm{pair}}$ can be dealt with by showing the possibility of a path connecting $x^{(f)}$ to a configuration $x'^{(I)}, I(x'^{(I)}, x'^{(I)}) > 2d_{\mathrm{pair}}$, reversing the path and taking its positive counterpart.

Adapting the expansion procedure in [5], it comes down to proving that there exists some $\delta > 0$ so that, for any $(x, v) \in \Omega \times \mathcal{V}$ with $I(x, x) < 2d_{\mathrm{pair}}$, there exists a path γ_δ such that $\gamma_\delta(0) = (x, \bar{v})$, $\gamma_\delta(1) = (x', \bar{v}')$ and $I(x', x') \geq I(x, x) + \delta$. Indeed, assuming such a $\delta > 0$ exists, we consider the maximal pairwise distance M achievable from $x^{(0)}$ by a path γ, i.e.

$$M = \max_{y \in \mathcal{I}(x^{(0)})} I(y, y) \text{ with } \mathcal{I}(x^{(0)}) = \{y \in \Omega; \exists \gamma \in C([0,1], \Omega \times \bar{\mathcal{V}}), \gamma(0) = (x^{(0)}, \bar{v}^{(0)}), \gamma(1) = (y, \bar{v}_y)\},$$

As I is a bounded function, M is finite and given $\eta \in]0, \delta/2[$, there exists $y_1 \in \mathcal{I}(x^{(0)})$ such that $I(y_1, y_1) \geq M - \eta$. If $I(y_1, y_1) < 2d_{\mathrm{pair}}$, we can consider a path γ_δ so that $\gamma_\delta(0) = (y_1, \bar{v})$ and $\gamma_\delta(1) = (y_2, \bar{v}')$ and $I(y_2, y_2) \geq I(y_1, y_1) + \delta$. By construction, $y_2 \in \mathcal{I}(x^{(0)})$ and $I(y_2, y_2) > M$, which is impossible. It then shows that there exists $y \in \mathcal{I}(x^{(0)})$ such that $I(y, y) > 2d_{\mathrm{pair}}$. It leads to the construction of an intermediate configuration $x^{(I)}$, with $I(x^{(I)}, x^{(I)}) > 2d_{\mathrm{pair}}$ with a valid flow starting from $x^{(0)}$, and conversely by reverting the flow one may then find a flow to collapse the configuration into $x^{(f)}$.

Starting from $(x^{(0)}, v^{(0)})$, the system evolves to $(x, v^{(0)})$ until a first refreshment time t_0 updating the state to $(x, v) \in \Omega \times \mathcal{V}$ Let us now prove that there exists some $\delta > 0$ so that, for any $x \in \Omega$ with $I(x, x) < 2d_{\mathrm{pair}}$, there exists a path γ_δ and $v \in \mathcal{V}$ such that $\gamma_\delta(0) = (x, \bar{v})$, $\gamma_\delta(1) = (x', \bar{v}')$ and $I(x', x') \geq I(x, x) + \delta$. To do so, we will use the induction strategy of the proof of [5, Lem. 4.2], and adapt it here to the PDMP scheme and torus setting.

We proceed by induction and thus have to prove that there exists $\delta = \delta(N, d_{\mathrm{pair}}, L)$ and

$\rho = \rho(N, d_{\text{pair}}, L)$ such that $\forall J \in \{1, \cdots, N\}$,

$$(P(J)) \qquad \begin{array}{l} \forall x \in \Omega(J)\, s.t.\, I(x,x) < 2d_{\text{pair}}, \\ \exists v \in \mathcal{V}, \exists \gamma \in C([0,1], \Omega(J) \times \bar{\mathcal{V}}), \text{ with } \begin{cases} \gamma(0) = (x, \bar{v}),\ \gamma(s) = (x(s), \bar{v}(s)), \\ I(x(1), x(1)) \geq I(x,x) + \delta, \\ \sup_t \max_i d(x_i, x(t)_i) \leq J\rho \end{cases} \end{array}$$

where we remind that

$$\Omega(J) = \{x \in (\mathbb{R}/L\mathbb{Z})^{2J}; \forall (i,j) \in [\![1, J]\!]^2, i \neq j, (x_i, x_j) \in \Omega_{\text{pair}}\},$$

stands for the system with only J spheres. Let us choose $\delta = d_{\text{pair}}/(600N^2)$ and $\rho = d_{\text{pair}}/(6N)$.

Let us start our induction with $J = 1$ (only one sphere) for which there is nothing to prove. Suppose now that $P(J-1)$ is verified. Let us divide, as equivalence class, spheres that can be connected by a path in $\cup_1^J B(x_k, d_{\text{pair}} + J\rho)$. If there are more than two classes, then one can consider each class individually, which then contains strictly less than N spheres, and use the induction hypothesis. Indeed, in this case one has $\{1, \cdots N\} = I \cup \tilde{I}$ and for all $i \in I$, $j \in \tilde{I}$ one has $d(x_i, x_j) > 2d_{\text{pair}} + 2J\rho$. The induction hypothesis enables us to build two paths γ_I and $\gamma_{\tilde{I}}$ each satisfying $(P(I))$ and $(P(\tilde{I}))$ and this defines a path γ for all spheres. As along γ_I, $\sum_t \max_i d(x_i, x(t)_i) \leq |I|)$ (and respectively along $\gamma_{\tilde{I}}$, we have to impose here that $2d_{\text{pair}} + 2J\rho\delta - (|I| + |\tilde{I}|)\rho > 2d_{\text{pair}} + \delta$ resuming in $J\rho > \delta$, to get that γ is a valid path and $I(x(1), x(1)) > I(x,x) + \delta$, $\sup_t \max_i d(x_i, x(t)_i) < \max(|I|, |\tilde{I}|)\rho \leq (J-1)\rho$.

Thus we are reduced to consider the case where there is only one equivalence class, so that the spheres are quite packed. Recall that our density assumption ensures that there is in fact sufficient space for at least $3N$ spheres of radius d_{pair}. One can then choose a direction $\nu = (1,0)$ or $(0,1)$ and introduce an ordering $\sigma : [\![1, N]\!] \to [\![1, N]\!]$ so that the reordered positions $\{x_{\sigma(i)}\}_{i=1}^J$ satisfy $\langle x_{\sigma(i)}, \nu\rangle \leq \langle x_{\sigma(j)}, \nu\rangle$ for all $(i,j) \in [\![1, N]\!]^2$ with $\sigma(i) < \sigma(j)$. As $\{\langle x_{\sigma(i)}, \nu\rangle\}_{i=1}^J \in [0, L]^J$, we can now consider a pair of furtherst apart $\sigma-$successive spheres along the ν-direction, i.e. a pair of spheres i_J and i_1 so that $\sigma(i_J) = (\sigma(i_1) + 1) \mod J$ and

$$(\langle x_{i_J} - x_{i_1}, \nu\rangle) \mod L = \max_i \left(\langle \left(x_{\sigma^{-1}(\sigma(i)+1 \bmod J)} - x_i\right), \nu\rangle \mod L\right),$$

which is, for a well-chosen direction ν, larger than $\max\{d \in]d_{\text{pair}}, +\inf[; J \leq \lfloor L/d \rfloor \lfloor (L/d)(2\sqrt{3}/3) \rfloor\}$ which is in turn larger than $\max\{d \in]d_{\text{pair}}, +\inf[; N \leq$

$\lfloor L/d \rfloor \lfloor (L/d)(2\sqrt{3}/3) \rfloor \} \geq 2(2d_{\text{pair}}/\sqrt{3})$. Indeed, given the density condition, one can pack $3N$ spheres of radius d_{pair}. Considering the densest hexagonal packing of these $3N$ spheres, we can pack N spheres of radius $(2d_{\text{pair}}/\sqrt{3})$ corresponding to the circumscribed circles of the equilateral triangles forming up the $3N$-hexagonal packing.

We then note the subset of indices matching i_J in its ν-coordinate $\mathcal{I}_J = \{i \in [\![1, N]\!] \setminus \{i_J\}; \langle x_i, \nu \rangle = \langle x_{i_J}, \nu \rangle\}$. From there, we build on the ordering σ to obtain a sequence $(i_l)_{l=1}^J$ with i_J and i_1 as previously defined and i_l so that $\sigma(i_l) = (\sigma(i_{l-1}) - 1) \mod J$ for $2 \leq l \leq J - 1 - |\mathcal{I}_1|$ and $i_l \in \mathcal{I}_J$ for $J > l \geq J - |\mathcal{I}_J|$. Now, for $j \in \{1, ..., J\}$, choose $a_j = (J + 1 - j)\rho$ and consider $v = (\nu, i_1)$ and the valid continuous path γ set by the sequences

$$\mathbf{t} = (a_l)_{l=1}^J \,, \; \mathbf{v} = ((\nu, i_l))_{l=1}^J \tag{67}$$

It is easy to verify as in [5] that in this case $(P(J))$ is verified. Indeed, we first have that $\sup_t \max_i d(x_i, x(t)_i) \leq J\rho$. Note that there is no periodicity effect to take care of here, as $J\rho < L/2$ since $L^2 > 3N\pi d_{\text{pair}}^2 > (d_{\text{pair}}/3)^2$.

Then, we consider the evolution of $d(x_{i_l}(t), x_{i_m}(t))$ for all $1 \leq l < m \leq J$. The periodic distance d refers to the shortest distance between every periodic copies of the spheres i_l and i_m. We refer to the initially involved copies as $x_{i_l}^c$ and $x_{i_m}^c$. A change of the copy involved in the computation of d means that the relative displacement $(m - l)\rho > L/2 - |\langle x_{i_l}^c - x_{i_m}^c, \nu \rangle|$. However, as $N\rho < L/2 - 2d_{\text{pair}} - \delta$, it means that, first the initial periodic distance is bigger than $2d_{\text{pair}} > I(x, x)$ and second that the final periodic distance is $L - (|\langle x_{i_l}^c - x_{i_m}^c, \nu \rangle| + (m - l)\rho) > 2d_{\text{pair}} + \delta > I(x, x) + \delta$.

Now, for pairs of spheres $2 \leq l < m < J - |\mathcal{I}_1|$ with unchanged involved periodic copies, we have,

$$|(x_{i_l}^c + a_l\nu) - (x_{i_m}^c + a_m\nu)|^2 \;=\; |x_{i_l}^c - x_{j_l}^c|^2 + 2(a_l - a_m)\langle x_{i_l}^c - x_{i_m}^c, \nu \rangle + |a_l - a_m|^2 \geq |x_{i_l}^c - x_{i_m}^c|^2 + \rho^2.$$

For pairs of spheres $J - |\mathcal{I}_J| \leq l < m \leq J$, we have,

$$|(x_{i_l}^c + a_l\nu) - (x_{i_m}^c + a_m\nu)|^2 \;=\; |x_{i_l}^c - x_{i_m}^c|^2 + |a_l - a_m|^2 \geq |x_{i_l}^c - x_{i_m}^c|^2 + \rho^2.$$

And finally for $J - |\mathcal{I}_J| \leq l < m \leq J$ and $2 \leq m < J - |\mathcal{I}_1|$, with unchanged involved periodic copies, we have,

$$|(x_{i_l}^c + a_l\nu) - (x_{i_m}^c + a_m\nu)|^2 \;=\; |x_{i_l}^c - x_{i_m}^c|^2 + 2(a_l - a_m)\langle x_{i_l}^c - x_{i_m}^c, \nu \rangle + |a_l - a_m|^2$$

If $\langle x^c_{i_l} - x^c_{i_m}, \nu\rangle < 0$, then

$$|(x^c_{i_l} + a_l\nu) - (x^c_{i_m} + a_m\nu)|^2 \geq |x^c_{i_l} - x^c_{i_m}|^2 + \rho^2.$$

Otherwise,

$$\begin{aligned}|(x^c_{i_l} + a_l\nu) - (x^c_{i_m} + a_m\nu)|^2 &\geq |\langle (x^c_{i_J} + a_J\nu) - (x^c_{i_1} + a_1\nu), \nu\rangle|^2 \\ &\geq \left(\frac{4}{\sqrt{3}}d_{\text{pair}} - (J-1)\rho\right)^2 > 4d^2_{\text{pair}} + \rho^2 > I(x,x)^2 + \rho^2\end{aligned}$$

We then deduce $I(x(1), x(1))^2 \geq I(x,x)^2 + \rho^2 \geq (I(x,x) + \delta)^2$.

Remark that using the reversed-path scheme, as described in the paragraph **(i)**, we also have a valid collapse scheme. Therefore using the expansion then collapse procedure we may go from a collapsed initial configuration to an intermediate separated configuration by expansion then move to an other intermediate separated configuration and then use a collapse procedure (if needed) to reach the final configuration.

(v) Gaining density. Considering any $(x^{(0)}, v^{(0)}), (x^{(f)}, v^{(f)}) \in \Omega \times \mathcal{V}$, there exist admissible deterministic sequences $(\mathbf{t} = (t_i)_{i=1}^m, \mathbf{v} = (v_i)_{i=0}^m) \in \mathbb{T}_m$, $m \in \mathbb{N}^*$, so that the corresponding flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ pushes $(x^{(0)}, v^{(0)})$ to $(x^{(f)}, v^{(f)})$ and $\mathbf{v}$ admits every pair in $\mathcal{V}$ at least once. Recalling the notation $T_k = \sum_{i=1}^k t_k$, we consider a bounded neighbourhood $\mathcal{U}_k$ of T_k for $1 \leq k \leq m$. The neighbourhoods $(\mathcal{U}_k)_{k=1}^m$ can be chosen so that they do not intersect and so that, for any sequences $(\boldsymbol{\tau}, \mathbf{v}) \in \mathcal{T}$, with $\mathcal{T} = \{\boldsymbol{s} \in \mathbb{T}_m; \sum_{l=1}^k s_l \in \mathcal{U}_k\}$, the flow $\phi^{\mathbf{v}}_{\boldsymbol{\tau}}$ preserves a minimal pairwise interdistance strictly greater than d_{pair}, as the initial flow $\phi^{\mathbf{v}}_{\mathbf{t}}$ already does.

Following [37, section 6] and as done in the proof of lemma 8 in [38], we only need to show that, for some $t' > T_m$, the partial map $\boldsymbol{\tau} \to \phi^{v^{(f)}}_{t' - \sum_{k=1}^m \tau_m} \circ \phi^{\mathbf{v}}_{\boldsymbol{\tau}}(x^{(0)})$, defined on $\boldsymbol{\tau} \in \mathcal{T}, \sum_{k=1}^m \tau_k < t'$, has full rank with

$$\phi^{v^{(f)}}_{t' - \sum_{k=1}^m \tau_k} \circ \phi^{\mathbf{v}}_{\boldsymbol{\tau}}(x^{(0)}) = x^{(0)} + \tau_1\bar{v}_1 + \tau_2\bar{v}_2 + \cdots + \tau_m\bar{v}_m + (t' - \tau_m)\bar{v}^{(f)}.$$

The image of the differential of the partial mapping is spanned by the vector family,

$$\{g_i\}_{i=1}^m = \left\{(\bar{v}_1 - \bar{v}_2), (\bar{v}_2 - \bar{v}_3), \ldots, (\bar{v}_m - \bar{v}^{(f)})\right\}.$$

As shown by the construction in the procedure **(ii)**, the family $\{g_i\}_{i=1}^m$ includes the following family of $2N$ vectors,

$$\left\{(\bar{v}_{\mathrm{x},1} - \bar{v}_{\mathrm{y},1}), (\bar{v}_{\mathrm{y},1} - \bar{v}_{\mathrm{x},2}), (\bar{v}_{\mathrm{x},2} - \bar{v}_{\mathrm{y},2}), \ldots, (\bar{v}_{\mathrm{x},N} - \bar{v}_{\mathrm{y},N}), (\bar{v}_{\mathrm{y},N} - \bar{v}^{(f)})\right\},$$

with $\bar{v}_{\mathsf{x},i}, \bar{v}_{\mathsf{y},i}$ corresponding to $(u_{\mathsf{x}}, i), (u_{\mathsf{y}}, i)$ up to the $v \to \bar{v}$ mapping defined in **(i)**. Thus, the family $\{g_i\}_{i=1}^m$ spans Ω, as one can reconstruct the basis $\{\bar{v}_{\mathsf{x},i}\}_{i=1}^N \cup \{\bar{v}_{\mathsf{y},i}\}_{i=1}^N$ from this family by composition since $\bar{v}_{\mathsf{y},N} \neq \bar{v}^{(f)}$ and $\bar{v}^{(f)}$ appears elsewhere in $\{g_i\}_{i=1}^m$.

The partial mapping $\boldsymbol{\tau} \to \phi^{v^{(f)}}_{t'-\sum_{k=1}^m \tau_k} \circ \phi^{\mathbf{v}}_{\boldsymbol{\tau}}(x^{(0)})$ then has full rank and is a submersion at $\mathbf{t}$, proving Lemma 1.

2. Irreducibility of the Δ-skeleton

The Δ-chain $(X_{k\Delta}, V_{k\Delta})_{k\in\mathbb{N}}$ of the process, or its skeleton chain, is the sampled chain at times $t_k = k\Delta$ with $k \in \mathbb{N}$ and $\Delta \in \mathbb{R}_+^*$. It is irreducible if for all $(x, v) \in \Omega \times \mathcal{V}$ and $(y, v') \in \Omega \times \mathcal{V}$, there exist a neighbourhood $\mathcal{Y}$ of y and $n \in \mathbb{N}$ such that $\mathbb{P}_{(x,v)}((X_{n\Delta}, V_{n\Delta}) \in \mathcal{Y} \times \{v'\}) > 0$.

Let $((x, v), (y, v')) \in (\Omega \times \mathcal{V})^2$ and let $(w, u) \in \Omega \times \mathcal{V}$. Applying Lemma 1 between the pairs $((x, v), (w, u))$, $((w, u), (y, v'))$ and $((w, u), (w, u))$ (looping around) yields that there exists $\epsilon \in \mathbb{R}_+^*$ and $\tau, c > 0$ such that for any $t \in [\tau, \tau + \epsilon]$, there exists a neighbourhood $\mathcal{Y}$ of y such that,

$$\mathbb{P}_{(x,v)}((X_t, V_t) \in \cdot \times \{v'\}) \geq c\mathrm{Leb}(\cdot \cap \mathcal{Y}) > 0. \tag{68}$$

While τ and c depends on $(x, v), (y, v')$ and (w, u), ϵ can be set so as to depend only (w, u) and the ability for the process to loop around an arbitrary point. We refer to [38] for the successive applications of Lemma 1 and corollary (59) resulting in (68).

Finally, setting $\Delta = \epsilon$ and $n = \left\lfloor \frac{\tau}{\epsilon} + 1 \right\rfloor$ such that $n\epsilon \in [\tau, \tau + \epsilon]$, we obtain $\mathbb{P}_{(x,v)}(X_{n\Delta}, V_{n\Delta} \in \cdot \times \{v'\}) > 0$.

C. Towards uniform ergodicity in the soft-sphere case

Let us see now how we can consider a modification of the reachability procedure described in **(ii)**, so that the initial condition dependence only appears in travel times. It may be seen as a first step towards uniform ergodicity and coupling. The described procedure does not behave optimally in the number of spheres and, consequently we only describe it qualitatively. The notations of the previous subsection apply and we consider the soft-sphere case ($d_{\mathrm{pair}} = 0$).

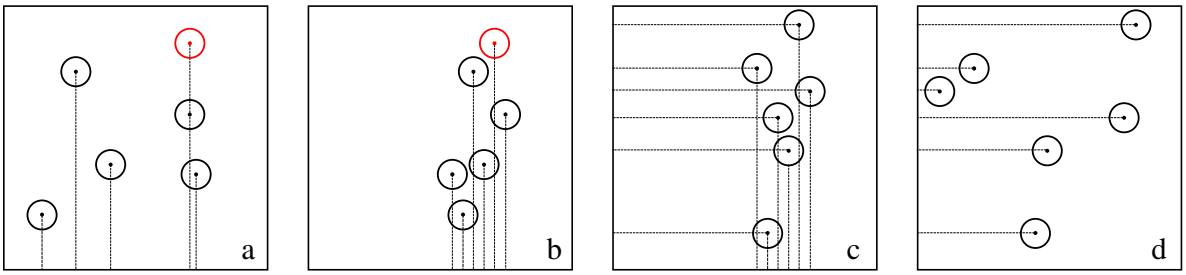

FIG. 2: In the case $\alpha > 0$, to reach the configuration *(d)* from any initial configuration *(a)*, the x-coordinates of the spheres are first gathered in configuration *(b)* in a segment of size $\frac{L}{N}$ with L the size of the box side and N the number of spheres *(b-d)*. They are then moved successively along their y-coordinates until they reach their final y-position in configuration *(c)*. From *(a)* to *(b)* and from *(b)* to *(c)*, a distance of $\frac{L}{N^2}$ in the x-coordinates is preserved between any pair of spheres. They are finally updated to their final x-position in the configuration *(f)*, while a distance of α is preserved in the y-coordinates.

The same could be done in the hard sphere case however with a far more stringent density condition than (57).

We introduce the quantity,

$$\alpha = \max_{k\in\{0,1\}} \min_{i\neq j} \left(\min(|x_{i,k}^{(f)} - x_{j,k}^{(f)}|, L - |x_{i,k}^{(f)} - x_{j,k}^{(f)}|) \right)$$

and consider out of simplicity that α is reached along the y-coordinate ($k = 1$) as, otherwise, the following points still hold, up to exchanging $k = 0$ and $k = 1$. Note that $v^{(f)}$ is not really important as we consider a final refreshment to reach it. The followed strategy is illustrated in Fig. 2.

Starting from $(x^{(0)}, v^{(0)})$, the system evolves to $(\tilde{x}^{(0)}, \tilde{v}^{(0)})$ until a first refreshment time. There, we consider the same ordering σ along the x-coordinate as described in **(iv)** to determine the furthest apart successive spheres along the x-axis. We note i_1 and i_N the indices of these spheres, so that $\left(\tilde{x}_{i_N,0}^{(0)} - \tilde{x}_{i_1,0}^{(0)}\right) \mod L$ is either 0, in the case where all x-coordinates are the same in $\tilde{x}^{(0)}$, or larger than L/N otherwise. We then note the subset of indices matching i_N in its x-coordinate $\mathcal{I}_N = \{i \in [\![1, N]\!] \setminus \{i_N\}; \tilde{x}_{i,0}^{(0)} = \tilde{x}_{i_N,0}^{(0)}\}$. We obtain a sequence $(i_k)_{k=1}^N$ where i_1 and i_N as previously defined, i_l so that $\sigma(i_l) = (\sigma(i_{l-1} - 1)) \mod N$ for $2 \leq l \leq N - 1 - |\mathcal{I}_N|$ and $i_l \in \mathcal{I}_N$ otherwise.

We now *stack* the x-coordinates of the spheres on a segment

$$\left[x^{(0)}_{i_N,0} - (N - |\mathcal{I}_N|)L/N^2, x^{(0)}_{i_N,0} + |\mathcal{I}_N|L/N^2\right]/(L\mathbb{Z}),$$

by following the trajectories defined by the sequences,

$$\begin{aligned}
\mathbf{t}_{\mathsf{x}} &= \left(\left(\tilde{x}^{(0)}_{i_N,0} - \tilde{x}^{(0)}_{i_l,0}\right) \mod L - \frac{lL}{N^2}\right)_{l=1}^{N-1-|\mathcal{I}_N|}, \ \mathbf{v}_{\mathsf{x}} = ((u_{\mathsf{x}}, i_l))_{l=1}^{N-|\mathcal{I}_N|-1} \\
\mathbf{t}_{\mathsf{x}}^{\mathcal{I}_N} &= \left(\frac{(|\mathcal{I}_N| - l)L}{N^2}\right)_{l=0}^{|\mathcal{I}_N|-1}, \ \mathbf{v}_{\mathsf{x}}^{\mathcal{I}_N} = ((u_{\mathsf{x}}, i_l))_{l=N-|\mathcal{I}_N|}^{N-1}.
\end{aligned} \tag{69}$$

The corresponding flow $\phi^{\mathbf{v}_{\mathsf{x}}^{\mathcal{I}_N}}_{\mathbf{t}_{\mathsf{x}}^{\mathcal{I}_N}} \circ \phi^{\mathbf{v}_{\mathsf{x}}}_{\mathbf{t}_{\mathsf{x}}}(\tilde{x}^{(0)}) = x^{(\mathsf{x})}$ exists as it preserves a bound for all pair event rates $\lambda_{j\neq i_l}(x, (u_{\mathsf{x}}, i_l)) \leq \lambda_{i_{l-1}}(x, (u_{\mathsf{x}}, i_l)) \leq \gamma\sigma^\gamma/(L/N^2)^{\gamma+1}$, thanks to the $(i_l)_{l=1}^N$ ordering.
Case $\alpha > 0$**.** From the configuration $x^{(\mathsf{x})}$, we then updates the y-coordinates of the spheres to their final values by introducing the following sequences,

$$\mathbf{t}_{\mathsf{y}} = \left(\left(x^{(f)}_{i,1} - \tilde{x}^{(0)}_{i,1}\right) \mod L\right)_{i=1}^{N}, \ \mathbf{v}_{\mathsf{y}} = ((u_{\mathsf{y}}, i))_{i=1}^{N}, \tag{70}$$

and the corresponding flow $\phi^{\mathbf{v}_{\mathsf{y}}}_{\mathbf{t}_{\mathsf{y}}}(x^{(\mathsf{x})}) = x^{(\mathsf{y})}$ exists as it preserves the same bound by keeping a minimum pairwise distance of at least L/N^2.

Eventually, the sphere x-coordinates are updated to their final values by considering the sequences,

$$\mathbf{t}_{\mathsf{f}} = \left(\left(x^{(f)}_{i,0} - x^{(\mathsf{x})}_{i,0}\right) \mod L\right)_{i=1}^{N}, \ \mathbf{v}_{\mathsf{f}} = ((u_{\mathsf{x}}, i)_{i=1}^{N}, v^{(f)}), \tag{71}$$

and the corresponding flow $\phi^{\mathbf{v}_{\mathsf{f}}}_{\mathbf{t}_{\mathsf{f}}}(x) = x^{(f)}$ exists as it preserves a minimum pairwise distance of at least α and the total composite flow $\phi^{\mathbf{v}}_{\mathbf{t}} = \phi^{\mathbf{v}_{\mathsf{f}}}_{\mathbf{t}_{\mathsf{f}}} \circ \phi^{\mathbf{v}_{\mathsf{y}}}_{\mathbf{t}_{\mathsf{y}}} \circ \phi^{\mathbf{v}_{\mathsf{x}}^{\mathcal{I}_N}}_{\mathbf{t}_{\mathsf{x}}^{\mathcal{I}_f}} \circ \phi^{\mathbf{v}_{\mathsf{x}}}_{\mathbf{t}_{\mathsf{x}}}$, $(\mathbf{t}, \mathbf{v}) \in \mathbb{T}_{3N}$, preserves a minimum pairwise distance of

$$\alpha^{\neq 0}_{\text{tot}} = \min\left(\alpha, \frac{L}{N^2}\right).$$

Case $\alpha = 0$**.** We define the subset of indices $\mathcal{I}_f = \{l \in [\![1, N]\!]; \exists i \in [\![1, N]\!], i \neq l, x^{(f)}_{i,1} = x^{(f)}_{l,1}\}$, the equivalence classes $[l] = \{i \in \mathcal{I}_f; x^{(f)}_{i,1} = x^{(f)}_{l,1}\}$ and the bijections $\nu_l : [l] \to [\![0, \text{Card}(l) - 1]\!]$ so that $\nu_l(i) > \nu_l(j)$ if $i > j$. We also now consider the quantity

$$\alpha^{\neq 0} = \min\left\{\min\left(|x^{(f)}_{i,1} - x^{(f)}_{j,1}|, L - |x^{(f)}_{i,1} - x^{(f)}_{j,1}|\right); i \in [\![1, N]\!] \setminus \mathcal{I}_f, j \in [\![1, N]\!], i \neq j\right\} + \mathbb{1}_{\{[\![1,N]\!]\}}(\mathcal{I}_f)L.$$

From the configuration $x^{(\mathsf{x})}$, we update the y-coordinates of the spheres $i \in [\![1, N]\!] \setminus \mathcal{I}_f$ to their final values as,

$$\mathbf{t}_{\mathsf{y}}^{\neq 0} = \left(\left(x_{i,1}^{(f)} - \tilde{x}_{i,1}^{(0)} \right) \mod L \right)_{i \in [\![1,N]\!] \setminus \mathcal{I}_f}, \ \mathbf{v}_{\mathsf{y}}^{\neq 0} = ((u_{\mathsf{y}}, i))_{i \in [\![1,N]\!] \setminus \mathcal{I}_f}, \tag{72}$$

the corresponding flow $\phi_{\mathbf{t}_{\mathsf{y}}^{\neq 0}}^{\mathbf{v}_{\mathsf{y}}^{\neq 0}}$ being well-defined, as it preserves a minimum pairwise distance of at least L/N^2. We now update the y-coordinates of the spheres $i \in \mathcal{I}_f$ as,

$$\mathbf{t}_{\mathsf{y}}^{=0} = \left(\left(\left(x_{i,1}^{(f)} - \tilde{x}_{i,1}^{(0)} \right) \mod L \right) - \frac{\alpha^{\neq 0} \nu_i(i)}{|[i]|} \right)_{i \in \mathcal{I}_f}, \ \mathbf{v}_{\mathsf{y}}^{=0} = ((u_{\mathsf{y}}, i))_{i \in \mathcal{I}_f}, \tag{73}$$

the corresponding flow $\phi_{\mathbf{t}_{\mathsf{y}}^{=0}}^{\mathbf{v}_{\mathsf{y}}^{=0}}$ being well-defined, as it preserves a minimum pairwise distance of at least L/N^2.

Now, the x-coordinates of all the spheres are updated to their final values by considering the sequences,

$$\mathbf{t}_{\mathsf{f},\mathsf{x}} = \left(\left(x_{i,0}^{(f)} - x_{i,0}^{(\mathsf{x})} \right) \mod L \right)_{i=1}^{N}, \ \mathbf{v}_{\mathsf{f},\mathsf{x}} = ((u_{\mathsf{x}}, i))_{i=1}^{N}, \tag{74}$$

and the corresponding flow $\phi_{\mathbf{t}_{\mathsf{f},\mathsf{x}}}^{\mathbf{v}_{\mathsf{f},\mathsf{x}}}$ exists as it preserves a minimum pairwise distance of at least $\alpha^{\neq 0} / \max_i |[i]|$.

Eventually, the y-coordinates of the spheres $i \in \mathcal{I}_f$ are also updated to their final values by considering the sequences,

$$\mathbf{t}_{\mathsf{f},\mathsf{y}} = \left(\frac{\alpha^{\neq 0} \nu_i(i)}{|[i]|} \right)_{i \in \mathcal{I}_f}, \ \mathbf{v}_{\mathsf{f},\mathsf{y}} = ((u_{\mathsf{y}}, i)_{i \in \mathcal{I}_f}, v^{(f)}), \tag{75}$$

and the corresponding flow $\phi_{\mathbf{t}_{\mathsf{f},\mathsf{y}}}^{\mathbf{v}_{\mathsf{f},\mathsf{y}}}$ exists as it preserves a minimum pairwise distance of at least

$$\alpha_{\mathcal{I}_f} = \min_{i \in \mathcal{I}_f} \left\{ \min_{\substack{l \in [i] \\ l \neq i}} \left(\min \left(|x_{i,0}^{(f)} - x_{j,0}^{(f)}|, L - |x_{i,0}^{(f)} - x_{j,0}^{(f)}| \right) \right) \right\} > 0.$$

Eventually, the total composite flow $\phi_{\mathbf{t}}^{\mathbf{v}} = \phi_{\mathbf{t}_{\mathsf{f},\mathsf{y}}}^{\mathbf{v}_{\mathsf{f},\mathsf{y}}} \circ \phi_{\mathbf{t}_{\mathsf{f},\mathsf{x}}}^{\mathbf{v}_{\mathsf{f},\mathsf{x}}} \circ \phi_{\mathbf{t}_{\mathsf{y}}^{=0}}^{\mathbf{v}_{\mathsf{y}}^{y=0}} \circ \phi_{\mathbf{t}_{\mathsf{y}}^{y \neq 0}}^{\mathbf{v}_{\mathsf{y}}^{\neq 0}} \circ \phi_{\mathbf{t}_{\mathsf{x}}^{\mathcal{I}_0}}^{\mathbf{v}_{\mathsf{x}}^{\mathcal{I}_0}} \circ \phi_{\mathbf{t}_{\mathsf{x}}}^{\mathbf{v}_{\mathsf{x}}}$, $(\mathbf{t}, \mathbf{v}) \in \mathbb{T}_{3N+|I_f|}$, preserves a minimum pairwise distance of

$$\alpha_{\text{tot}}^{=0} = \min \left(\alpha_{\mathcal{I}_f}, \frac{\alpha^{\neq 0}}{\max_i |[i]|}, \frac{L}{N^2} \right).$$

Thus, this procedure shows how to obtain a lower bound of the reachability probability which depends only on the travel times between initial and final positions, impacting the

probability to get the target number of refreshment events, ruled by a homogeneous Poisson process. In future works, it could be interesting to build on this alternative procedure to obtain a coupling strategy.

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[48] We will note $\langle a, b\rangle_+ \coloneqq \max(0, a \cdot b)$ and $\langle a, b\rangle_- \coloneqq -\min(0, a \cdot b)$.

[49] The extended domain $\mathcal{D}(\mathcal{A})$ of the generator corresponds to functions f such that $(f(X_t, V_t) - f(X_0, V_0) - \int_0^t \mathcal{A}f(X_s)\mathrm{d}s)_{t\geq 0})$ is a local martingale ([27]). The description of such domain $\mathcal{D}(\mathcal{A})$, and a suitable core [27, Th. 5.5,], proves to be a strenuous task for almost all considered PDMP-MCMC schemes (see [31, 38]). Here we consider the case where we may associate to (X_t, V_t) a strongly continuous semigroup so that $\mathcal{A}$ (associated to its domain $\mathcal{D}(\mathcal{A})$) is the strong generator of our process. The fact that the continuous and continuously differentiable functions form a core follows from the same approximation procedure that in [31, Prop. 21, Prop 23] for the Bouncy Particle Sampler, for which one of the difficulty here may be that the jump rate may be non smooth.