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Cell list algorithms for nonequilibrium molecular dynamics

Matthew Dobson *, Ian Fox, Alexandra Saracino

Department of Mathematics and Statistics, University of Massachusetts, 710 N. Pleasant Street, Amherst, MA 01003-9305, United States

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ABSTRACT

We present two modifications of the standard cell list algorithm that handle molecular dynamics simulations with deforming periodic geometry. Such geometry naturally arises in the simulation of homogeneous, linear nonequilibrium flow modeled with periodic boundary conditions, and recent progress has been made developing boundary conditions suitable for general 3D flows of this type. Previous works focused on the planar flows handled by Lees–Edwards or Kraynik–Reinelt boundary conditions, while the new versions of the cell list algorithm presented here are formulated to handle the general 3D deforming simulation geometry. As in the case of equilibrium, for short-ranged pairwise interactions, the cell list algorithm reduces the computational complexity of the force computation from $O(N^2)$ to $O(N)$, where N is the total number of particles in the simulation box. We include a comparison of the complexity and efficiency of the two proposed modifications of the standard algorithm.

1. Introduction

Recent developments in the simulation of nonequilibrium molecular dynamics for homogeneous flow have greatly increased the types of flows that can be simulated for long simulation times [1,2]. In a simulation of homogeneous, linear background flow with periodic boundary conditions, the simulation box deforms with the background flow. If care is not taken in the alignment of the simulation box, this can lead to a breakdown of the numerics. However, boundary conditions have been devised for shear flow [3], planar elongational flow [4–6] based on the original study of Kraynik and Reinelt [7], and subsequently for most 3D flows in [1,2].

The deforming geometry of the simulation box presents new challenges when developing efficient algorithms. Many techniques have been developed to increase simulation speed and scalability for the equilibrium case with a static simulation box. One prominent example is the cell list algorithm, which reduces the computational complexity of the simulation from $O(N^2)$ to $O(N)$ by exploiting the short range interaction of the particles to eliminate unnecessary computation. In this paper we present two new versions of the cell list algorithm generalized for simulations using the generalized Kraynik–Reinelt boundary conditions. Previous work by Matin et al. [8] has produced cell list algorithms to treat the deforming simulation box undergoing shear flow or planar elongational flow, which used precomputed cell neighborhood lists based on the specific form of the flow. The versions described here extend the types of flows handled and allow for robust handling of general 3D flows including planar, uniaxial, and biaxial flows.

In Section 2, we describe periodic boundary conditions for equilibrium and nonequilibrium flows. In Section 3, we review the cell list algorithm for equilibrium molecular dynamics before introducing the new modifications for nonequilibrium

* Corresponding author.
E-mail address: dobson@math.umass.edu (M. Dobson).

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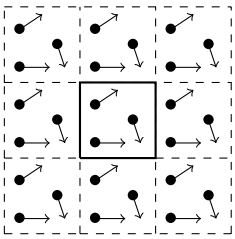

Fig. 1. Periodic boundary conditions at equilibrium. The center square shows a simulation box with three particles. Image particles all experience identical forces and move in sync for all time.

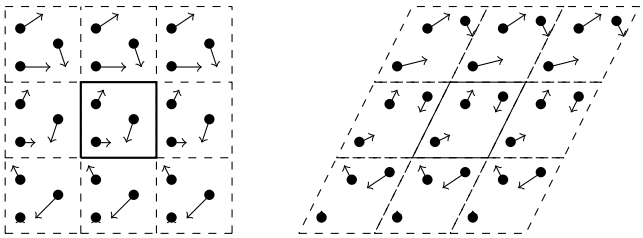

Fig. 2. Periodic boundary conditions under a shear flow. In (a), the initial configuration is shown, with a square simulation box. Note that the image particles have differences in the horizontal component of the velocity depending on the vertical position, consistent with the background shear flow. In (b), the simulation box and all replicas have deformed along with the flow. Again, image particle velocities are position dependent, consistent with the background flow.

flows in Section 4. Two variants are described, the dynamic size cell list and the dynamic offset cell list, and the efficiency of these two algorithms is compared in Section 5.

2. Periodic boundary conditions

Periodic boundary conditions allow the simulation of bulk fluid states by replicating each of the simulated particles in a periodic fashion so that each particle has infinitely many images. We review the formulation of periodic boundary conditions for equilibrium and nonequilibrium molecular dynamics in order to fix notation and describe the setting for the cell list algorithms presented here.

2.1. Equilibrium periodic boundary conditions

The simulation geometry is defined by three basis vectors written together in matrix form:

$$L = [\mathbf{v}_1\ \mathbf{v}_2\ \mathbf{v}_3] \in \mathbb{R}^{3\times 3}. \tag{1}$$

These vectors define a lattice in $\mathbb{R}^3$ whose points are given by $\{L\mathbf{n} = n_1\mathbf{v}_1 + n_2\mathbf{v}_2 + n_3\mathbf{v}_3 \mid \mathbf{n} \in \mathbb{Z}^3\}$. The simulation box is the unit cell of the lattice,

$$\Omega = \{\lambda_1\mathbf{v}_1 + \lambda_2\mathbf{v}_2 + \lambda_3\mathbf{v}_3 \mid 0 \le \lambda_1, \lambda_2, \lambda_3 < 1\}. \tag{2}$$

We explicitly track the position of each particle within the simulation box, and a particle with position $\mathbf{q}$ has an infinite number of images, whose positions are at $\mathbf{q} + L\mathbf{n}$ for all $\mathbf{n} \in \mathbb{Z}^3$, see Fig. 1. Each of the image particles has the same velocity, so that for all times the images move in sync with one another, and a particle with phase coordinates $(\mathbf{q}, \mathbf{p})$ has images with coordinates $(\mathbf{q} + L\mathbf{n}, \mathbf{p})$ for all $\mathbf{n} \in \mathbb{Z}^3$.

2.2. Nonequilibrium flow and the deforming simulation box

In a nonequilibrium simulation of steady, incompressible, homogeneous flow, there is a background flow represented by the trace-free flow matrix $A \in \mathbb{R}^{3\times 3}$. This represents a linear flow field where at spatial position $\mathbf{x} \in \mathbb{R}^3$, the macroscopic velocity equals $\mathbf{u}(\mathbf{x}) = A\mathbf{x}$. We construct periodic boundary conditions where the image particle velocities are consistent with the background flow, as seen in Fig. 2. The lattice vectors are now necessarily time dependent and are denoted:

$$L_t = [\mathbf{v}_{1,t}\ \mathbf{v}_{2,t}\ \mathbf{v}_{3,t}], \tag{3}$$

and in this case a particle with phase coordinates $(\mathbf{q}, \mathbf{p})$ has images with coordinates $(\mathbf{q} + L_t\mathbf{n}, \mathbf{p} + mAL_t\mathbf{n})$ for $\mathbf{n} \in \mathbb{Z}^3$.