Minimum image convention in non-cubic simulation cells

ESDG talk by Zoltán Radnai

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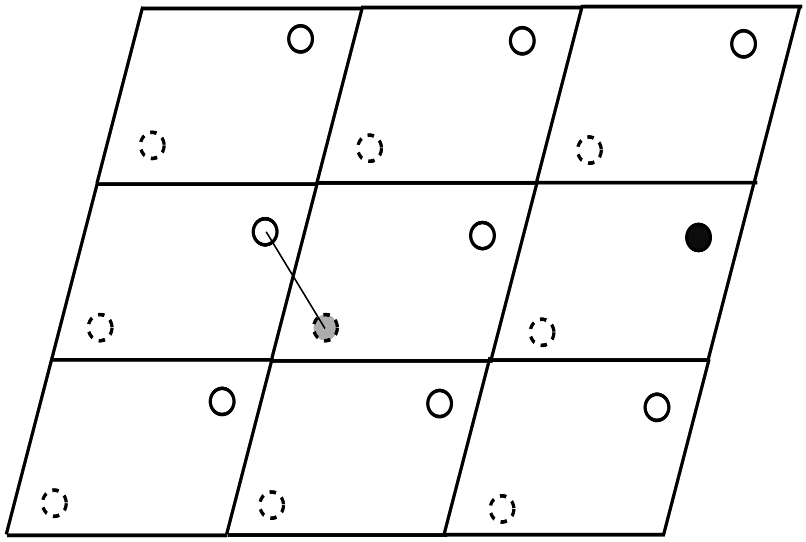
Introduction

- Minimum image convention is often used when a simulation is carried out under periodic boundary conditions.

- The distance between two particles is taken to be the shortest distance between their periodic images:



- Examples of use: interaction between atoms in MD or Jastrow factor in QMC.

Challenges

- This part is one of the most time-consuming (visited often), therefore has to be very efficient. Good algorithms exist for special cell shapes (cubic, FCC, BCC etc.), but not for general Bravais lattices.

- Difficulty arises because minimum image may not be in same simulation cell.

- If we place the origin at one of the particles, the question is mapped to the Closest Vector Problem, or equivalently, to finding the Wigner-Seitz cell in which the other particle is located.

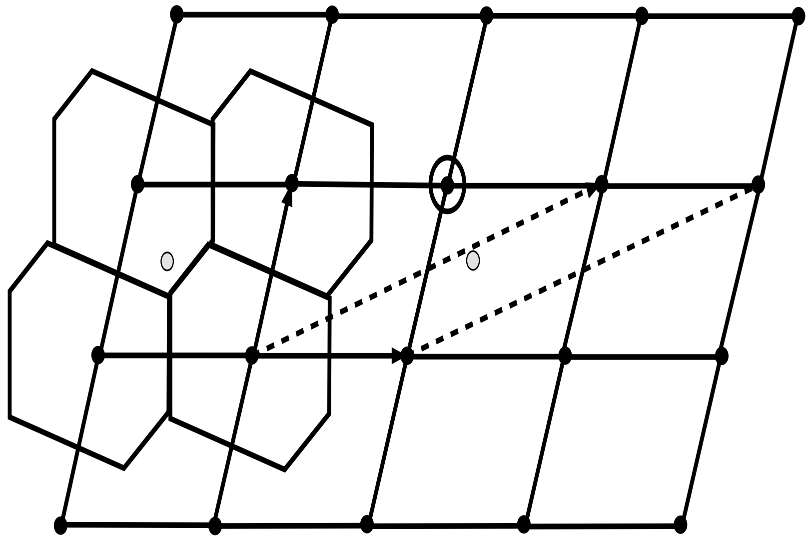
Reduced basis

- Any given lattice has infinitely many possible choice of basis.

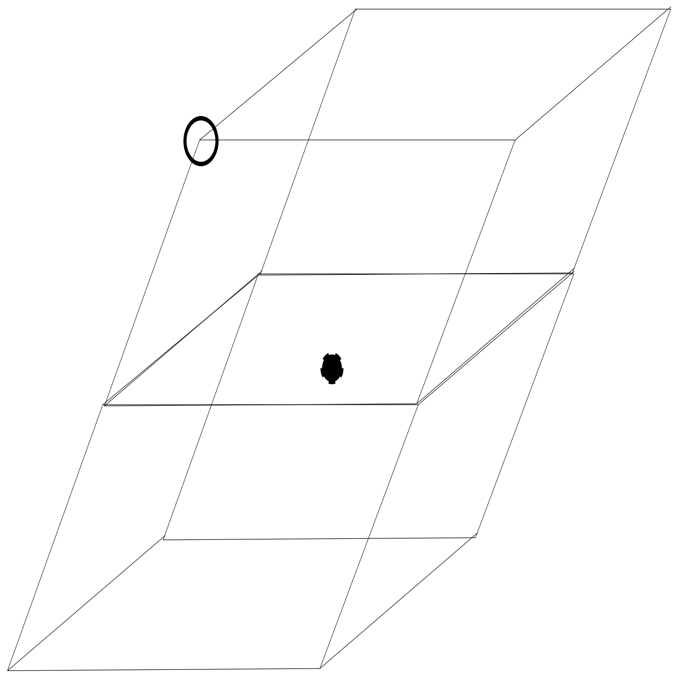
- A “sensible” choice is the shortest possible set of lattice vectors, called the reduced basis. All other lattice vectors (except $\mathbf{0}$) are longer than any of the basis vectors.

- If a lattice is given in terms of any basis, it is possible (at least in 2D and 3D) to *efficiently* find the reduced basis. (Can always do an exhaustive search of lattice vectors).

2D minimum image convention is straightforward. If the basis is reduced, then only need to check the four corners of parallelogram unit cell.



3D is more complicated. It is *not* sufficient to just check the eight corners of the parallelepiped unit cell.



Need to know which lattice points have to be considered, but don't want to consider unnecessary ones.

An efficient algorithm

- One-time pre-screening at start of simulation
  1. Find reduced basis
  2. Find Wigner-Seitz cell
  3. Find which parallelepiped unit cells does WS cell intersect with
  4. The inverse of this gives a list of lattice points that matter

  (2 and 3 can be combined and done simply as a linear programming problem, without need to fully find WS cell.)

- During simulation, only compare distances to those lattice points in the list.

- Can further improve by dividing unit cell into small parallelepipeds, and doing pre-screening for each of those. Most of the parallelepipeds will only have one lattice point that matters, hence there is large improvement in efficiency.

Conclusion

Minimum image convention as often implemented fails for some lattices. It is not straightforward to come up with a general algorithm. However, with well-designed set-up at the start of the simulation, it is possible to have an algorithm that does not sacrifice efficiency.