Questions for Day 05 (20-Aug-2020)

Questions related to Classical Atomistic Modeling

- [Name] Question (leave the template)
- [Dahvyd] (molecular statics slide 53) It looks like conjugate gradient is just taking into account the previous step: i.e. if the forces are increasing in the same direction as compared to the last step, then increase d, if the forces are decreasing then decrease d, if the last step moved orthogonally to the present step then keep moving in the previous direction as well. Is that the correct interpretation?
- [Biswarup, Ariel Perera] (slide 57) Is the verlet list useful only for short-range interaction? For example, if particles are interacting via Coulomb interaction we need to compute interaction between all the particles. Is there any way to make the calculation faster under such situations? (Ewald, Particle mesh, fast multipole)
- [Dahvyd] (molecular statics slide 57) Is delta_max in the two max sum the total displacement of the atom from when the last verlet list was calculated or the maximum movement of just that time step?

- [Daniel P] *Periodic Boundary Conditions (Slides 59 - 61):* When simulating a system in which we focus of the center while the rest of the simulated medium serves as a buffer between the volume of interest and the edges of our simulation, it is clear that some volume is *sacrificed* to get a good approximation of an infinite crystal about out volume of interest. **How** can the replication of our volume of interest in all directions (slide 61) give us a similar picture to the method in slide 59 (where 40% of the volume is thrown out)? It seems like we create our own periodic lattice by replicating the volume of interest - **how** does that compare with reality? Once we generate the initial lattice by replication of the cell of interest in all directions, **how** do we go on if we want to introduce a change into that one cell? Say, do we modify the whole lattice (because it is stored in a formula that references the initial cell), or do we change the inner cell only (because after construction the whole lattice now stored in the memory regardless of further changes), or anything else? I.e., I am not convinced this is a good method.

- [Maria] Slide 61 (still boundary conditions) - What if one of the atoms in the small system approaches the boundary of that system? Meaning, can it cross to the neighboring system? Will it “bounce” on the wall of that system? How do you treat such a case?

- [Gilad M, Daniel K] After explaining the last equation on slide 62, Ellad said “It means you need to run with a larger cell than you actually need to. It may be that it’s larger than your true periodicity because of the neighbor list size.” I don’t understand this. What’s the cell size you “actually need?” What’s the “true periodicity?” Isn’t twice the neighbor list size the bare minimum periodicity you should be using anyway so that you don’t interact with the same atom twice?

- [Gilad M, Alon Inbar,Chen Oppenhime] Error in slide 65; FCC unit cell contains 4 atoms, not 1
- [Biswarup, Amir K., Arkady K] (General question about the periodic boundary condition) If we take a square box of length L and use periodic boundary condition then the lowest possible mode will be k_min = 2pi/L. Thus, we can't have excitation with a lower value of momentum. But the real bulk system may have lower excitations. Does this restriction (imposed by PBC) have any consequences?
- [Di] Would the periodic boundary condition introduce artefacts if we need to apply a field (ex: E-field in z-direction with PB on z as well)
- [Di] If we want to simulate a system of layered materials, for example, solid-liquid-solid, and in real experiments, they don't repeat in the direction perpendicular to normal of the layers, what kind of boundary condition is suitable?>
- [Di, Oksana Yanshyna] Slide 57. I couldn't understand the "two max sum" criterion. It would make more sense to me, if it is the radial component of 0.5*(dmax,1+dmax,2) > dskin.
- [Galit] Slide 56- didn't fully understand the answer to the second question.. What causes the energy barrier? Or how can one compute it?
- [Tahe,Chen Oppenhime] If we are only modeling the minimum of the energy surface (global and local) without the maximum peaks, how can we predict its structure in certain conditions (equilibrium)? Meaning, do we have other tool to know whether there will be enough energy in the system to overcome maximum peaks?
- [Georgia, Tami] molecular statics-slide 53: Would it make sense to combine the methods? Like start with steepest descent or conjugate gradient and when we are close to an area around the minimum, switch to newton-raphson? To my understanding NR would be better around the minimum since it is based on second derivatives.
- [Di] Since bonded force fields are not included in KIM. Any advice on how to choose? Is there any equivalent of KIM for bonded force fields?
- [Vlada] Slide 70, Are all of those results represent evolution of exactly the same system? Or rather it is an evolution with some changed parameters, like temperature, etc?
- [Israel Greenfeld] What would be a minimum cell size for a non-periodic material? How to calculate it?
- [Israel Greenfeld] slide 59 - how do you set the far field BC?