

Multiscale methods for soft matter physics

Maurizio Gilioli

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Chapter 1

Questions

All in notes if not specified

Legend:

- tuckerman: Tuckerman book
- not notes
- demonstrate: make the demonstration
- LJ: Lennard-Jones potential

Lessons questions

- Lesson 1
 1. What is soft matter?
 2. Is active moving matter soft material?
 3. What is the definition of soft matter?: Soft matter or soft condensed matter is a subfield of condensed matter comprising a variety of physical systems that are deformed or structurally altered by thermal or mechanical stress of the magnitude of thermal fluctuations.
 4. What does it mean to define soft matter as mesoscopic? what are the consequences?
 5. How should be defined the bigger compounds? what happens to time and space scale when those are utilized?
 6. Will have the force to be specific?
 7. What is the approximation that allow to simplify quantum mechanical problems with classical mechanics?
 8. How are thermal systems driven?
 9. What is the Helmholtz free energy? Which system is described? How is it obtained? (Tuckerman)
 10. What is the critical point? (See tuckerman) What happens?
 11. What is the Ising model? How can you describe with it the critical point?
 12. What is necessary to make Multiscale methods relevant? (hierarchy) The use of a mapping function
 13. What procedure allows the coarse-graining?
- Lesson 2
 1. Where are defined experimental observations? In a Universe

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2. What is the Newton principle of determinacy
 3. What elements are defined in your experimental space?
 4. What is Galilean invariance? In which conditions it is maintained?
 5. What is a model? and what allows to build? A definition of a system
 6. Is invariance maintained in case of isolated systems? and in the case of systems with several bodies?
 7. When are forces conservative? In physics, a force is considered conservative if the work done by the force on an object is independent of the path taken by the object. In other words, the total mechanical energy of the system (kinetic energy plus potential energy) remains constant as the object moves within the force field.
 8. What is the action integral? What does it tell? What does satisfy a path called stationary? (demonstrate) (tuckerman)
 9. What does the action integral concept suggest? (tuckerman)
 10. Write Euler lagrange equation
 11. What is the formula of the Lagrangian?
 12. What is the Legendre transformation (tuckerman)
 13. What is the Hamiltonian? how is it obtained? (tuckerman)
 14. Which are the Hamilton equations?
 15. What happens to the Hamiltonian when the Lagrangian is conserved?
 16. What is an ensemble? In classical statistical mechanics, the ensemble is a probability distribution over phase points (as opposed to a single phase point in ordinary mechanics), usually represented as a distribution in a phase space with canonical coordinate axes.
 17. How is the value of a macroscopic observable normally obtained? (through a time average ...)
 18. To what a time average can be converted? what is a phase space average?
 19. When is a stochastic process called ergodic? relating to or denoting systems or processes with the property that, given sufficient time, they include or impinge on all points in a given space and can be represented statistically by a reasonably large selection of points
 20. How do we obtain a microcanonical ensemble? N, V, E TODO
 21. What are Poisson brackets? When is a quantity conserved? (tuckerman)
 22. What does the Liouville theorem say? It says that as the systems contained in a tiny region of phase space evolve according to classical mechanics, the volume they occupy remains constant. TODO explain why
 23. When is the average of a quantity constant in time?
 24. How can you write the average of that quantity?
 25. What is a partition function? what type of coefficient it has? TODO
 26. Formula for entropy in the microcanonical ensemble TODO

- Lesson 3

1. Describe the canonical partition function, what is the related coefficient? TODO
2. What is a Boltzmann weight? it is the probability of a certain configuration, the lower is the energy associated to the configuration, the higher is the Boltzmann weight and viceversa
3. What type of ansatz you assume to simplify your work? What is the adiabatic approximation TODO

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4. Describe the Born-Oppenheimer approximation TODO
 5. What is meant by separability when talking about the potential energy? and additivity?
 6. What is a multi-body potential? What type of truncation you can perform?
 7. What are the differences between VdW and Coulomb interactions?
 8. What is the Newton Raphson method? TODO
 9. What is the difference between bonded and non-bonded interactions?
- Lesson 4
 1. How can be non bounded interactions truncated?
 2. What is a periodic boundary condition? A periodic boundary is an important technique in a molecular dynamics simulation. It is a clever trick to make a simulation that consists of only a few hundred atoms behave as if it was infinite in size.
 3. Why should you use periodic boundary conditions
 4. How do you write the energy due to cut-off short distance interactions, what's the tail correction?
 5. In which case you can't absolutely ignore the epsilon tail energy?
 6. What is the typical length for the cut-off distance?
 7. What is the correction for LJ?
 8. How do you compute the Coulombic and LJ interactions?
 9. How are interactions classified as short and long?
 10. Write formula for short potential and long range potential (consider PBC)
 11. How do you select a cut-off for the short range interactions?
 12. What is the minimum image convention?
 13. What is the Verlet list algorithm
 14. How do you avoid bumps in short potential?
 15. How do you calculate long range potential?
 16. Which is the fundamental concept around statistical mechanics?
 17. What is an integrator? How does it use time?
 18. Write Euler integrator
 19. What is the problem with the Euler integrator?
 20. What is the Euler-Cromer integrator?
 21. What is the mathematical difference between the two previous integrators?
 22. What is the meaning of symplectic?
 23. What is a unitary matrix
 - Lesson 5
 1. How do you express the average of a quantity in equilibrium? Introduce the Liouville operator
 2. How can you decompose the Liouville operator? What changes do the parts produce?
 3. What problem do you face by doing that separation? what expansion comes into play?
 4. Write the Velocity Verlet algorithm, do the evolutions remind you of something?
 5. What is conserved by applying the Velocity Verlet algo?
 6. How is different the shadow H with respect to the real Hamiltonian?

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7. How would you call then the Velocity Verlet algo?
 8. _____
 9. How can you transform a time evolution? and in which condition?
 10. How do time dependent correlation functions behave in time? Write the formula
 11. How would you find in general a quantity A? But what's the problem with the integration process?
 12. What's the idea behind stochastic integration?
 13. How do you write an integration performed by using a uniform distribution?
 14. How can you improve this stochastic sampling?
 15. What's the limit of stochastic sampling? What is the Bulk problem? (topic included also in the next lecture)

- Lesson 6

1. What happens when you sample with more and more dimensions?
2. What is the objective of Markov chains?
3. On which configuration Markov chain structures depend upon?
4. What the transition probability matrix? how transitions are formalized?
5. What is the definition of ergodic (ergodicity expresses the idea that a point of a moving system, either a dynamical system or a stochastic process, will eventually visit all parts of the space that the system moves in, in a uniform and random sense. This implies that the average behavior of the system can be deduced from the trajectory of a "typical" point. Equivalently, a sufficiently large collection of random samples from a process can represent the average statistical properties of the entire process.)
6. What does the Frobenius theorem say?
7. What is the behavior of the eigenvectors of a transition matrix over time? What is the detailed balance?
8. How are computed the elements in the transition matrix?
9. Write the Metropolis algorithm using the Boltzmann equation for the distribution
10. What can you calculate at the end
11. What if a transition is rejected?
12. What is a sweep? When is an operation of order n? (make use of the example with the spins)
13. When do you prefer to use Markov chains? instead of Molecular Dynamics?
14. What is the difference between Markov chains and Molecular Dynamics?

- Lesson 7

1. In which relation are the short atomistic time scales, the relaxation times of the colloids and the diffusion time?
2. To what depends the diffusion time?
3. What steps would you alike to follow to proceed with the coarse graining?
4. what does the Markov property say?
5. What is the Smoluchowski equation?
6. How do you write the infinitesimal change of f in time?
7. Find the probability of finding a particle at position r after time t (Fokker Plank equation)

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8. How are newtonian systems positions related to the time of simulation
 9. How Diffusion dynamics is different? What is the general solution?
 10. Make an example of solving equation of dynamics for diffusion
- Lesson 8A
 1. What case we considered up to now?
 2. What is the fine grained effective description of a system?
 3. Is a normal system (like a biological solution) Hamiltonian?
 4. Describe the forces in that system, average? correlation?
 5. What is τ ?
 6. Find the diffusion formula?
 7. How do you find the amplitude of correlation?
 8. What does the Fluctuation-Dissipation theorem say? What are the important points?
 9. What is a Langevin thermostat?
 - Lesson 8B
 1. What is a partition function
 2. How can you simplify the calculation of the average of a quantity a ($\langle A \rangle$)?
 3. How do you obtain the correlation function?
 4. How do you obtain the partition function?
 5. How is the radial function for a non-interacting system (ideal gas)
 6. How is the radial function taking into consideration just a single particle
 7. How is the radial function taking into consideration just two particle, what assumptions do you make?
 8. What is the radial distribution function?
 9. How is the graph of that distribution? why are there bumps?
 10. How can you calculate energy, pressure and compatibility on the base of that?
 11. What theorem could you apply to gain information about the fluctuations of a system? on the base of the radial distribution function?
 - Lesson 9: Free Energy calculation
 1. which is the partition function of the canonical ensemble
 2. How is it calculated in case of ideal gas?
 3. How do you write a difference in free energy? Write it taking also as reference the system 1
 4. With what type of integral you can rewrite the difference formula. Write consequently the Kirkwood Thermodynamical Integration theorem
 5. What does the Kirkwood Thermodynamical Integration theorem allows you to do?
 6. Obtain $P_0(v)$, which shape does it have?
 7. Supposing the Gaussian shape, what's the problem that you have with the curve that you generated?
 8. What does the calculation of the free energy difference allows you to do?
 9. How can you simplify the calculation? make the example regarding the solvated ion

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10. What is a reaction coordinate
 11. Make the example taking the distance as collective coordinate
- Lesson 10: Renormalisation group
 1. what is a renormalization group in biophysics and why it is called a group? In biophysics, as in other fields of physics, the renormalization group (RG) is a theoretical framework used to understand the behavior of complex systems across different scales. The term "group" in renormalization group refers to a mathematical structure, specifically a group of transformations. The renormalization group provides a systematic way to analyze how physical properties change as we zoom in or out, or as we move through different energy or length scales.
 2. what happens to a liquid with high Temperatures? and with low temperatures? What happens to the partition function?
 3. How is entropy while varying the temperature?
 4. What is phase transition?
 5. What is the order of a phase transition? What happens at the critical point
 6. How is correlation changing outside the CP and in the CP?
 7. When is a system self-similar? what does it mean? To how many parameters depend the correlation length?
 8. How would you write the hamiltonian of the Ising model by making use of the renormalisation group? And the partition function?
 9. What is the meaning of defocusing? How can defocusing be done?
 10. What is a projection operator?
 11. How are the partition function and the free energy after defocusing?
 12. What happens when you defocus your system in terms of entropy? And what free energy do you obtain?
 13. What happens to a correlation function at each step if not on a critical point? what if on a critical point?
 - Lesson 11: The process of coarse graining and the multibody potential
 1. What is the aim of Coarse Graining?
 2. How are interactions called in Coarse Graining?
 3. What is a reference?
 4. What are the possible modelling approaches?
 5. How is the partition factor for the all atom model? and for the CG model?
 6. What free energy formula can you obtain from the CG partition function?
 7. How is the degeneracy factor?
 8. How can you write the mapping process? How mapping has to be? (specific)
 9. How is the CG process?
 10. Is mapping invertible?
 11. What is the consistency condition?
 12. Obtain the potential energy that you get coarse-graining the system
 13. When is your CG system ok?
 14. What is transferability?

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15. What is the multibody potential mean energy? write the process to obtain the related force
 16. How do you allow the consistency condition for the momenta?
- Lesson 12: How is it possible to equate our potential to the multibody potential?
 1. Which condition should be affirmed?
 2. How can we force $U(R)$ to satisfy that condition?
 3. What is relative entropy?
 4. How do you compute the distance between two distributions? What is the most important probability?
 5. what is the degeneracy factor?
 6. What is the formula for the partition function?
 7. What is the mapping entropy
 8. How do you average the atomic probabilities? what does this allow you to do with the mapping entropy?
 9. When and how does the mapping entropy change?
 10. What do you obtain by mapping in terms of relative entropy?
 11. What formula of relative entropy do you obtain that should be minimized? (Gibbs-Bogoliubov inequality)
 12. What is the potential energy that you have at the minimum of the relative entropy
 13. What is also conserved in case in which the relative entropy is at the minimum?
 - Lesson 13
 1. What is the Boltzmann inversion process?
 2. Write the process to obtain the potential energy through Boltzmann inversion
 3. What is a more general way to write the Boltzmann inversion?
 4. What happens if we have more than a single collective coordinate? explain the two possible cases
 5. What is the double counting problem?
 6. What is the solution? (explain with formulae)
 7. What is another problem with the iterative Boltzmann inversion process? What kind of properties do not converge for example?
 - Lesson 14: Inverse Monte Carlo
 1. What is the problem that you have with Boltzmann Inversion?
 2. How do you solve the limitation?
 3. What is Inverse Monte Carlo?
 4. What do you have to compute by using inverse Monte Carlo? (susceptibility matrix)
 5. What does the susceptibility matrix tell you?
 6. How do you calculate the infinitesimal change in potential energy after
 7. How does Monte Carlo converge?
 8. obtain from relative entropy the susceptibility matrix
 9. What softer do you generally use to parametrize the CG potential?
 10. Is the cut-off important in Boltzmann inversion?

11. Is parametrization always correct or is it specific?

- Lesson 15: Force Matching

1. What is force matching?
2. What is the MB force field and how can you write it?
3. How do you compare force fields?
4. How can you also write the comparison of the atomic force field and the coarse grained force field (in terms of the multibody force field)?
5. What do you deduce from that relation?
6. How can you find an F (coarse grained f.f.) which is as close as possible to f (atomistic f.f.) (concept)? (χ^2 method)
7. What is the meaning of χ^2 applied to this problem? (until plane explanation)
8. How do you find the minimum in the difference $\underline{f} - \underline{F}$
9. What happens when all your interactions are all independent?
10. How does χ^2 differentiate himself from relative entropy?
11. Why Force Matching does not produce very good radial distribution functions?

- Lesson 16: Protein models

1. what does the Anfisen experiment tell us?
2. what is the protein folding funnell?
3. why to use CG?
4. what type of approaches are available?
5. what models are available?
6. what is a lattice model?
7. which types protein models exist?
8. what is a martini model?
9. what is a go model?
10. what is inferred by saying that proteins are conformationally selected by ligands?
11. How is the vibrational nature of proteins involved?
12. what is a elastic network model?
13. how can you evaluate slow modes in ENMs?
14. what are quasi-rigid domain description models?

- Lesson 17:

1. what is a polymer?
2. what are the types of a polymer?
3. what quantities you should consider?
4. what is the contour length
5. what is hte end to end distance?
6. what is the radius of gyration?
7. what are the models generally used for polymer modelling?
8. what are freely jointed chains?

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9. what is a kramers-fox model?
 10. what is the persistence length? and the Kuhn length?
 11. what are self-avoiding chains? how can you describe the average difference in volume?
 12. what is the Kuhn-Grest model?
 13. how can you evaluate the stiffness of a polymer?
 14. main characteristics of DNA
 15. what is ssDNA
 16. what are the resolutions types used on the base of the length wanted
 17. what is a crumpled globule model?
- Lesson 18
 1. what is a topological problem in soft matter?
 2. what are for example topologies in biology?
 3. what is a knot mathematically?
 4. how do you define a knot?
 5. which are the most common types of knots?
 6. what are Reidemeister moves?
 7. can you define knots in open chains?
 8. what is the concept of minimally interfering closure? with what process do you find it?
 9. what is a knotoid? how can it help you?
 10. what are in-protein links?
 11. what is a Gauss number in this context?
 12. to what is proportional the folding rate? to what is negatively correlated?
 13. what is knot dynamics? what type of chain model is normally used in this context?
 14. what is the transmission coefficient?
 15. where do the knots tend to position themselves? why not on the stationary nodes?
 16. how can you intend the position of a knot on a length? what type of ... you expect on the stationary points?
 17. what is interesting about knots in proteins? why you don't expect them?
 18. what characteristics are necessary for self-folding? what type of measures do you adopt as a consequence?
 19. what is an elastic folder model? what is its main role?
 20. what is the process through which you evaluate the folding rate through the elastic folder model
 21. What type of measure do you adopt to evaluate the folding process?
 22. what is the RMSD?
 23. what is a LASSO protein?
 - Lesson 19 - multi-resolution and dual resolution models
 1. which are the top-down and the bottom-up models?
 2. what is the purpose of adaptive resolution simulations?
 3. what is the objective of multi-resolution models?

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4. what are the two types?
 5. what is a switching function?
 6. how do you write the force of a system described by a multi-resolution model?
 7. what is the purpose of quasi-grand canonical (AdResS) simulations? what is changing and in what condition?
 8. what are the problems related to AdResS?
 9. what is the hamiltonian version of AdResS? what kind of force you obtain?
 10. what is the problem that you observe by looking to the force formula? In which way do the particles behave on the interface between AA and CG?
 11. what kind of correction you have to give to compensate the drift force (precedent point)?
 12. what kind of system do you have after the first correction?
 13. how can you obtain a system that has instead equal density? make a scheme at the end
 14. Is it possible to have a system with same density and pressure?
 15. what type of advantage you have by using a multi-resolution scheme in the water-gas model?
 16. how do you measure normally the chemical potential? how can you use the multi-resolution scheme to improve it?
 17. what is the fast calculation of solvation energy process?
 18. what can you also investigate with the multi-resolution models? of proteins
 19. what is a dual resolution? what are the main problems?
 20. how you solve them?
 21. how does the free energy can help you when coarse graining the active site of an enzyme?
 22. what is the problem that you encounter in the previous point?
 23. what can you solve with both the methods?
- Lesson 20: Fluids?
 1. what does the navier stokes law sais? why you can't use it in MD
 2. what is a celular automata?
 3. what is multiparticle collision dynamics? what is the reasoning behind stochastic rotation dynamics?
 4. is it possible to use multiparticle collision dynamics with different types of particles
 5. how can you study hydrodynamics?
 6. what can you observe?
 7. what is Dissipative particle dynamics? endenumerate