Exercise Instructions for Students

1. Name which computation method you would use to calculate a force interaction between atoms, assuming that you do not have an equation that describes the attraction or repulsion between the atoms?
2. What do you think the advantages and disadvantages are of “course-graining” an atomistic model?
3. Is there a computational approach that can make a prediction or correlation about a system, without having any actual knowledge about it works?
4. Could you use molecular dynamics to simulate cosmic body trajectories?
5. Explain for which situations it is okay to assume that matter is continuous (i.e., there are no atoms or molecules) and conservation equations (e.g., force, mass and energy balances) are sufficient to describe the behavior of a system.