Bioinformatics Practicum

Phase transitions of argon

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1 Introduction

1.1 Molecular dynamics (MD)

Molecular dynamics is an integrative field of physics and computer science that aims to model the behavior of all atoms in a relatively small virual sample volume. To reduce the complexity of this problem, most MD simulations ignore quantum mechanics and model only covalent bonds, Van-der-Waals radii and electrostatic interactions and try to solve the trajectory and position of each atom for all time steps of a simulation.

This approach is aided by deriving all forces the atoms exert on each other from a force field equation, a mathematical model that serves to lookup the gradient of potential energy on each atom at a given timepoint. The Amber force field (Eq. 1.1) for example adds the potential energy of covalent bond distances (first term), covalent bond angles (second term), rotations on covalent bonds and stiffness of covalent double-bonds (third term), Lennard-Jones potential (fourth term) and Coloumb - interatomic electrostatic - potential (fifth term).

$$\begin{aligned} V_{AMBER} = & \sum_{i}^{n_{bonds}} b_i(r_i - r_{i,eq})^2 + \Sigma_i^{n_{angles}} a_i(\theta_i - \theta_{i,eq})^2 \\ & \&quad + \Sigma_i^{n_{dihedrals}} \Sigma_n^{n_{i,max}} (V_{i,n}/2)[1 + \cos(n\psi_i - \gamma_{i,n}] \\ & \&quad + \Sigma_{i<j}^{n_{atoms}} \left(\frac{A_{ij}}{r_{ij}^{12}} - -racB_{ij}r_{ij}^{6} \right) + \Sigma_{i<j}^{n_{atoms}} \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} \end{aligned}$$

2 Some LaTeX examples

2.1 Paragraphs, citations, and footnotes

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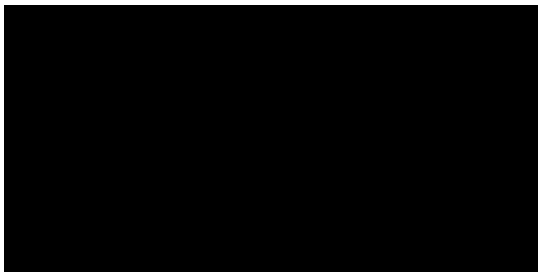

Figure 1: Always provide a short description of the figure.

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2.2 Equations

You can "in-line" small equations like this: $\vec{F}(\vec{r}) = -q\vec{\nabla}\varphi(\vec{r})$. Otherwise, equations should be in a separate line like this:

$$H : \mathrm{T}^*\mathcal{Q} \to \mathbb{R}^+ \cup \{0\}\,,\ (q,p) \mapsto \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$$

If you want to refer to them somewhere in your text, you should assign a number (Eq. 1).

$$H : \mathrm{T}^*\mathcal{Q} \to \mathbb{R}^+ \cup \{0\}\,,\ (q,p) \mapsto \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \tag{1}$$

2.3 Tables and figures

Figure placement can be automatically decided on the basis of a set of restraints given in brackets (see comments in the code). For example, Fig. 1 is always located at the top area of a page (`[t]`).

Row No.	Left	Centered	Right
1	lorem	a	3.14
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3	elit	ef	1.618

Table 1: Always provide a short description of the table.

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Each table and figure should be referred to in your text, no matter their exact location (Table 1).

References

[1] J. Schröder, H. Schröder, S. J. Puglisi, R. Sinha, and B. Schmidt. SHREC: a shrot-read error correction method. *Bioinformatics*, 25(17): 2157–2163. 2009.

[2] P. Meinicke. UProc: tools for ultra-fast protein domain classification. *Bioinformatics*, 31(9): 1382–1388. 2015.