Indian Institute of Technology Delhi  
School of Interdisciplinary Research (SiRe)

PhD Project

Project Details

<table>
<thead>
<tr>
<th>Role</th>
<th>Faculty</th>
<th>Academic Unit in IITD</th>
<th>Email ID</th>
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<tbody>
<tr>
<td>Supervisor 1</td>
<td>Prof. Anoop Krishnan</td>
<td>Civil</td>
<td><a href="mailto:krishnan@iitd.ac.in">krishnan@iitd.ac.in</a></td>
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<tr>
<td>Supervisor 2</td>
<td>Prof. Manidipa Banerjee</td>
<td>Kusuma School of Biological Sciences</td>
<td><a href="mailto:mbanerjee@iitd.ac.in">mbanerjee@iitd.ac.in</a></td>
</tr>
<tr>
<td>Supervisor 3</td>
<td>Dr. Manish Agarwal</td>
<td>CSC</td>
<td><a href="mailto:zmanish@iitd.ac.in">zmanish@iitd.ac.in</a></td>
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The order of supervisors may be switched for some students.

Project requirements (Student qualifications, experience required, etc)

- B.Tech/BE/M.Sc, or higher
- Basic knowledge of statistical mechanics, experience with molecular simulations packages (at least one)
- CSIR/ICMR/DBT-A JRF qualification or valid GATE score, if applicable

Source of funding (IRD/FITT Project details, if any)

PDF or IRD project funds may be used.

Role of Faculty Members involved:
Prof. Anoop Krishnan and Dr. Manish Agarwal would guide the student in the setup and analysis of all-atom and coarse-grained molecular dynamics simulations of biological molecules. Force fields would be generated using traditional and recent AI/ML methods. Prof. Manidipa Banerjee would guide the biological fidelity, along with experimental insights.

Design of coarse-grained force fields for molecular simulations of biologically relevant molecules

Currently available all atom and coarse-grained forcefields lack sufficient fidelity for the relevant temporal and physical timescales. Starting from molecules which exhibit self-assembled moieties, this work aims to establish forcefields for use in commonly available molecular simulation packages. Biological assemblies such as peptide/protein cages, nanoparticles and virus capsids will be analyzed.