



# CSSI Element: Highly Efficient and Scalable Software for Coarse-Grained Molecular Dynamics

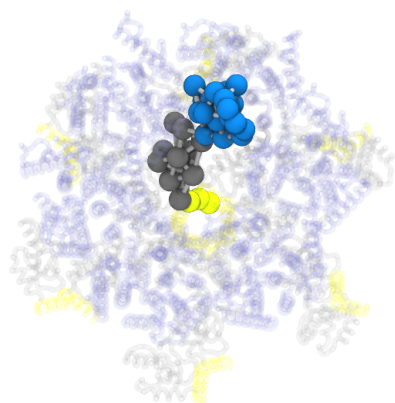
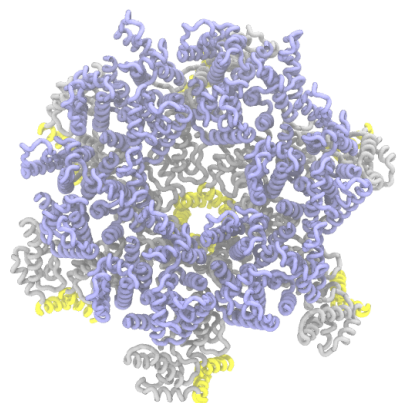
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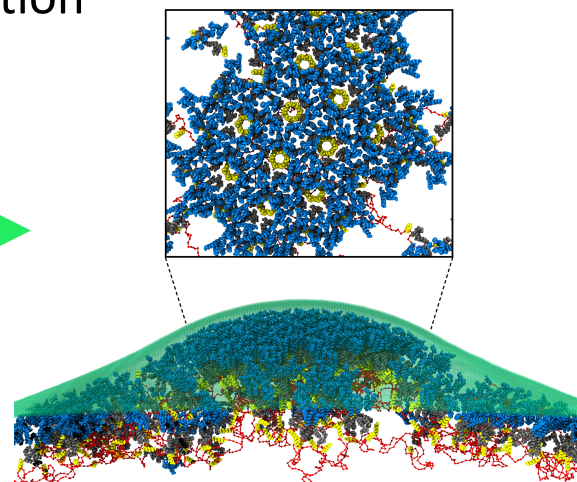
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## Model Generation



## Simulation



## KEY CHALLENGES

- Systematic CG development is difficult and fragmented
- Bottlenecks slow simulation implementation and runtime

## OUR APPROACH

- Integrated tools for bottom-up CG development and simulation
- Open-source network to enable community-driven development

The screenshot shows the homepage of the Multiscale Coarse-Graining (MSCG) project. The header includes navigation links: Home, About, Downloads, Tutorials, and Community. The main title is "Multiscale Coarse-Graining" with the subtitle "Systematic methods for multiscale phenomena in biology and materials science". Below the title is a diagram showing the transition from "All-Atom" to "Coarse-Grain" with four numbered steps. A mathematical equation is displayed: 
$$\frac{\partial U(v, \mathbf{R}^{N_v})}{\partial \mathbf{R}^N} = \left( M_{R,v}^{N_v} \left( \frac{\partial}{\partial \mathbf{r}^a} \left( u(\mathbf{r}^a) - \frac{1}{\beta} \ln p_{\Sigma}(\mathbf{v}, \mathbf{r}^a) \right) \right) \right)_{\mathbf{R}^{N_v}, v}$$
 The "Downloads / MSCGFM" section describes the MSCG method as a variational force-matching technique and provides links to "From GitHub" and "GitLab Server". The "Features" section lists: Range-Finder (Generate pair lists from LAMMPS or GROMACS trajectory files), Reweight (Weight frames in a trajectory differently in force matching), Tabulated (Generate tabulated interaction potentials by force matching), Iterative (Iterative force-matching method for CG distribution functions), Multi-Body (Linear approximations to solve 3-body and 4-body interactions), and Dynamic (Dynamic state sampling technique to build UCG interactions).