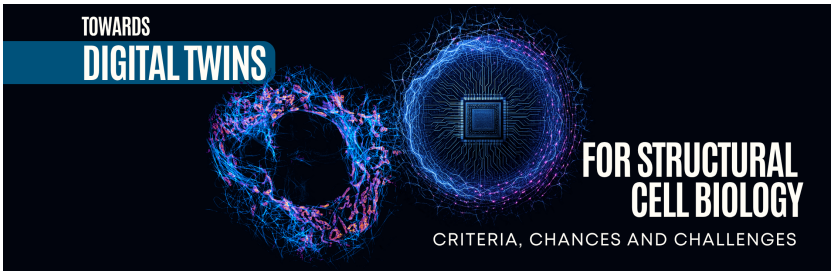


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# In-cell structural systems modeling

*Thursday, 5 March 2026 17:30 (45 minutes)*

One of the central goals of computational biology is to build a realistic model of a cell –one that can simulate cellular processes, predict the effects of perturbations, and support rational drug design. This vision has gained new momentum through recent technological advances, for example, in single-cell omics, structural proteomics, and visual mapping of cells using in-cell cryo-electron tomography (cryo-ET) and volume electron microscopy. The emergence of AI-based methods such as AlphaFold and other AI-driven models of biological complexity further contributes to this renewed interest. Although the form of such a comprehensive cell model remains undefined, the recent technological advances now allow us to build components that were previously out of reach. In this context, I will present our contribution toward modeling a cell by leveraging some of these recent technological advances. I will show the computational tools we are developing as part of an effort to build a computational framework for in-cell structural systems biology, aimed at enabling spatial and systems-level mapping of the cellular environment. These will include methods for data-driven modeling macromolecular assemblies and interaction networks, as well as approaches for identifying and modeling molecules and membranes in cryo-ET data.

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