

**Wojtek Potrzebowski**, working in Janusz Bujnicki's group at the International Institute of Molecular and Cell Biology in Warsaw, Poland, will give a seminar this Monday (22nd) at 13.30 in the biochemistry library. He will describe his work of developing a new method of fitting atomic structures into cryo-electron microscopy models. Welcome!

Host: Ingemar André

## **Fitting of Structures Into Density Maps**

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Experimental advances in producing electron microscopy data on structures of macromolecular assemblies have paved the way for theoretical methods that dock atomic models into low-resolution electron density maps. Although considerable progress has recently been made in building pseudo-atomic models based on combination of cryo-EM and X-ray crystallography, putting together macromolecular assemblies consisting of tens or even hundreds of components remains a challenging and open issue. The same is true for combining structures with partial information e.g. with known molecular shape.

I developed a method for fitting atomic models or any user-defined shapes into cryo-EM maps by means of reduced mesh representation. The program achieves this goal by calculating the Minkowski sum of polyhedrons of the structure or any user-defined shape and the map. The exact position of the fitted component is obtained by finding "tight passages" in the configuration space defined by the Minkowski sum. This method has been inspired by an approach used in mobile robotic navigation control in obstacle environment. The method can be applied to infer the fit and orientation of individual components in low-resolution electron density maps of macromolecular assemblies