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### Macromolecular computational crystallography: Looking forward and backward

Addressing to more and more difficult problems of molecular structural biology requires development of new methodological, mathematical and computational tools. For macromolecular crystallography, that is one of the principal methods for the structure determination, the well-known lines of development are automation, structure analysis at very high and at very low resolutions, as well as model and data validation. Other developments are relevant to determination of very large or/and very flexible structures. There is also an evolution of crystallographic tools with a goal to apply them to non-crystallographic samples like isolated objects in XFEL or cryo electron microscopy images. In general, integration of other structural techniques with macromolecular crystallography is an ongoing process. While completely new and original ideas are required to go forward, some structural problems of macromolecular crystallography could be addressed by 'recycling' the tools and ideas known for a while. However, sometimes their routine use may result in misleading or in meaningless results. This requires properly revisiting the corresponding tools and notions. The talk will develop these issues illustrating them by several practical examples.

### Biography

Alexandre Urzhumtsev is a full Professor at the Université de Lorraine, Nancy, and a Researcher at the IGBMC, Illkirch, France. He completed his PhD in X-ray Macromolecular Crystallography. His main research interests include "The development of computational methods and programmes for structure solution, refinement and validation, as well as solution of difficult structures where development and application of original algorithms are required".

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