GI-MS48-P14 | TEACHING OLD TRICKS: ROTATION CONVENTIONS IN CRYSTALLOGRAPHY AND CRYOEM

Urzhumtsev, Alexandre (IGBMC, Illkirch, FRA); Urzhumtseva, Ludmila (IBMC, Strasbourg, FRA)

An unambiguous descriptor of rotations is the matrix that links two sets of Cartesian coordinates of each point of a rotated object, those before and after rotation. However, the matrix elements are mutually dependent and hardly interpretable in a straightforward way. To overcome these difficulties, crystallographic and cryo-EM software usually refers to polar (a single rotation about an axis in a general orientation) or to Euler angles (three consecutive rotations about the chosen coordinate axes). Different software uses different sets of parameters as: both polar and Euler angles may be defined with respect to different coordinate axes; Euler angles may be defined with respect to both fixed and rotating axes; positive rotation direction may be chosen in opposite ways; one can consider the object rotating with respect to a fixed coordinate system or *vice versa*.

All these possible parametrizations of rigid-body rotations can be interactively illustrated with the program *py_convrot*. It deals with all kinds of Euler angles, including all choices of rotation axes and rotation directions, and with all possible choices of polar angles. Using a kind of 'lego', a user can build their own rotation convention and view its action using an interactive *Demo*. An extended *Help* describes details of these parameterizations. Available *Tables* explain all possible interpretations of the rotation matrices in terms of various parameters and v*ice versa*. The program can be used both as a teaching and as a practical tool converting one set of rotation parameters to another.