Poster

Slice'N'Dice: Maximising the value of predicted models for structural biologists

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With the advent of next generation modelling methods, such as AlphaFold2, structural biologists are increasingly using predicted structures to obtain structure solutions via Molecular Replacement (MR) or model fitting in Cryo Electron Microscopy (Cryo-EM). Inaccuracy in domain-domain orientations is often a key limitation when using predicted models. Slice'N'Dice is a software package designed to address this issue by first slicing models into distinct structural units and then automatically placing the slices using either Phaser [1], Molrep [2], or PowerFit [3]. The slicing step can use AlphaFold2's predicted aligned error (PAE) [4], or can operate via a variety of Cα atom based clustering algorithms, extending the applicability to structures of any origin. The number of splits can either be selected by the user or determined automatically. Slice'N'Dice is available from CCP4 8.0 for MR and will be available with automated map-fitting for Cryo-EM from CCP4 9.0.

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