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3-D TEM Reconstructions with EMAN2

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Transmission Electron Microscopy (TEM), in both negative stain and cryo, is a powerful technique for determining 3-D structural information about biological molecules/ macromolecules. EMAN was originally developed a decade ago to ease the task of performing high resolution single particle reconstructions, by automating portions of the reconstruction process which were considered robust and providing an easy to use graphical user interface (GUI) for tasks not considered ready for automation[1]. The techniques used for reconstruction were a hybrid of some methods not then in common use, such as direct Fourier inversion for reconstruction and full amplitude and phase CTF correction, as well as other established techniques pioneered in earlier software packages such as SPIDER[2] and IMAGIC[3]. EMAN evolved to offer additional techniques for 2-D analysis, 2-D and 3-D population dynamics studies, and various post-processing operations such as secondary structure localization, skeletonization and crystal-structure docking. The resolution capabilities of single particle reconstruction have advanced rapidly over the last decade. In the last year, several single particle reconstructions have been solved at ~4 Å resolution, and subnanometer resolutions have been achieved in numerous labs around the world.

We have just completed a ~3 year effort to develop EMAN2, a major new version of EMAN, which includes numerous new algorithms, a completely refactored C++ library and a new OpenGL-based user-interface with a complete workflow mechanism to ease the process of single particle reconstruction[4]. While small or low-resolution reconstructions can be completed on a desktop workstation, larger structures or work at high resolutions still requires more substantial computing resources. EMAN2 supports both traditional Linux clusters as well as the new GPU computing paradigm, making use of commodity 3-D graphics cards for computation. EMAN2 was designed to be highly modular, and new algorithms for specific tasks such as image alignment, similarity metrics, reconstruction, etc. can be added to the core library and immediately become available in all of the end-user programs without additional programming. While the core image processing library is written in highly efficient C++ code, all end-user programs, including the GUI interfaces are written in the Python scripting language, meaning they can be customized by knowledgeable end-users without need to recompile the entire package. EMAN2 includes a completely redesigned CTF model and automated correction scheme as well as a new semi-automated particle picking tool based on techniques developed earlier in the SWARM$_{PS}$ software package[5].

In this talk, I will give an overview of single particle processing in general, and an introduction to EMAN2, and how it can be used to complete this, and other TEM-related tasks.

Bibliography
[1] S.J. Ludtke *et al.*. J Struct Biol. 128 (1999) 82.
[2] J. Frank *et al.*. J Struct Biol. 116 (1996) 190.
[3] M. van Heel *et al.*. J Struct Biol. 116 (1996) 17.
[4] G. Tang *et al.*. J Struct Biol. 157 (2007) 38.
[5] D. Woolford *et al.*. J Struct Biol. 157 (2007) 174.
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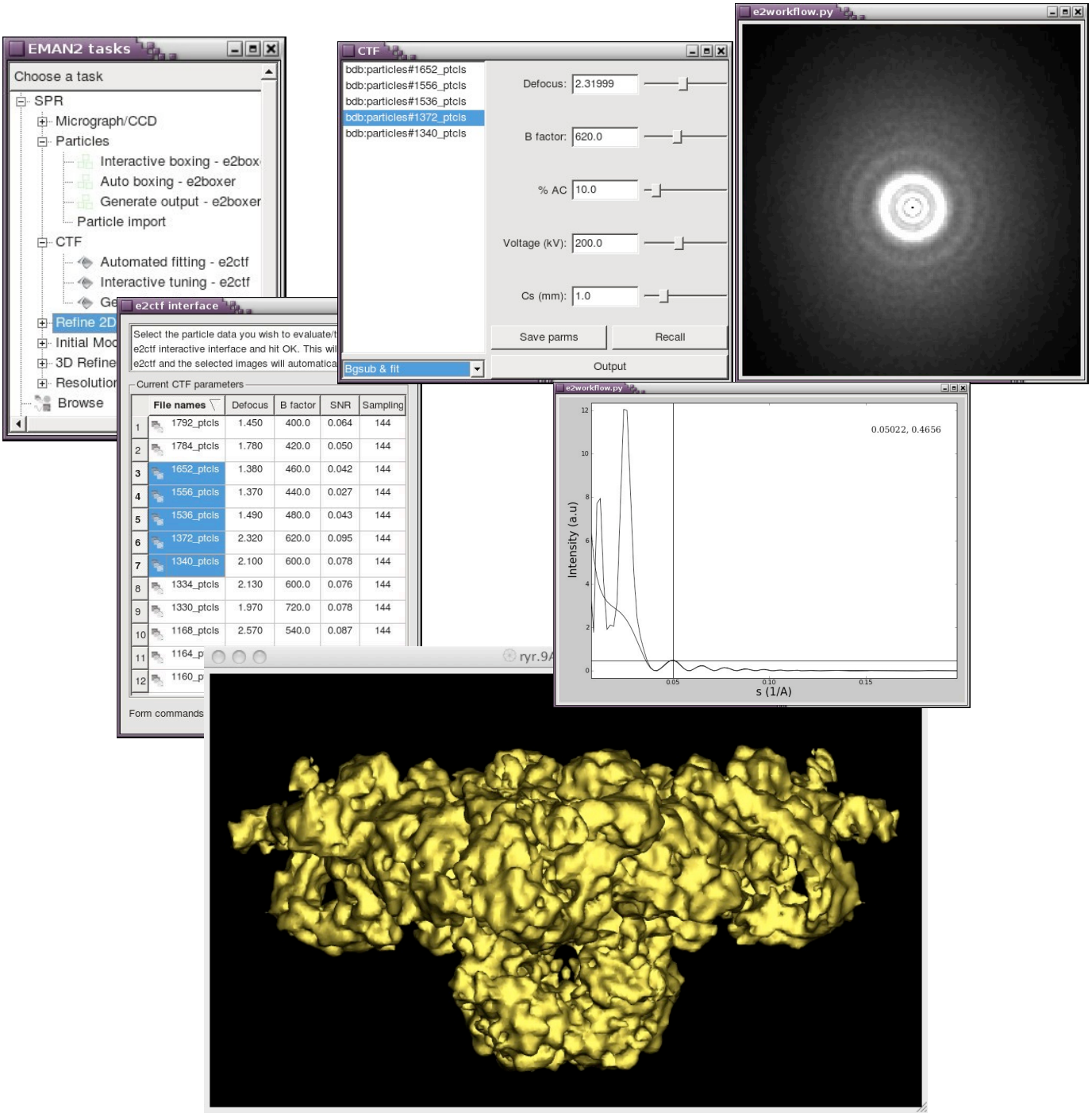

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