VISUALIZATION IN SPACE AND TIME:
Seamless Pipelines Now Available

By Katharine Miller

The pathway from raw data to valuable visualization of molecules, cells or organs being simulated over time involves several potentially painstaking steps. Typically, researchers must generate a set of initial images from raw data; give them some kind of context (often through image registration); segment the images into meaningful parts; figure out how to analyze the images to understand the system being studied; determine how the display of the objects being studied can assist in that analysis; and, finally, produce a compelling graphic for a published work. Here we describe three examples of recent efforts to simplify the process.

Molecular Dynamics Hollywood Style: ePMV

To watch and understand complex biological molecules in action, researchers want fast physics, easy manipulation of objects, and an intuitive interface—all features that Hollywood has already developed in high-end graphics software. To access those capabilities, some researchers have coded their own molecular viewers into their favorite professional 3-D animation applications while others have coded ani-

ePMV allows a user to go from an idea (the proverbial napkin sketch) to a press-ready image. An online movie at http://epmv.scripps.edu/ shows how this can be done in a matter of minutes with practice. Courtesy of Graham Johnson.

Scene objects rendered from Cinema 4D
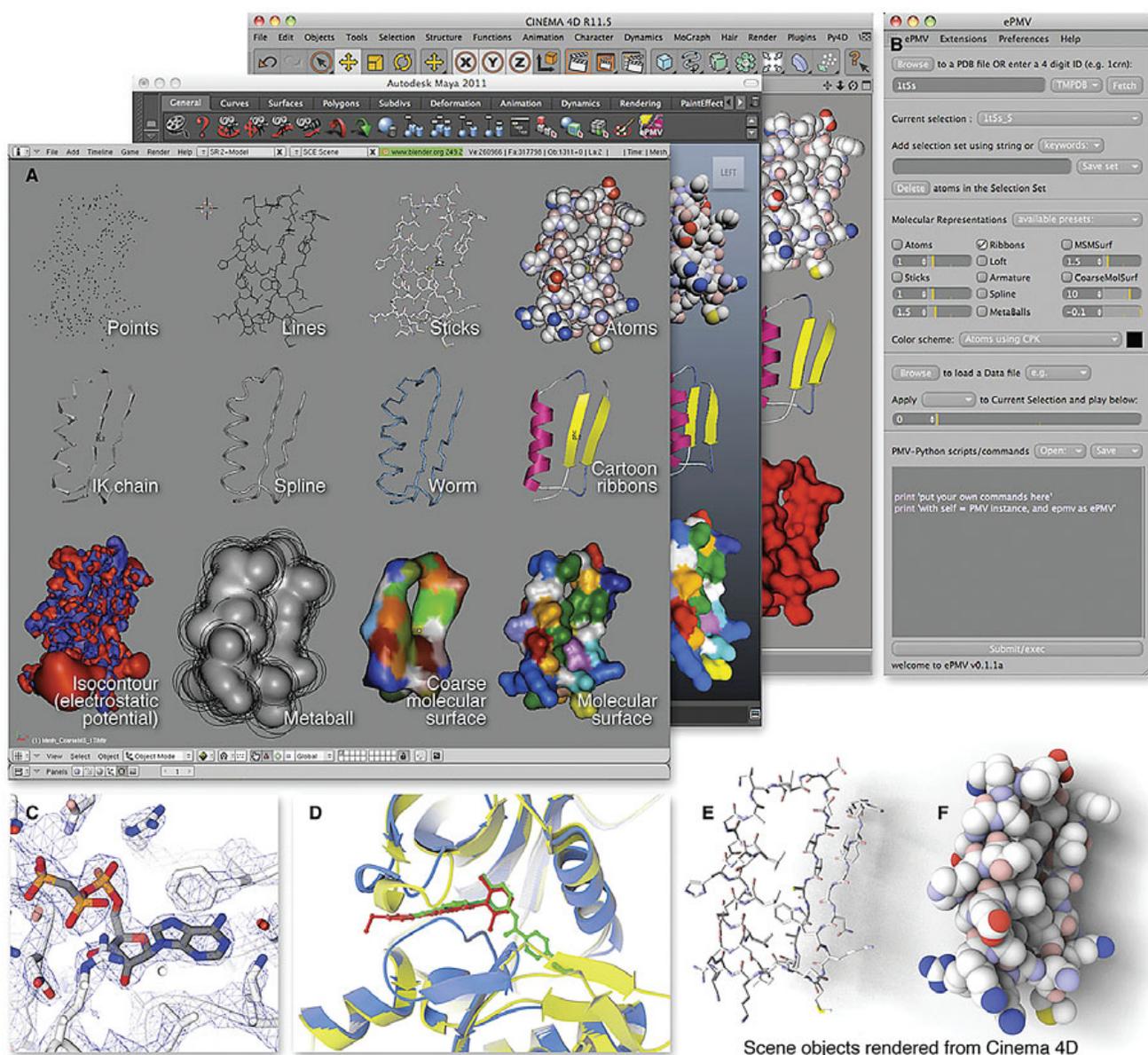
mation capabilities into molecular viewers. The members of Art Olson's lab saw the folly of this redundant effort and took action, producing embedded Python Molecular Viewer (ePMV).

"We developed ePMV to pool the strengths of both types of existing software (pro 3-D animation and scientific modelers/viewers/simulators) by merging them with Autin Ludovic's ubiquitous translator," says **Graham Johnson**, **PhD**, who developed the software along with **Autin Ludovic**, PhD, **David Goodsell** and **Michel Sanner**, **PhD**, in **Art Olson**'s Molecular Graphics Lab at the Scripps Research Institute. ePMV is described in the March 2011 issue of *Structure* and available for download at http://epmv.scripps.edu.

The value of Hollywood's tools goes well beyond creating pretty pictures. For example, they provide great character animation controls. "Picture the simplified skeletons that underlie the meshes of your favorite Pixar characters and control the motion," Johnson says.

And because "Hollywood works on a time-is-money model," Johnson says, the software allows fast physics within a relatively intuitive interface; multiple simultaneous views; easy assembly of mesoscale models; efficient and intuitive real-time construction of repeating units such as actin monomers into an actin filament; positioning of transmembrane proteins into a bilayer; and click-and-drag interfaces for manipulating lights and textures and adding text and arrows. "And that's just scratching the surface," he says.

Some of the early enthusiasm for ePMV has come from illustrators, Johnson notes. But, "what's most exciting about ePMV for biologists is that it allows you to interoperate an unlimited number of Python scientific algorithms on the same model in the same user interface at the same time," he says.

In addition, ePMV makes computational tools relatively approachable for structural biologists and molecular biologists, letting them interact with molecular dynamics experts in an intuitive way, Johnson says.

Olson notes that although scientists can use ePMV to do their research, the question is: Will they? "There is an energy barrier to learning these high level graphics codes," he says. But, Johnson says, it's mostly a matter of legacy and momentum. "Clean-slate audiences can be brought up to similar levels in both approaches in similar amounts of time." Olson adds, "You learn what you need to learn to do your work."
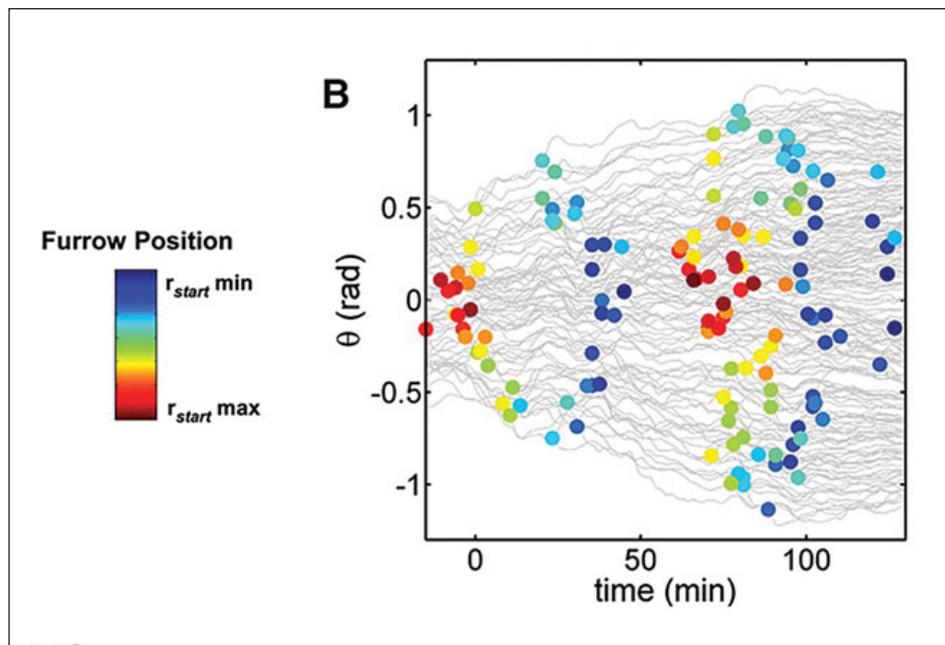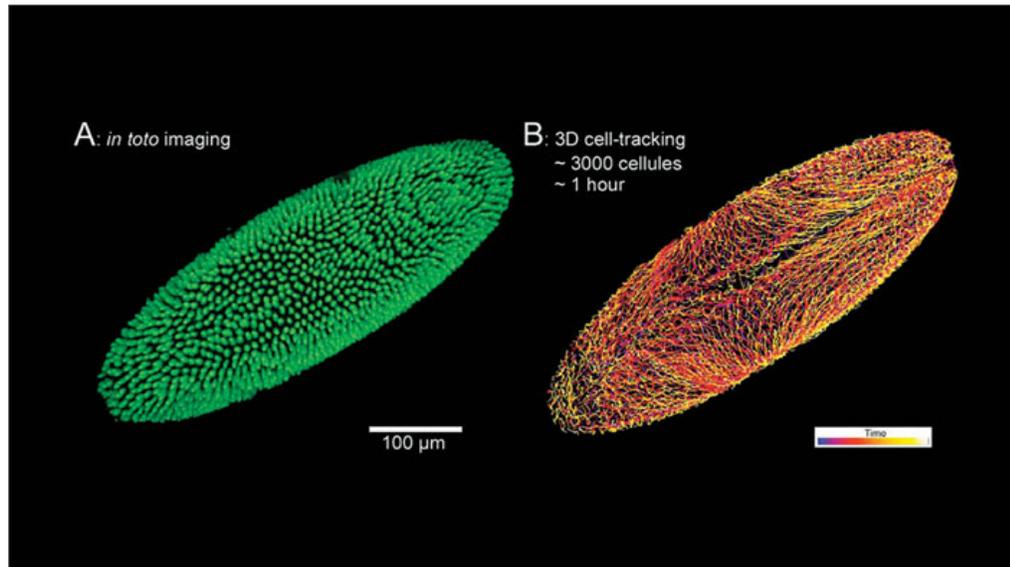
Understanding Cells on the Move

With recent advances in microscopy tools, developmental biologists can now image and track live cells as they move and divide. The information gathered has the potential to explain much about cell growth and differentiation. Although the field of developmental biology is still at the early stages of developing visualization tools to analyze the accumulating data, says **Willy Supatto, PhD**, a researcher at Ecole Polytechnique, Palaiseau, France, some progress has been made.

First, of course, developmental biologists must visualize the data itself. The entire pipeline from embryo preparation to live imaging and image analysis can be extremely painstaking. Many researchers still do some steps manually—for example, clicking on the mouse to pick out

Visualized tracking of a Drosophila *embryo during gastrulation produced a lovely image (top) and movie, but it was only when the cells' movements were decomposed and visualized with a color code (bottom) that the researchers understood what was happening. The color code represents the position of the cells in the furrow at a particular time. The graph shows when each of those cells divided as it moved along its trajectory. Cells that started nearest the ectoderm divided first, followed by cells nearer to the top of the ventral furrow. Embryo images reprinted with permission from Truong, TV, and Supatto, W., Toward high-content/high-throughput imaging and analysis of embryonic morphogenesis,* Genesis *49:555–569 (2011). Graphs reprinted with permission from McMahon, A et al., Dynamic Analyses of* Drosophila *Gastrulation Provide Insights into Collective Cell Migration,* Science *322: 1546-1550 (2008).*