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Subject: Re: Molecular models and contour maps  
Posted by [Rick Matthews](#) on Thu, 01 Aug 2002 20:40:24 GMT  
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David Fanning wrote:

> Rick Matthews (matthews@wfu.edu) writes:

>> Newbie question:

> Oh, oh. :-(

>> I want to use IDL for help with 3-D visualization of

>> electron density calculations. I want like IDL to display a ball and

>> stick model of a molecule, with interleaved contour maps of the density

>> surrounding the atoms in planes of my choosing.

<snip>

> Do you mean you are a programming newbie, or an IDL

> newbie?

IDL newbie. 33 years (Oh my, am I that old?) in other languages.

> If the former, and you don't have any 3D

> graphics or object experience,

I have zero 3-D graphics experience.

> you may be looking

> at quite a project here.

I was afraid of that. However, visualizing 3-D charge density maps are going to be a recurring need for my next decade, so it may be worth the investment.

> If it's the latter, and

> you are a proficient C++ programmer, then maybe

> there is some hope ahead.

More in Fortran and a few other languages than C++, but I think I understand objects well enough if that is critical. The 3-D experience may be a problem.

> But what you want to do is in no way a trivial

> programming exercise in IDL, I'm afraid. I'm hoping

> Ronn Kling's latest book, due out soon, will shed

> some light on this sort of thing. But you are going

> to have to pretty much build this yourself, I think.

> I'm reasonably sure it can be done with IDL, just not

> as easily as you were probably hoping.

Thanks for the heads up. I have also looked at OpenDX,  
where this particular task might be easier, but

1. IDL is closer to the languages I use most, and
2. IDL seems to be better equipped to make movies, which  
will be the next step in the project.

I appreciate your help.

Rick

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Rick Matthews	matthews@wfu.edu
Department of Physics	<a href="http://www.wfu.edu/~matthews">http://www.wfu.edu/~matthews</a>
Wake Forest University	336-758-5340 (Voice)
Winston-Salem, NC 27109-7507	336-758-6142 (FAX)
USA	

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