Subject: Molecular Modelling really possible with pv-wave?
Posted by Bernd Ihmels on Thu, 08 Feb 1996 08:00:00 GMT
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Hello, you pv-wave / idl gurus!

I tried to do some Molecular Modelling with pv-wave, i.e. to draw a molecule. When I scanned the libraries of pv-wave, the only routine I found to do some kind of modelling was molecules.pro. But this works extremly slow and if I change the numbers of atoms (balls) to a more realistic number (i.e. several thousands of atoms (normal proteins)), the code immediadly breaks down, even if I set the ..locals parameter to an approproate number.

So I wonder, if anyone of you ever wrote a program do draw large molecules, with a fast algorithm, so that you won't have to wait several minutes for just one image? Or even better, a program, able to turn a molecule ones created, so that you don't have to create a new image for every new view-angle?

Or is something like that impossible to do with pv-wave?

Any help will be appreciated. Thanks in advance,

Bernd
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Subject: Re: Molecular Modelling really possible with pv-wave?
Posted by hewat on Fri, 16 Feb 1996 08:00:00 GMT
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Bernd Ihmels <bihmels1@gwdg.de> writes:

> To display large molecules is only a first step on a longer road to get more
> sophisticated graphics of molecules, like displaying densities around a molecule
> or to show two molecules in different colors in one picture. I tink both is
> impossible to do with rasmol. I don't know much about vrml, but I think there's no
> version for SUNSolaris, so it won't run on my SUN-workstation.

There is an excellent VRML viewer for SUN and most other Unix stations on:
http://hyperg.iicm.tu-graz.ac.at/Cvrweb;sk=D4A601A3

There are already several applications of VRML to molecular modelling,
including the features you mention. See eg http://www.ch.ic.ac.uk/VRML/

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ftp://ftp.ill.fr/pub/dif http://193.49.43.3/dif/3D_crystals.html

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