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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* Bernd Ihmels, Max-Planck-Institut fuer biophysikalische Chemie *
* Biocomputation Group, AG 061 *
* Am Fassberg, 37077 Goettingen *
* Tel: +49+551-201-1762 Fax: +49+551-201-1467 *
* Email: bihmels1@gwdg.de *
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