

Re: Simulating an assembler?

Source: <http://sci.tech-archive.net/Archive/sci.nanotech/2005-08/msg00016.html>

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 - *Date:* Thu, 18 Aug 2005 05:38:45 -0000
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In article <11f0d1q8o4gf2b7@xxxxxxxxxxxxxxxxxxxx>, boblarson@xxxxxxxxxxxx says...

> Do we now have computers capable of designing and testing an assembler in
> software? Has it been done yet?

http://www.nanoengineer-1.com/mambo/index.php?option=com_content&task=view&id=66&Itemid=2

The URL above links to an article describing the simulation of a Drexler-Merkle differential gear, in a software package called nanoengineer-1. For scale purposes, the gear has 8292 atoms. The six degree of freedom manipulator arm designed by (I think) Merkle has something like 3000 atoms, as I recall. And the full scale assembler designs (I should put those in scare quotes, really) are on the order of three to four million atoms.

So, since this is considered to be significant (nanodot.org is claiming it to be a first) I wager to say that the very much larger simulations of full assemblers are not yet feasible. 65 ps of simulation took almost 8 hours on a midrange laptop; even under the dubious assumption that simulations of this type are linear in the number of atoms, a full assembler would take about a thousand times as long to simulate.

Now, some healthy skepticism:

- o I can't evaluate the accuracy of the software used to simulate this, since it is not yet released. (Although apparently it will be released under GPL next year.)
- o There is no documentation of the software. (It asks me to log in to the website, but doesn't give a way to obtain a login, that I see, so it may not be intended as public access.) In any event, it is not possible for me to even eyeball what sorts of effects the simulator is *supposed* to model, much less how well it does so. (Granted, not being a chemist, I might not be qualified.)
- o A (very) brief search reveals no peer-reviewed publications by the

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author, Mark Sims. This is complicated somewhat by a Mark Sims at Amherst who is active in the multi-agent software community; I doubt they are the same person. (People may note that I'm big on peer review by respected, established journals and institutions, like the IEEE, ACM, and ACS.)

o I'm not aware of the software package being sanity tested against other molecular modelling software.

In light of all that, I take this simulation with a grain of salt in itself... but henceforth, the debates are going to shift from "Has such and such been simulated?" to "Has it been simulated properly and do we believe the results?"

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John S. Novak, III
The Humblest Man On The Net

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◇ *From:* John Devereux

• *References:*

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◇ *From:* Bob Larson

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