

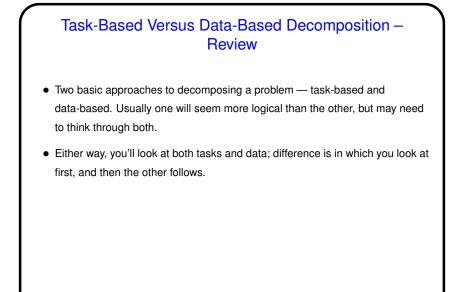
 Reminder: Homework 2 due Monday. (Unless ... I'm having trouble making leapfrogging work with OpenCL. I'll send e-mail probably tomorrow, either giving you some hints about how to make it work or — something.)

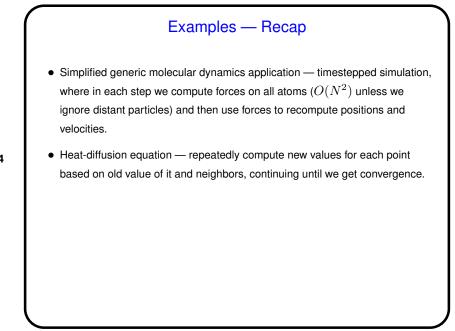
Slide 1

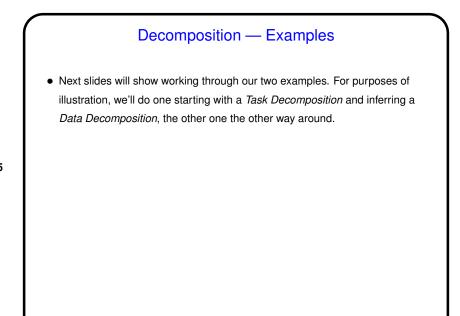
Numerical Integration Revisited

• The OpenMP version of this example is simple and compact. However, it might not be the best model for the OpenMP version of Homework 2 — seems like you want to be able to control which random sequence each iteration of the main loop uses, and no obvious way to do that with OpenMP parallel for.

- So instead we could try an SPMD-style approach ...
- Also note that while declaring variable x outside the parallel block allows it to be an example of how to deal with such data, really it could be local to the thread or even to the loop, no?
- (Example revised.)







Molecular Dynamics Example — Task Decomposition

- Tasks that find the vibrational forces on an atom.
- Tasks that find the rotational forces on an atom.

(Together, these are tasks to compute "bonded forces" — those due to chemical bonds.)

- Tasks that find the non-bonded forces on an atom (the ones due to electrical charges).
- Tasks that update the position and velocity of an atom.
- Tasks that update the neighbor list for an atom. (Or we could consider updating all the neighbor lists as one task, as in the book, if we think it won't be done very often and therefore is not worthwhile to parallelize.)

