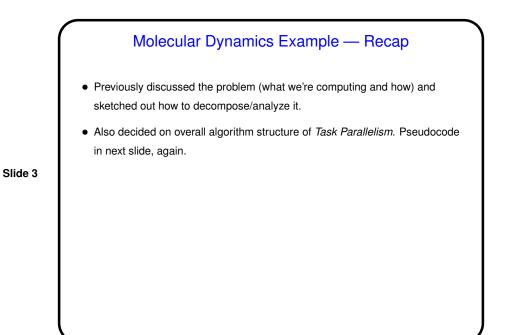
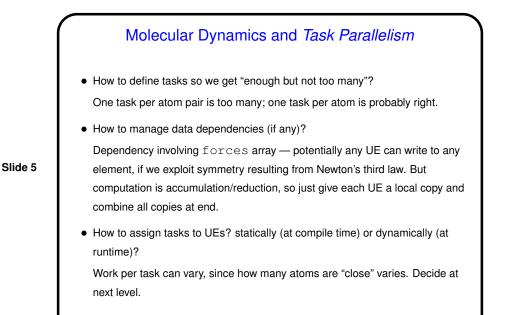


Supporting Structures — Recap
Program structuring patterns — we've talked about these. How to decide? Tables in section 5.3 should be helpful.
Data structure patterns — Distributed Array is widely useful. Shared Queue less so since many programming environments will provide something. Shared Data is good general advice.



<text>



Design of Program for Molecular Dynamics

- Finally, we turn the design into code, probably using patterns from *Supporting Structures* design space, and possibly some information/understanding from *Implementation Mechanisms* (to be discussed later).
- Based on previous design steps, consider *Loop Parallelism* and/or *SPMD*. Decide based mostly on target platform.

Molecular Dynamics and *Loop Parallelism* — Key Design Decisions

- Parallelize computationally intensive loop only (the one for non-bonded forces).
- Figure out what to do about shared variables:

Slide 7

Slide 8

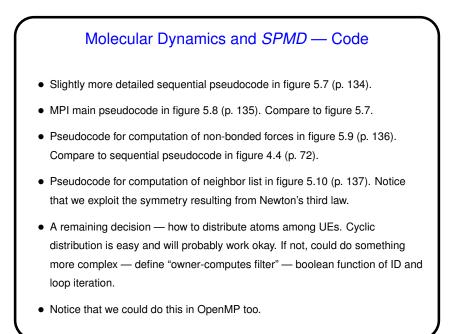
- Make forces array a reduction variable.

- Make temporary variables used inside loop private.

- Decide how to map iterations onto UEs. Dynamic schedule works well if available (as it is in OpenMP).
- OpenMP-based pseudocode as shown in figure 5.25 (p. 161) and following pragma omp directives). Compare to pseudocode in figure 4.4 (p. 72).



- Only parallelize computation of non-bonded forces, since that's most of the computational load.
- Keep a copy of the full force and coordinate arrays on each node.
- Have each UE redundantly update positions and velocities for the atoms (i.e., assume it's cheaper to redundantly compute these terms than to do them in parallel and communicate the results).
- Have each UE compute its contributions to the force array and then combine (or reduce) the UEs' contributions into a single global force array copied onto each UE.



Heat Diffusion Example — Recap

- Previously discussed the problem (what we're computing and how) and sketched out how to decompose/analyze it.
- Also decided on overall algorithm structure of *Geometric Decomposition*.

