





• Write your own "thread-safe" RNG — one that can be called from multiple threads concurrently without ill effects. (Think about how to do that in Java versus C.)

(References to some reasonable choices to be included in writeup on Web.)

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- Modify your programs to use your RNG. Do something you think is reasonable so that each UE starts with a different seed.
- Measure your programs' accuracy and performance and plot results.
- Make a second version of your code in which all UEs start from the same seed but each works on a different part of the problem space (domain decomposition). Measure its accuracy and performance.







Slide 6







Molecular Dynamics and Task Parallelism
How to define tasks so we get "enough but not too many"? One task per atom pair is too many; one task per atom is probably right.
How to manage data dependencies (if any)? Dependency involving forces array — potentially any UE can write to any element, if we exploit symmetry resulting from Newton's third law. But computation is accumulation/reduction, so just give each UE a local copy and combine all copies at end.
How to assign tasks to UEs? statically (at compile time) or dynamically (at runtime)? Work per task can vary, since how many atoms are "close" varies. Decide at next level.

Slide 10





