

General MD Algorithm

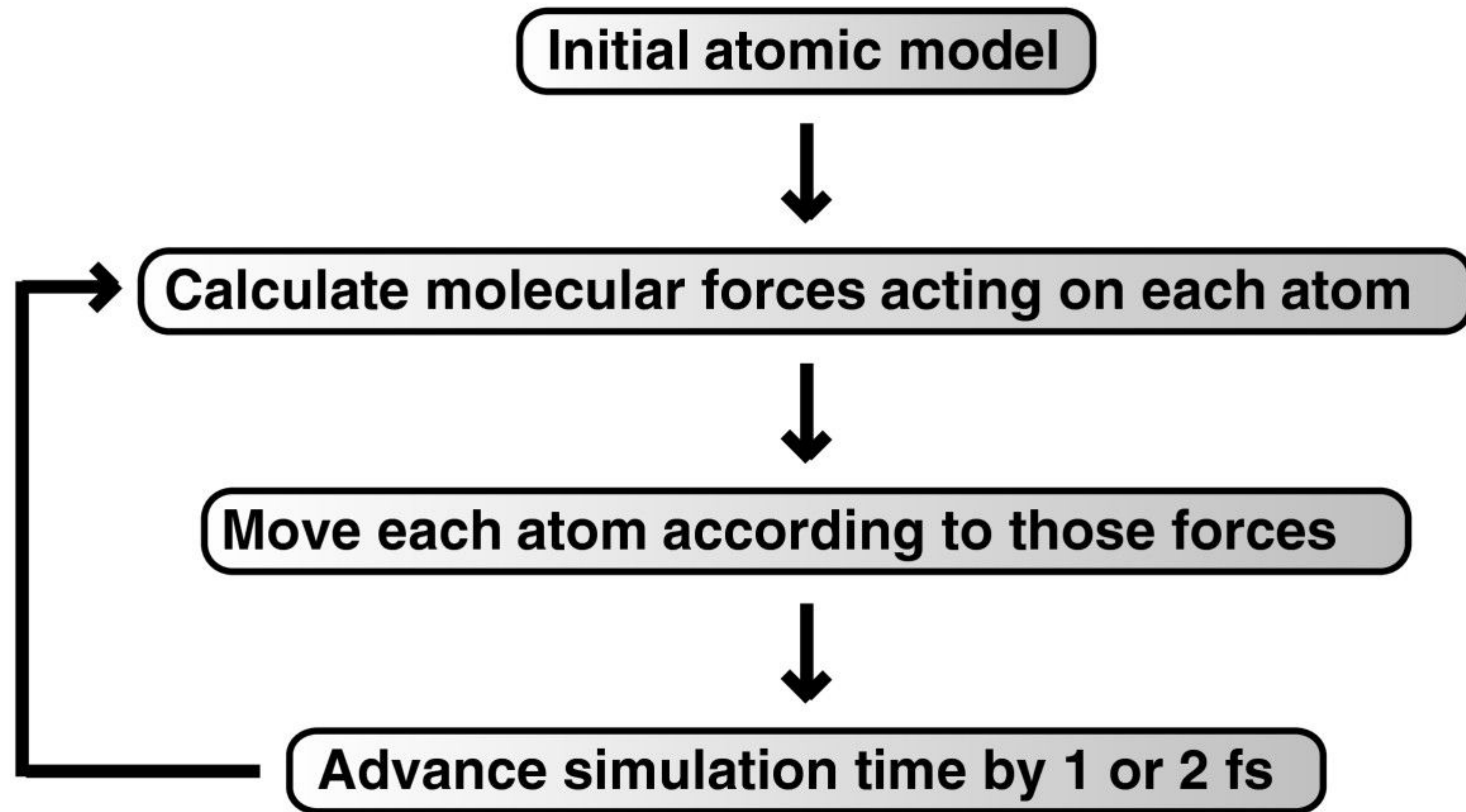


Figure 2 of Durrant & McCammon, 2011

Why do biological molecular dynamics?

- “everything that living things do can be understood in terms of the jiggings and wiggings of atoms” - Richard Feynman
- Check out my molecular dynamics YouTube playlist: https://www.youtube.com/playlist?list=PLYEyeVFrqfAu0ft6sF4vVe5FOEbJYyi_L