

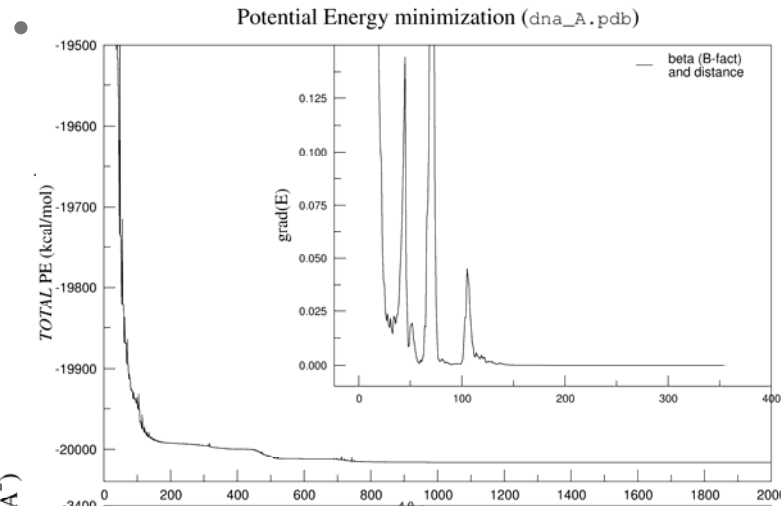
MD practice, IV: How to actually do it...

Overall steps in a typical work-flow, from PDB to MD:

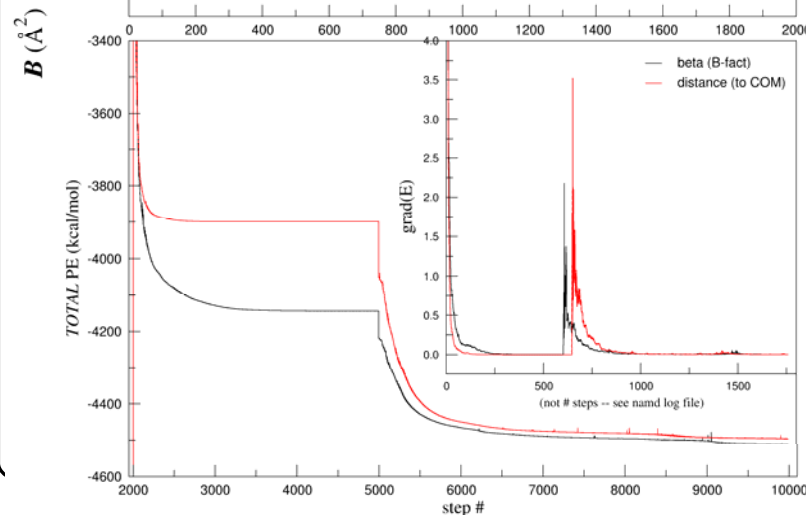
System preparation

- Obtain (and validate?) a 3D structural model – X-ray, NMR, even cryo-EM or homology models

Energy minimization



Heating of the system



System equilibration

Dynamics

Data analysis

