

# MD practice, II: Force fields and their potentials

## Some of the available (atomistic) force fields

### ➤ AMBER & CHARMM

- The classic “second-generation” MD FFs for biomolecules, developed by Cornell, Kollman, *et al.* starting in mid-1990s (AMBER) and by Karplus, Brooks, MacKerell, *et al.* starting in 1980s (CHARMM)
- Particularly widespread application in DNA and RNA worlds (AMBER)
- Includes a “GLYCAM” FF for carbohydrates (AMBER)
- Polarizable version of both FFs exist (based on point charges)

### ➤ GROMOS

- Developed as part of the GROMOS molecular dynamics program (largely superceded by Gromacs)
- United-atom FF – only polar hydrogens explicitly represented
- Commonly used for lipid and detergent systems

### ➤ OPLS

- **O**ptimized **P**otentials for **L**iquid **S**imulations, by Jorgensen *et al.*
- Parameterized so as to optimally match experimental properties of liquids ( $\rho$ ,  $\Delta H_{vap}$ , *etc.*), not just gas phase torsional profiles
- Very similar functional form to the Amber FF; UA and AA forms exist