AMBER AND CHARMM FORCE FIELDS
FORCE FIELD

• Function for calculating the nuclear motion of the particle.
• **AMBER** is an acronym for **Assisted Model Building with Energy Refinement**.

• It is a family of force fields for molecular dynamics of biomolecules originally developed by the late Peter Kollman's group at the University of California, San Francisco.
The functional form of the AMBER force field is

\[ V(r^N) = \sum_{\text{bonds}} k_b(l - l_0)^2 + \sum_{\text{angles}} k_a(\theta - \theta_0)^2 \]

\[ + \sum_{\text{torsions}} \frac{1}{2} V_n[1 + \cos(n\omega - \gamma)] \]

\[ + \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} \left\{ \epsilon_{i,j} \left[ \left( \frac{r_{0ij}}{r_{ij}} \right)^{12} - 2 \left( \frac{r_{0ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{4\pi \epsilon_0 r_{ij}} \right\} \]
Parameter sets

- To use the AMBER force field, it is necessary to have values for the parameters of the force field (e.g. force constants, equilibrium bond lengths and angles, charges).

- A fairly large number of these parameter sets exist, and are described in detail in the AMBER software user manual. Each parameter set has a name, and provides parameters for certain types of molecules.
• Peptide, protein and nucleic acid parameters are provided by parameter sets with names beginning with "ff" and containing a two digit year number, for instance "ff99".

• GAFF (General AMBER force field) provides parameters for small organic molecules to facilitate simulations of drugs and small molecule ligands in conjunction with biomolecules.

• The GLYCAM force fields have been developed by Rob Woods for simulating carbohydrates.
Software

• It is written in Fortran 90 and C with support for most major Unix-like systems and compilers.
Programs

- **LEaP** is used for preparing input files for the simulation programs.
- **Antechamber** automates the process of parameterizing small organic molecules using GAFF.
- **SANDER** (Simulated Annealing with NMR-Derived Energy Restraints) is the central simulation program and provides facilities for energy minimization and molecular dynamics with a wide variety of options.
• **pmemd** is a somewhat more feature-limited reimplementation of sander by Bob Duke. It was designed with parallel processing in mind and has significantly better performance than sander when running on more than 8–16 processors

• **nmode** calculates normal modes

• **ptraj** provides facilities for numerical analysis of simulation results. AMBER does not include visualization capabilities; visualization is commonly performed with **VMD**. A new visualization alternative is **Sirius**.

• **MM-PBSA** allows for implicit solvent calculations on snap shots from molecular dynamics simulations
CHARMM

• CHARMM is Chemistry at HARvard Macromolecular Mechanics

• is the name of a widely used set of force fields for molecular dynamics as well as the name for the molecular dynamics simulation and analysis package associated with them

• The CHARMM Development Project involves a network of developers throughout the world working with Martin Karplus and his group at Harvard to develop and maintain the CHARMM program.
The CHARMM force fields for proteins include:

- For united-atom: CHARMM19
- For all-atom: CHARMM22
- For dihedral potential corrected variant: CHARMM22/CMAP
- For DNA, RNA, and lipids: CHARMM27

Some force fields may be combined, for example CHARMM22 and CHARMM27 for the simulation of protein-DNA binding.
SOFTWARE

• It is written in Fortran 77/95 with support for most major Unix-like systems and compilers
• More advanced features include free energy perturbation (FEP), quasi-harmonic entropy estimation, correlation analysis and combined quantum, and molecular mechanics (QM/MM) methods.
References

• http://en.wikipedia.org/wiki/Force_field_(chemistry)
• en.wikipedia.org/wiki/AMBER
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THANK YOU