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.

Functional form

- The functional form of the AMBER force field is
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$$V(r^N) = \sum_{\text{bonds}} k_b(l - l_0)^2 + \sum_{\text{angles}} k_a(\theta - \theta_0)^2$$

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

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

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**
- http://onlinelibrary.wiley.com/doi/10.1002/jcc.21425/abstract
- http://en.wikipedia.org/wiki/Force_field_(chemistry)

THANK YOU