CHAMBER – A CHARMM format converter to enable the use of CHARMM forcefields within AMBER

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The similarity of the CHARMM force field's energy functional form with that of the AMBER force field, gives the potential for direct translation of common bonding and non-bonding terms, along with their parameters, present in CHARMM's topology and parameter files for use in the AMBER software.

To this extent, we have created a tool; CHAMBER, which can take a CHARMM PSF file and associated forcefield files and convert these to an AMBER topology file (prmtop) and associated coordinate file (inpcrd). Differences in the the two functional forms, such as CHARMM's additional two body Urey-Bradley term, which extends over all 1-3 bonds, a four body quadratic improper term and CHARMM's numerical energy correction to two sequential dihedrals (CMAP), are accommodated by the creation of additional sections within AMBER's topology file.

In concert to these prmtop additions, modifications were made to AMBER's code to enable the calculation of the energy and derivatives corresponding to these new terms. Backwards compatibility within the prmtop file is maintained.

CHAMBER opens a conversion route which will enable the simulation of CHARMM parameterized models using AMBER's PMEMD engine; thus enabling improved serial efficiency as well as parallel efficiency over higher numbers of CPUs.