Run MCCE on Multiple PDBs at Once

p_batch is a program included in MCCE, under the folder MCCE_bin. It accepts a directory containing ".pdb" files, and runs MCCE with identical settings on each protein file. Usage: p_batch protein_dir [custom_script.sh] By default, default_script.sh is created by p_batch at run time, if it does not exist. The default scripts calls for steps 1-4 of MCCE to be run at level 1, assumes a dielectric constant of 8 with NGPB as the Poisson Bolztmann solver, and sets entropy control on. For additional control over MCCE, more options are accessible via run.prm files, examples of which can be found in MCCE4-Alpha/runprms. For example, if I wanted to add neutral atoms to simulate a membrane slab on my runs, I would create a file named "run.prm.custom" in the same directory I plan to run p_batch. The run.prm.custom file would contain the following text: f (IPECE_ADD_MEM) Now, in addition to the regular MCCE files, another file named "mem_pos" will be created.