Overview

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PSCF+ is a software package for solving the polymer self-consistent field (SCF) theory in continuum. It is based on the nice GPU framework of PSCF (which is only for the "standard" or known as the Edwards-Helfand model, *i.e.*, incompressible melts of continuous Gaussian chains with the Dirac δ-function interactions, commonly used in polymer field theories) originally developed by Prof. David Morse and co-workers, but is improved with better numerical methods, less GPU memory usage and more flexible algorithms, and is extended to various discrete-chain models. Similar to the C++/CUDA version of PSCF, PSCF+ described here is written primarily in C++ with GPU accelerated code in CUDA.

Same as the C++/CUDA version of PSCF, PSCF+ is applicable to mixtures containing arbitrary acyclic copolymers, and preserves all of the nice features already implemented in the former, including the use of cuFFT on GPU, the use of Anderson mixing (which is performed on GPU) combined with a variable-cell scheme to simultaneously solve the nonlinear SCF equations and find the bulk periodicity for the ordered phases formed by block copolymer self-assembly (which speeds-up the calculation by about one order of magnitude), and the documentation produced by Doxygen. Their differences and expected advantages of the latter include:

- PSCF is only applicable to the "standard" model, while PSCF+ can also be applied to various discrete-chain models with finite-range non-bonded interactions commonly used in molecular simulations, thus providing the mean-field reference results for such simulations; see Models.pdf for more details.
- For the continuous-Gaussian-chain models, PSCF+ uses the Richardson-extrapolated pseudo-spectral methods (denoted by REPS-*K* with *K*=0,1,2,3,4) to solve the modified diffusion equations (which is the crux of SCF calculations of such models), while PSCF uses only REPS-1. A larger *K*-value gives more accurate result at larger computational cost; see REPS.pdf for more details.
- For 3D spatially periodic ordered phases such as those formed by block copolymer self-assembly, while PSCF uses fast Fourier transforms (FFTs) between a uniform grid in the real space and that in the reciprocal space, for the Pmmm supergroup PSCF+ uses discrete cosine transforms instead of FFTs to take advantage of the (partial) symmetry of an ordered phase to reduce the number of grid points, thus both speeding up the calculation and reducing the memory usage; see *Qiang and Li*, **Macromolecules 53**, 9943 (2020) for more details.
- In SCF calculations the (one-end-integrated) forward and backward propagators q and $q^\dagger$ of each block usually take the largest memory usage, but the GPU memory is rather limited. While in PSCF the size of these propagators is MN_s, where M denotes the number of grid points in real space and N_s the number of contour discretization points on a continuous Gaussian chain (or the number of segments on a discrete chain), in PSCF+ the "slice" algorithm proposed by Li and Qiang can be used to reduce the size of q to $M\sqrt{N_s}$ and that of $q^\dagger$ to just M, thus greatly reducing the GPU memory usage at the cost of computing q twice; see SavMem.pdf for more details.
- Since SCF equations are highly nonlinear, having a good initial guess is very important in practice as it determines not only which final solution (corresponding to a phase in block copolymer self-assembly) can be obtained but also how many iteration steps the solver (*e.g.*, the Anderson mixing) takes to converge these equations. PSCF+ uses automated calculation along a path (ACAP), where the converged solution at a

neighboring point is taken as the initial guess at the current point in the parameter space. While this is similar to the "SWEEP" command in PSCF, the key for ACAP to be successful and efficient is that it automatically adjusts the step size along the path connecting the two points. In PSCF+, ACAP is further combined with the phase-boundary calculation between two specified phases, making the construction of phase diagrams very efficient. See ACAP.pdf for more details.

- The approach used by PSCF to solve the SCF equations (for an incompressible system) does not allow any athermal species in the system, which has no Flory-Huggins-type interactions with all other species. This problem is solved in PSCF+; see SlvSCF.pdf for more details.

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