Richardson-Extrapolated Pseudo-Spectral (REPS) Methods

For continuous Gaussian chain (CGC) as used in the "standard" model (see Models.pdf for details), the chain propagators satisfy the modified diffusion equations. Here we consider as an example the (one-end-integrated) forward propagator $q(\mathbf{r},s)$ in a block of length N and the statistical segment length b (for CGC, individual values of N and b are not important; strictly speaking, $N\to\infty$ and $b\to 0$, and it is $\sqrt{N}b$ that matters), where $s\in[0,N]$ is the (continuous) variable along the block contour; the modified diffusion equation is then $\frac{\partial q}{\partial s}=\frac{b^2}{6}\nabla^2 q-\omega(\mathbf{r})q$ with given initial condition of $q(\mathbf{r},s=0)$, where $\omega(\mathbf{r})$ is the conjugate field interacting with segments on the block, and has the formal solution of $q(\mathbf{r},s+\mathrm{d}s)=\exp\left[\left(\frac{b^2}{6}\nabla^2-\omega(\mathbf{r})\right)\mathrm{d}s\right]q(\mathbf{r},s)$. Discretizing the block contour into n steps each of step-size $\Delta s=N/n$, one needs to numerically calculate $q(\mathbf{r},s+\Delta s)$ from $q(\mathbf{r},s)$, where $s=j\Delta s$ and $j=0,\ldots,n-1$. For block copolymer self-assembly under the periodic boundary conditions, the 2^{nd}-order pseudo-spectral (PS) method[1] gives $q(\mathbf{r},s+\Delta s)\approx\exp\left(-\frac{\omega(\mathbf{r})\Delta s}{2}\right)\exp\left(\frac{b^2\Delta s}{6}\nabla^2\right)\exp\left(-\frac{\omega(\mathbf{r})\Delta s}{2}\right)q(\mathbf{r},s)$, which has a ***global*** error of $O(\Delta s^2)$ and can be readily computed using fast Fourier transforms. Morse and co-workers first pointed out that the error of the PS method contains only even powers of Δs and thus proposed a 4^{th}-order method, which is used in PSCF, by linearly extrapolating the two results of $q(\mathbf{r},s+\Delta s)$ obtained via the PS method with the step-size of Δs and $\Delta s/2$, respectively, to the limit of $\Delta s\to 0$.[2] This is similar to the trapezoidal rule for numerical integration, the error of which also contains only even powers of the step-size; the K^{th}-order polynomial extrapolation of the $K+1$ results obtained via the trapezoidal rule with successively halved step-size to the limit of zero step-size then give the commonly used Romberg integration[3], with $K=1$ corresponding to the Simpson's 1/3 rule. We therefore refer to the PS method and that proposed by Morse and co-workers[2] as the REPS-0 and REPS-1 method, respectively, and have implemented the REPS-K (for $K=0,\ldots,4$) methods in PSCF+; polynomial extrapolation with $K>4$ is usually unstable.

To be more specific, let q_k ($k=1,\ldots,K+1$) be the result of $q(\mathbf{r},s+\Delta s)$ obtained via the PS method with a step-size of $\Delta s/2^{k-1}$, and q_0 be the extrapolated result given by the REPS-K method; one can then write $q_k=q_0+\sum_{i=1}^{K}a_i\left(\frac{\Delta s}{2^{k-1}}\right)^{2i}$. For given Δs and q_k's, solving q_0 and the coefficients a_i ($i=1,\ldots,K$) from these $K+1$ equations, we obtain $q_0=(4q_2-q_1)/3$ (*i.e.*, Eq. (A6) in Ref. 2) for $K=1$, $q_0=(64q_3-20q_2+q_1)/45$ for $K=2$, $q_0=(4096q_4-1344q_3+84q_2-q_1)/2835$ for $K=3$, and $q_0=(1048576q_5-348160q_4+22848q_3-340q_2+q_1)/722925$ for $K=4$. Note that the REPS-K method has a global error of $O(\Delta s^{2(K+1)})$; this requires the Romberg integration of the same (or higher) order to calculate the integral $\int_0^N \mathrm{d}s\,q(\mathbf{r},s)q^\dagger(\mathbf{r},s)$ involved in the volume-fraction field (*e.g.*, the Simpson's 1/3 rule is used in PSCF to match the REPS-1 method), which in turn requires n be an integer multiple of 2^K (see RI.pdf for details). We also note that the REPS-K method requires $2^{K+1}-1$ pairs of forward and backward fast Fourier transforms to obtain $q(\mathbf{r},s+\Delta s)$ from

$q(\mathbf{r},s)$.

References:

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