Richardson-Extrapolated Pseudo-Spectral (REPS) Methods

For a 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 effective bond length b (for CGC, individual values of N and b do not matter; 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 $q(\mathbf{r},s+\mathrm{d}s)=\exp\left\{\left[\left(b^2/6\right)\nabla^2-\omega(\mathbf{r})\right]\mathrm{d}s\right\}q(\mathbf{r},s)$. 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 2nd-order pseudo-spectral (PS) method[1] gives $q(\mathbf{r},s+\Delta s)\approx\exp\left(-\omega(\mathbf{r})\Delta s/2\right)\exp\left[\left(b^2/6\right)\Delta s\nabla^2\right]\exp\left(-\omega(\mathbf{r})\Delta s/2\right)q(\mathbf{r},s)$, 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 4th-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 Kth-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 gives 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 $q_k=q_0+\sum_{i=1}^{K}a_i\left(\Delta s/2^{k-1}\right)^{2i}$. 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 $q_0=\left(4q_2-q_1\right)/3$ (*i.e.*, Eq. (A6) in Ref. 2) for $K=1$, $q_0=\left(64q_3-20q_2+q_1\right)/45$ for $K=2$, $q_0=\left(4096q_4-1344q_3+84q_2-q_1\right)/2835$ for $K=3$, and $q_0=\left(1048576q_5-348160q_4+22848q_3-340q_2+q_1\right)/722925$ 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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