Fast and accurate implementation of Fourier spectral approximations of nonlocal diffusion operators and its applications

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Abstract

This work is concerned with the Fourier spectral approximation of various integral differential equations associated with some linear nonlocal diffusion and peridynamic operators under periodic boundary conditions. For radially symmetric kernels, the nonlocal operators under consideration are diagonalizable in the Fourier space so that the main computational challenge is on the accurate and fast evaluation of their eigenvalues or Fourier symbols consisting of possibly singular and highly oscillatory integrals. For a large class of fractional power-like kernels, we propose a new approach based on reformulating the Fourier symbols both as coefficients of a series expansion and solutions of some simple ODE models. We then propose a hybrid algorithm that utilizes both truncated series expansions and high order Runge-Kutta ODE solvers to provide fast evaluation of Fourier symbols in both one and higher dimensional spaces. It is shown that this hybrid algorithm is robust, efficient and accurate. As applications, we combine this hybrid spectral discretization in the spatial variables and the fourth-order exponential time differencing Runge-Kutta for temporal discretization to offer high order approximations of some nonlocal gradient dynamics including nonlocal Allen-Cahn equation, nonlocal Cahn-Hilliard equation, and nonlocal phase-field crystal models. Numerical results show the accuracy and effectiveness of the fully discrete scheme and illustrate some interesting phenomena associated with the nonlocal models.

Key Words. Nonlocal diffusion operator, peridynamic operator, Fourier spectral method, non-local Allen-Cahn equation, nonlocal Cahn-Hilliard equation, nonlocal phase-field crystal model.

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1 Introduction and motivations

In recent years, nonlocal models have been successfully applied in fields such as mathematics, physics, biology, mechanics and materials sciences, including the studies of nonlocal Dirichlet forms [3], phase transitions [5, 19], nonlocal heat conduction [6], kinetic equations [24], fluid mechanics [13] and peridynamics (PD) [30]. Among these, we are particularly interested in nonlocal diffusion and peridynamic models which have demonstrated the effectiveness in recent works [4, 6, 26, 32, 33]. To avoid the explicit use of spatial derivatives, a nonlocal operator $\mathcal{L}_\delta$ is introduced as follows to represent nonlocal spatial interactions

$$\mathcal{L}_\delta u(x, y) = \int_{\mathcal{B}(\mathbf{x}, \delta)} \rho_\delta(|\mathbf{y} - \mathbf{x}|) (u(\mathbf{y}) - u(\mathbf{x})) d\mathbf{y}, \quad (1.1)$$

where $\mathcal{B}(\mathbf{x}, \delta)$ is the δ -radius neighborhood of $\mathbf{x}$, δ is the horizon parameter, and the kernel $\rho_\delta(s)$ is a nonnegative radial-type function with a compact support in $[0, \delta]$. We also call $\mathcal{L}_\delta$ a nonlocal diffusion operator given the connection to the conventional local diffusion operator in the local limit:

$$\mathcal{L}_\delta u \rightarrow \mathcal{L}_0 u = \Delta u, \quad \delta \rightarrow 0, \quad \forall u \in C^\infty, \quad (1.2)$$

if the kernel $\rho_\delta(s)$ satisfies the following condition for R^d

$$\int_0^\delta r^{1+d} \rho_\delta(r) dr = \frac{2}{V_d} := C_d, \quad (1.3)$$

where V_d is the area of the unit sphere in R^d and is properly scaled to allow concentration near the origin as $\delta \rightarrow 0$.

For models associated with the above nonlocal operators, there have been a great deal of rigorous mathematical and numerical analysis [1, 2, 7–9, 11, 12, 15, 16, 23, 25, 28, 31, 37, 38]. Recently, asymptotically compatible discretizations that preserve the local limiting behavior of (1.2) on the discrete level have been proposed in [35, 36]. Fast solution algorithms exploring the matrix Toeplitz structure have been initiated in [37] which demonstrated significant saving in computational cost. Instead of finite difference or finite element methods, [14] successfully extended the asymptotic compatibility concept to the Fourier spectral methods for the numerical solution of a one-dimensional (1D) nonlocal Allen-Cahn equations. The numerical study in [14] contains only some one dimensional numerical examples with very special kernels. The implementation was limited to such special cases mainly due to the lack of accurate and efficient ways to evaluate the eigenvalues (or Fourier symbols)

of the nonlocal operators in general. Hence, how to evaluate these Fourier symbols efficiently and accurately, including both one and higher dimensional cases, becomes a very important motivation of this work.

In contrast to the classical Laplace operator in $[0, 2\pi]^3$ whose (l, m, n) th eigenvalue corresponding to the eigenfunction $e^{i(lx+my+nz)}$ is readily given as $-(l^2 + m^2 + n^2)$ [29], each (l, m, n) th eigenvalue of the nonlocal diffusion operator (1.1) with radial-type kernels is a triple integral of the form:

$$\lambda_\delta(l, m, n) = \int_0^\delta r^2 \rho_\delta(r) \int_0^\pi \sin \theta \int_0^{2\pi} (\cos(r(l \sin \theta \cos \phi + m \sin \theta \sin \phi + n \cos \theta)) - 1) d\phi d\theta dr.$$

It may be anticipated that the evaluation of the above Fourier symbols can be challenging and costly given the possible singularity in the kernel $\rho_\delta(r)$ and high oscillation for large $\delta\sqrt{l^2 + m^2 + n^2}$, even though this is mostly a preprocessing step since these computed Fourier symbols can be used over and over again when nonlocal models are numerically solved. Meanwhile, it is known that when solving the linear nonlocal diffusion equation $\mathcal{L}_\delta u = f$ (with a zero mean for f) by Fourier spectral method with approximated Fourier symbols $\tilde{\lambda}$, the overall error can be characterized by

$$\begin{aligned} \|u - u_N\|_2^2 &= \sum_{\|\mathbf{k}\|_\infty \leq N} \left| \frac{1}{\lambda(\mathbf{k})} - \frac{1}{\tilde{\lambda}(\mathbf{k})} \right|^2 |f_{\mathbf{k}}|^2 + \sum_{\|\mathbf{k}\|_\infty > N} \left| \frac{f_{\mathbf{k}}}{\lambda(\mathbf{k})} \right|^2 \\ &= \sum_{\|\mathbf{k}\|_\infty \leq N} \left| \frac{\tilde{\lambda}(\mathbf{k}) - \lambda(\mathbf{k})}{\tilde{\lambda}(\mathbf{k})} \right|^2 \left| \frac{f_{\mathbf{k}}}{\lambda(\mathbf{k})} \right|^2 + \sum_{\|\mathbf{k}\|_\infty > N} \left| \frac{f_{\mathbf{k}}}{\lambda(\mathbf{k})} \right|^2 := R_e + T_e \end{aligned}$$

The term T_e resembles the truncation error which is generically bounded by cN^{-2p} , where p depends on the regularity of f . The term R_e measures error due to numerical evaluation of the Fourier symbols and is bounded by $c\mu^2 \|f\|_2^2$, where μ is the maximum relative error of $\tilde{\lambda}(\mathbf{k})$. Clearly, it is necessary to compute the nonlocal eigenvalues very accurately to guarantee the overall high accuracy of spectral methods.

The major contribution of this work is to develop an efficient and accurate hybrid algorithm to compute the eigenvalues to nonlocal operators with following typical fractional power kernels combining with a horizon parameter δ given as

$$\rho_\delta(s) = \frac{3(5 - \alpha)}{2\pi\delta^{5-\alpha}} |s|^\alpha \chi_{[-\delta, \delta]}, \quad \alpha \in [0, 5).$$

Note that the characteristic function χ is to impose the limit on the range of interactions and the constant coefficient is to assure the moment condition (1.3) being satisfied. Together, we can

achieve both the spectral accuracy in approximation and fast $O(N \log(N))$ computational cost. We demonstrate the effectiveness of this hybrid algorithm computationally. Furthermore, we illustrate the applicability of this new approach for a number of nonlocal models such as the nonlocal Allen–Cahn, nonlocal Cahn–Hilliard and nonlocal PFC models that may have broad interests [17, 18, 20, 21].

The organization for the rest of this paper is as follows. In Section 2, a few different reformulations of the Fourier symbols are carefully derived. In the subsequent section, we develop a robust, efficient and accurate hybrid algorithm to compute nonlocal eigenvalues by utilizing the advantages of different formulations in different parameter regimes. Section 4 is devoted to numerical experiments, including the verification of the efficiency and accuracy of the hybrid algorithm, as well as applications of the hybrid algorithm to simulate several nonlinear time dependent nonlocal problems. Some concluding remarks are given in the final section.

2 Fourier symbols and their reformulation

In this section, we first present the standard forms of Fourier symbols of nonlocal diffusion operators with periodic boundary conditions in R^d ($d = 1, 2, 3$). Then we propose some alternative formulations. Without loss of of generalization, we consider problems on $[0, 2\pi]^d$. For clarity, we consider separately the cases in different space dimensions.

2.1 1-d case

First, in 1-d with periodic boundary condition, the nonlocal diffusion operator and its eigenvalues are given as

$$\mathcal{L}_\delta u(x) = \int_{|s| \leq \delta} \rho_\delta(s) (u(x+s) - u(x)) ds, \quad \lambda_\delta(n) = 2 \int_0^\delta \rho_\delta(s) (\cos(ns) - 1) ds.$$

with e^{inx} being an eigenfunction associated with $\lambda_\delta(n)$ for any nonzero integer n . For the following normalized cut-off fractional kernels

$$\rho_\delta(s) = \frac{3 - \alpha}{\delta^{3-\alpha} |s|^\alpha} \chi_{[-\delta, \delta]}, \quad \alpha \in [0, 3),$$

we can rewrite the above eigenvalues as

$$\lambda_\delta(n) = \frac{2(3 - \alpha)}{\delta^2} \int_0^1 r^{-\alpha} (\cos(n\delta r) - 1) dr.$$

Except for $\alpha = 0$, we do not expect a general analytical expansion of $\lambda_\delta(n)$. However, $\lambda_\delta(n)$ is an even function of $|n|\delta$ ($:= a$), and we have the series expansion of $\lambda_\delta(n)$ as

$$\begin{aligned}\lambda_\delta(n) &= \frac{2(3-\alpha)}{\delta^2} \sum_{k=1}^{\infty} \frac{(-1)^k n^{2k} \delta^{2k}}{(2k)!(2k+1-\alpha)} \\ &:= \frac{2(3-\alpha)}{\delta^2} \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k)!(2k+1-\alpha)} := \frac{2(3-\alpha)}{\delta^2} K(a).\end{aligned}$$

A simple calculation gives

$$aK'(a) = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k)!} \frac{2k}{(2k+1-\alpha)} = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k)!} + (\alpha-1)K(a).$$

It is noted that $\sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k)!} = \cos(a) - 1$. Hence, we end up with an ordinary differential equation (ODE) for K in term of a as

$$K'(a) = \frac{\alpha-1}{a} K(a) + \frac{\cos(a)-1}{a}.$$

Thus, once we have the solution to the above ODE, we can get the desired eigenvalues $\lambda_\delta(n)$ immediately.

2.2 2-d case

The nonlocal diffusion operator in 2D is defined as

$$\mathcal{L}_\delta \phi(x, y) = \int \int_{s^2+t^2 \leq \delta^2} \rho_\delta \left(\sqrt{s^2+t^2} \right) (u(x+s, y+t) - u(x, y)) ds dt,$$

For any integers m, n such that $m^2 + n^2 \neq 0$, it is easy to check that $e^{imx+iny}$ is an eigenfunction of $\mathcal{L}_\delta$ in $[0, 2\pi]^2$ with periodic boundary conditions, and the corresponding eigenvalue is given by

$$\begin{aligned}\lambda_\delta(m, n) &= \int_0^\delta r \rho_\delta(r) \int_0^{2\pi} (\cos(r(m \cos \theta + n \cos \theta)) - 1) d\theta dr \\ &= \int_0^\delta r \rho_\delta(r) \int_0^{2\pi} (\cos(r\sqrt{m^2+n^2} \cos \theta) - 1) d\theta dr,\end{aligned}$$

where in the last step, we have used a basic property

$$m \cos \theta + n \cos \theta = \sqrt{m^2 + n^2} \cos(\theta + \theta_{mn}), \quad (2.1)$$

and the fact that

$$\int_0^{2\pi} (\cos(r\sqrt{m^2+n^2} \cos(\theta + \theta')) - 1) d\theta \equiv \int_0^{2\pi} (\cos(r\sqrt{m^2+n^2} \cos \theta) - 1) d\theta, \quad (2.2)$$

for any r and θ' . In 2-d, the normalized cut-off fractional kernels becomes

$$\rho_\delta(s) = \frac{2(4-\alpha)}{\pi\delta^{4-\alpha}|s|^\alpha} \chi_{[-\delta,\delta]}, \quad \alpha \in [0, 4).$$

To this end, $\lambda_\delta(m, n)$ has the following form

$$\begin{aligned} \lambda_\delta(m, n) &= \frac{2(4-\alpha)}{\pi\delta^2} \int_0^1 r^{1-\alpha} \int_0^{2\pi} \left(\cos\left(r\delta\sqrt{m^2+n^2}\cos\theta\right) - 1 \right) d\theta dr, \\ &:= \frac{8(4-\alpha)}{\pi\delta^2} \int_0^1 \int_0^1 \frac{\cos(ar\theta) - 1}{r^{\alpha-1}\sqrt{1-\theta^2}} d\theta dr := \frac{8(4-\alpha)}{\pi\delta^2} K(a), \end{aligned}$$

where a represents $\delta\sqrt{m^2+n^2}$. Thus, we need to evaluate the following integrals

$$K(a) = \int_0^1 \int_0^1 \frac{\cos(ar\theta) - 1}{r^{\alpha-1}\sqrt{1-\theta^2}} d\theta dr.$$

Again, we have a series expansion of $K(a)$ with respect to a as

$$K(a) = \frac{\pi}{2} \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{4^k (k!)^2 (2k+2-\alpha)}.$$

To derive an ODE for $K(a)$ with respect to a , we define

$$I(a) = \int_0^1 \frac{\cos(a\theta)}{\sqrt{1-\theta^2}} d\theta,$$

and rewrite $K(a)$ as

$$K(a) = \int_0^1 \frac{I(ar) - \frac{\pi}{2}}{r^{\alpha-1}} dr = a^{\alpha-2} \int_0^a \frac{I(t) - \frac{\pi}{2}}{t^{\alpha-1}} dt.$$

For $I(a)$ and $K(a)$, we know some facts as

$$I''(a) + \frac{1}{a} I'(a) + I(a) = 0, \quad I(0) = \frac{\pi}{2}, \quad I'(a) = 0,$$

and

$$K'(a) = \frac{\alpha-2}{a} K(a) + \frac{1}{a} (I(a) - \frac{\pi}{2}), \quad K(0) = 0.$$

Unlike the 1-d case, we need to introduce another independent variable to close the ODE system.

Let $J(a) = I'(a)$, we get an ODE system of I , J and K as

$$\frac{d}{da} \begin{bmatrix} I \\ J \\ K \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & -\frac{1}{a} & 0 \\ \frac{1}{a} & 0 & \frac{\alpha-2}{a} \end{bmatrix} \begin{bmatrix} I \\ J \\ K \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ \frac{\pi}{2a} \end{bmatrix},$$

with initial values $I(0) = \frac{\pi}{2}$, $J(0) = 0$ and $K(0) = 0$. Moreover, the series expansion forms for $I(a)$

and $J(a)$ are given respectively as

$$I(a) = \frac{\pi}{2} \left(1 + \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{4^k (k!)^2} \right), \quad J(a) = \frac{\pi}{2} \sum_{k=1}^{\infty} \frac{2k(-1)^k a^{2k-1}}{4^k (k!)^2}.$$

2.3 3-d case

The nonlocal diffusion operator in 3-d is defined as

$$\mathcal{L}_\delta \phi(x, y, z) = \int \int \int_{r^2+s^2+t^2 \leq \delta^2} \rho_\delta \left(\sqrt{r^2 + s^2 + t^2} \right) (u(x+r, y+s, z+t) - u(x, y, z)) dr ds dt,$$

Similarly, for any integers l, m, n when $l^2 + m^2 + n^2 \neq 0$, $e^{ilx+imy+inz}$ is an eigenfunction of $\mathcal{L}_\delta$ in $[0, 2\pi]^3$ with corresponding eigenvalue

$$\begin{aligned} \lambda_\delta(l, m, n) &= \int \int \int_{r^2+s^2+t^2 \leq \delta^2} \rho_\delta \left(\sqrt{r^2 + s^2 + t^2} \right) \left(e^{ilr+ims+int} - 1 \right) dr ds dt \\ &= \int_0^\delta r^2 \rho_\delta(r) \int_0^\pi \sin \theta \int_0^{2\pi} (\cos(r(l \sin \theta \cos \phi + m \sin \theta \sin \phi + n \cos \theta)) - 1) d\phi d\theta dr, \\ &= \int_0^\delta r^2 \rho_\delta(r) \int_0^\pi \sin \theta \int_0^{2\pi} \left(\cos \left(r \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi + n \cos \theta \right) \right) - 1 \right) d\phi d\theta dr, \end{aligned}$$

where in the last step we use similar techniques (2.1) and (2.2) as for the 2d case. We still consider the normalized cut-off fractional kernels in 3-d as

$$\rho_\delta(s) = \frac{3(5-\alpha)}{2\pi\delta^{5-\alpha}|s|^\alpha} \chi_{[-\delta, \delta]}, \quad \alpha \in [0, 5).$$

In this setting, $\lambda_\delta(m, n)$ can be simplified as

$$\lambda_\delta(m, n) = \frac{3(5-\alpha)}{2\pi\delta^2} \int_0^1 r^{2-\alpha} \int_0^\pi \sin \theta \int_0^{2\pi} \left(\cos \left(r \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi + n \cos \theta \right) \right) - 1 \right) d\phi d\theta dr.$$

By Taylor expansion, we have

$$\begin{aligned} &\cos \left(r \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi + n \cos \theta \right) \right) - 1 \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k r^{2k} \delta^{2k}}{(2k)!} \left(\sum_{p=0}^{2k} C_{2k}^p \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi \right)^p n^{2k-p} \cos^{2k-p} \theta \right), \end{aligned}$$

where C_{2k}^p is the notation of combination number. Since $\int_0^\pi \cos^{2k+1} \phi d\phi = 0$ for any integer k , consequently,

$$\begin{aligned} &\int_0^\pi \sin \theta \int_0^{2\pi} \left(\cos \left(r \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi + n \cos \theta \right) \right) - 1 \right) d\phi d\theta \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k r^{2k} \delta^{2k}}{(2k)!} \left(\sum_{p=0}^k C_{2k}^{2p} (l^2 + m^2)^p n^{2k-2p} \int_0^\pi \sin^{2p+1} \theta \cos^{2k-2p} \theta d\theta \int_0^{2\pi} \cos^2 \phi d\phi \right) \\ : &= \sum_{k=1}^{\infty} \frac{(-1)^k r^{2k} \delta^{2k}}{(2k)!} G(l, m, n, k). \end{aligned}$$

Inspired by discussions in the 1 and 2-d cases, we conjecture that $G(l, m, n, k) = c_k(l^2 + m^2 + n^2)^k$. If this is right, we should have $c_k = 2\pi \int_0^\pi \sin \theta \cos^{2k} \theta d\theta = \frac{4\pi}{2k+1}$. Meanwhile, the following equalities hold for any nonnegative numbers p and k such that $p \leq k$

$$\int_0^{2\pi} \cos \phi^{2p} d\phi = 2\pi \frac{(2p-1)!!}{(2p)!!},$$

and

$$\int_0^\pi \sin^{2p+1} \theta \cos^{2k-2p} \theta d\theta = \frac{\Gamma(p+1)\Gamma(k-p+\frac{1}{2})}{2\Gamma(k+1+\frac{1}{2})} = \frac{2^p p! (2k-2p-1)!!}{(2k+1)!!},$$

where $(2k-1)!! = 1 \times 3 \times \cdots \times (2k-1)$, $(2k)!! = 2 \times 4 \times \cdots \times 2k$, $(0-1)!! = 1$ and $0!! = 1$. These two equalities can be proved by induction method or can be verified by Mathematica. We omit details here. This instantly yields

$$\frac{4\pi}{2k+1} C_k^p = C_{2k}^{2p} \int_0^\pi \sin^{2p+1} \theta \cos^{2k-2p} \theta d\theta \int_0^{2\pi} \cos \phi^{2p} d\phi,$$

which confirms our conjecture. Now we have

$$\begin{aligned} & \int_0^\pi \sin \theta \int_0^{2\pi} \left(\cos \left(r \left(\sqrt{l^2 + m^2} \sin \theta \cos \phi + n \cos \theta \right) \right) - 1 \right) d\phi d\theta \\ &= \sum_{k=1}^{\infty} 4\pi \frac{(-1)^k r^{2k} \left(\delta \sqrt{l^2 + m^2 + n^2} \right)^{2k}}{(2k+1)!} := \sum_{k=1}^{\infty} 4\pi \frac{(-1)^k r^{2k} a^{2k}}{(2k+1)!}, \end{aligned}$$

where $a = \delta \sqrt{l^2 + m^2 + n^2}$. Thus, we end up with a series expansion of nonlocal eigenvalue for the 3-d case as

$$\lambda_\delta(m, n) = \frac{6(5-\alpha)}{\delta^2} \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k+1)!(2k+3-\alpha)} := \frac{6(5-\alpha)}{\delta^2} K(a).$$

We have the similar calculation as in the 1-d case

$$aK'(a) = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k+1)!} \frac{2k}{(2k+3-\alpha)} = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k+1)!} + (\alpha-3)K(a).$$

We further observe that

$$\sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k+1)!} = \frac{\sin a - a}{a}.$$

Therefore, we derive an ODE for K as

$$K'(a) = \frac{\alpha-3}{a} K(a) + \frac{\sin a - a}{a^2}.$$

2.4 Summary

We provide a short summary of the discussions in the above subsections:

- **1D:** $\lambda_\delta(n) = \frac{2(3-\alpha)}{\delta^2}K(a)$ and $a = \delta|n|$, where $K(a)$ with following series form

$$K(a) = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k)!(2k+1-\alpha)} \quad (2.3)$$

satisfies the following ODE

$$K'(a) = \frac{\alpha-1}{a}K(a) + \frac{\cos(a)-1}{a}. \quad (2.4)$$

- **2D:** $\lambda_\delta(m, n) = \frac{8(4-\alpha)}{\pi\delta^2}K(a)$ and $a = \delta\sqrt{m^2 + n^2}$, where $K(a)$ has following series form

$$K(a) = \frac{\pi}{2} \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{4^k (k!)^2 (2k+2-\alpha)} \quad (2.5)$$

In this case, we need to introduce two auxiliary variables $I(a)$ and $J(a)$ with the following series expansions

$$I(a) = \frac{\pi}{2} \left(1 + \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{4^k (k!)^2} \right), \quad J(a) = \frac{\pi}{2} \sum_{k=1}^{\infty} \frac{2k(-1)^k a^{2k-1}}{4^k (k!)^2}, \quad (2.6)$$

to close the ODE system as

$$\frac{d}{da} \begin{bmatrix} I \\ J \\ K \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & -\frac{1}{a} & 0 \\ \frac{1}{a} & 0 & \frac{\alpha-2}{a} \end{bmatrix} \begin{bmatrix} I \\ J \\ K \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ \frac{\pi}{2a} \end{bmatrix}. \quad (2.7)$$

- **3D:** $\lambda_\delta(l, m, n) = \frac{6(5-\alpha)}{\delta^2}K(a)$ and $a = \delta\sqrt{l^2 + m^2 + n^2}$, where $K(a)$ has the following series form

$$K(a) = \sum_{k=1}^{\infty} \frac{(-1)^k a^{2k}}{(2k+1)!(2k+3-\alpha)} \quad (2.8)$$

satisfying the following ODE

$$K'(a) = \frac{\alpha-3}{a}K(a) + \frac{\sin a - a}{a^2}. \quad (2.9)$$

Remark 1. From (2.9), we can further get an integral form of the solution for K as

$$K(a) = a^{\alpha-3} \int_0^a \theta^{1-\alpha} (\sin \theta - \theta) d\theta.$$

Hence, we simplify the original form of $K(a)$ from a triple integral into a single integral.

Remark 2. From the ODEs for nonlocal eigenvalues, we can see that $\alpha = d$ in R^d is a critical value for power-law type kernels. When $0 \leq \alpha < d$, it is easy to get a bound only depending on α for K , which means that the nonlocal diffusion operator is a bounded linear operator in this case. Hence, the energy space E_{per}^δ defined via $\mathcal{L}_\delta$ as $E_{per}^\delta(\Omega) = \{u \in L_{per}^2(\Omega) \mid -(\mathcal{L}_\delta u, u) \leq \infty\}$ is equivalent to L^2 -space. On the other hand, more delicate analysis can show that E_{per}^δ is equivalent to $H_{per}^{\frac{\alpha-d}{2}}(\Omega)$ for $d \leq \alpha < d+2$.

3 A hybrid algorithm to compute nonlocal eigenvalues

In all three cases for $d = 1, 2$ and 3 , we now have three different forms of nonlocal eigenvalues, namely the original integral form, the series expansion form and the ODE form. Computing the integral form directly requires considerable work on numerical quadrature. Direct computation of the series expansion form is also problematic, for example, for $a \geq 50$, the expansion does not converge numerically in Matlab no matter how many truncated terms we compute. On the other hand, the ODE form also has its own issues such as its singular nature at $a = 0$. Taking these considerations into account, a hybrid algorithm is designed by combining truncated series expansion and ODE form. Our basic idea is that we evaluate nonlocal eigenvalues by truncated series expansion for small a , while we obtain them by solving the ODE form with RK4 for large a . In particular, when solving for $K(a)$ with RK4, we do not start at $a = 0$. Instead, we start at some a_0 , e.g. $a_0 = 1$, with an initial data computed by truncated series expansion. We only take 3D as an example to illustrate the main idea. The details are given in **Algorithm 1**.

We emphasize that even though the distribution of those needed positions of a (i.e. $\delta\sqrt{l^2 + m^2 + n^2}$) is not uniform, we do not need to compute each $K(a_{lmn})$ from the beginning. As in the Step 3 of the algorithm, we evaluate $K(a)$ from a_0 to a_M equally in advance, which is called the phase one RK4. Then we compute each $K(a_{lmn})$ for large $\delta\sqrt{l^2 + m^2 + n^2}$ by additional RK4 processes starting from the nearest available K , which is implemented in Step 5. This is called the phase two RK4. Hence, this means we can do one single phase one RK4 time-stepping procedure followed by another phase two RK4 to get all eigenvalues simultaneously. Comparing to evaluating each eigenvalue with quadratures for the integral form one by one, this two-phase RK4 hybrid algorithm can enhance the efficiency significantly. The accuracy can be guaranteed by solving ODEs with smooth

Algorithm 1 Hybrid algorithm computing eigenvalues

Given: L, M, N, δ and fractional order α .

Step 1. Compute $a_M = \delta\sqrt{L^2 + M^2 + N^2}$, choose fixed step Δa and choose $a_0 = 1$.

Step 2. Compute K_0 by the series expansion (2.8) with $a = a_0$.

Step 3. Let $a_k = a_0 + k\Delta a$, and solve (2.9) by RK4 with stepsize Δa and get K_k , $1 \leq k \leq \frac{a_M - 1}{\Delta a}$.

Step 4. For $0 \leq l \leq L, 0 \leq m \leq M, 0 \leq n \leq N$, compute $a_{lmn} = \delta\sqrt{l^2 + m^2 + n^2}$,

if $a_{lmn} \leq a_0$, **then**

 Compute $K(a_{lmn})$ by the series expansion (2.8) with $a = a_{lmn}$.

Step 5. **else**

 Calculate $k' = \lceil \frac{a_{lmn} - a_0}{\Delta a} \rceil$ and $\Delta a' = a_{lmn} - a_0 - k'\Delta a$. Find $K_{k'}$ prepared in **Step 3**,
 solve (2.9) by RK4 with initial data $K_{k'}$ and step $\Delta a'$ one step to get $K(a_{lmn})$.

Step 6. **endif.**

Step 7. Compute $\lambda_\delta(l, m, n) = \frac{6(5-\alpha)}{\delta^2} K(l, m, n)$.

Step 8. **endfor**

coefficients through RK4 with a sufficiently small time step since we only solve the ODE away from the singularity point $a = 0$.

4 Numerical examples

In this section, we apply the hybrid algorithm to solve nonlocal problems. For all numerical examples, we choose the 2D case to demonstrate its effectiveness. We point out that all numerical methods and techniques are valid for 1D and 3D cases as well.

4.1 Comparisons of three approaches computing eigenvalues

First, we show the efficiency and accuracy of **Algorithm 1** by comparing the three approaches for the computation of eigenvalues to nonlocal operators with fractional power type kernels, namely the truncated series expansion (TSE), a mid-point Riemann sum quadrature (RSQ) and the hybrid algorithm (HA).

Example 1. *We first make comparisons on the accuracy and efficiency for computing the eigen-*

values. Let $m = 400$, and $n = 300$, i.e., $a = 500\delta$. We take $\alpha = 1$ (integrable) and $\alpha = 3.99$ (non-integrable) and vary δ as 0.01, 0.04 and 0.2 respectively. We use TSE

$$\lambda = \frac{4(4-\alpha)}{\delta^2} \sum_{k=1}^N \frac{(-1)^k (a)^{2k}}{4^k (k!)^2 (2k+2-\alpha)},$$

RSQ

$$\lambda = \frac{8(4-\alpha)}{N^2 \pi \delta^2} \sum_{j=1}^N \sum_{k=1}^N \frac{\cos(ar_{j-\frac{1}{2}} \theta_{k-\frac{1}{2}}) - 1}{r_{j-\frac{1}{2}}^{\alpha-1} \sqrt{1 - \theta_{k-\frac{1}{2}}^2}}$$

and HA **Algorithm 1** to compute the (400, 300)th eigenvalue.

	N	$\delta = 0.01(a = 5)$		$\delta = 0.04(a = 20)$		$\delta = 0.2(a = 100)$	
		λ	CPU	λ	CPU	λ	CPU
$\alpha = 1$	10	-1.02832512e+05	0.0001	1.21770916e+09	0.0002	9.90477134e+21	0.0003
	1000	-1.02832514e+05	0.0006	-7.10310794e+03	0.0007	-9.70815151e+24	0.0007
	100000	-1.02832514e+05	0.0552	-7.10310794e+03	0.0552	-9.70815151e+24	0.0556
$\alpha = 3.99$	10	-2.48585685e+05	0.0001	4.44518671e+06	0.0003	3.84680357e+19	0.0002
	1000	-2.48585685e+05	0.0007	-2.45337919e+05	0.0007	-1.06237650e+23	0.0007
	100000	-2.48585685e+05	0.0559	-2.45337919e+05	0.0558	-1.06237650e+23	0.0561

Table 1: (Example 1) Computing eigenvalues by TSE.

In RSQ, we choose the centered quadrature to avoid singularities on lines $r = 0$ and $\theta = 1$. The eigenvalues computed by TSE, RSQ and HA are presented in Table 1, 2 and 3, respectively. In Table 1, we see that TSE takes the least CPU time. It is also observed that TSE can obtain highly accurate eigenvalues for small δ as $a = 5$ and $a = 20$ as TSE converges very fast. This can be further verified by the unreported digits. However, for large δ as $a = 100$, the instability starts to occur even with 100000 truncated terms. Comparing to TSE with small a , the RSQ (Table 2) gets eigenvalues with very low accuracy. For instance, when $\delta = 0.01$ it has only three significant digits for the most computational intensive experiments using 10000×10000 quadrature nodes. This drops to a single digit for $a = 20$. The eigenvalues obtained by HA are shown in Table 3. For all cases, HA converges very fast with a decreasing step size. Referring to Table 1, the HA can ensure high accuracy for $\delta = 0.01$ and $\delta = 0.04$. On the other hand, it is still stable and get at least nine significant digits using $\Delta a = 0.01$ for a large $\delta = 0.2$. Moreover, the HA only consumes moderate CPU time. More visibly, we first take small $a = 32$, $\alpha = 1$ and the case TSE with $N = 100000$

as the exact solution given the high accuracy in this regime. The relative errors and CPU time of other cases are shown in the left of Fig. 1. For large $a = 128$, we take the case HA with $\Delta = 0.0001$ as the exact solution, which is presented in the right part. We clearly see that for small a (or δ), TSE converges fastest with highest accuracy. Meanwhile, for large a (or δ), HA is superior in the performances with a very reasonable CPU time.

	N	$\delta = 0.01(a = 5)$		$\delta = 0.04(a = 20)$		$\delta = 0.2(a = 100)$	
		λ	CPU	λ	CPU	λ	CPU
$\alpha = 1$	100	-9.89415196e+04	0.0006	-6.90830808e+03	0.0005	-2.89038878e+02	0.0005
	1000	-1.01601124e+05	0.0312	-7.04147784e+03	0.0365	-2.94636047e+02	0.0327
	10000	-1.02443089e+05	2.4035	-7.08361779e+03	2.5815	-2.96410986e+02	2.6031
$\alpha = 3.99$	100	-1.37221950e+04	0.0007	-1.06573809e+04	0.0005	-6.95976710e+03	0.0006
	1000	-1.94865386e+04	0.0374	-1.62966019e+04	0.0358	-1.24587190e+04	0.0323
	10000	-2.48947256e+04	2.5063	-2.16652447e+04	2.6233	-1.77814449e+04	2.6872

Table 2: (Example 1) Computing eigenvalues by RSQ.

	Δa	$\delta = 0.01(a = 5)$		$\delta = 0.04(a = 20)$		$\delta = 0.2(a = 100)$	
		λ	CPU	λ	CPU	λ	CPU
$\alpha = 1$	0.1	-1.02832522e+05	0.0090	-7.10310878e+03	0.0038	-2.97232018e+02	0.0186
	0.01	-1.02832514e+05	0.0128	-7.10310794e+03	0.0414	-2.97232012e+02	0.1817
	0.001	-1.02832514e+05	0.1018	-7.10310794e+03	0.3631	-2.97232012e+02	1.8072
$\alpha = 3.99$	0.1	-2.48584346e+05	0.0140	-2.45336597e+05	0.0040	-2.41431562e+05	0.0184
	0.01	-2.48585685e+05	0.0125	-2.45337919e+05	0.0530	-2.41432863e+05	0.1794
	0.001	-2.48585685e+05	0.0837	-2.45337919e+05	0.3820	-2.41432863e+05	1.7807

Table 3: (Example 1) Computing eigenvalues by HA.

These three tables together with Fig. 1 demonstrate that, by combining series expansion and ODE strategy, the HA approach is robust, accurate and efficient for different situations, including small and big δ and integrable (such as, $\alpha = 1$) and non-integrable (such as, $\alpha = 3.99$) kernels. We also point out that doing the two-phase RK4 can provide all the rest eigenvalues below the largest one, which is implemented in **Algorithm 1**. This can enhance the overall efficiency significantly.

Figure 1: (Example 1) Errors and CPU time comparisons: left (small δ) and right (large δ).

4.2 Implementation of full discretizations for nonlocal models

Next we provide the full discretization of some nonlocal models in two dimensional domain $[0, L_x] \times [0, L_y]$. We consider some typical time dependent nonlinear nonlocal problems with following form

$$\frac{\partial u}{\partial t} = Lu + N(u).$$

Solving by Fourier spectral methods in space, the solutions are of the form as

$$u_{MN} = \sum_{m=-M}^M \sum_{n=-N}^N a_{mn}(t) e^{i\left(\frac{2\pi m}{L_x}x + \frac{2\pi n}{L_y}y\right)}.$$

Fourier coefficients $A(t) = \{a_{mn}(t)\}_{(2M+1) \times (2N+1)}$ satisfy the following ODE system

$$\frac{d}{dt}A = L * A + N(A),$$

where $'.*'$ denotes element-by-element multiplication, L is a polynomial of the matrix Λ formed by nonlocal eigenvalues $\{\lambda_\delta(m, n)\}$ for $-M \leq m \leq M$, $-N \leq n \leq N$, and $N(A)$ is the L^2 -Fourier projection of nonlinear term to P_{MN} . To match the high accuracy of spectral method in space, we take fourth-order exponential time differencing Runge–Kutta (ETDRK4) time stepping

scheme [10, 22] to solve the above ODE system given as

$$\begin{aligned}
a_n &= e^{\frac{\tau}{2}L} * A_n + L^{-1} * (e^{\frac{\tau}{2}L} - I) * N(A_n), \\
b_n &= e^{\frac{\tau}{2}L} * A_n + L^{-1} * (e^{\frac{\tau}{2}L} - I) * N(a_n), \\
c_n &= e^{\frac{\tau}{2}L} * a_n + L^{-1} * (e^{\frac{\tau}{2}L} - I) * (2N(b_n) - N(A_n)), \\
A_{n+1} &= e^{\tau L} * A_n + \tau^{-2} L^{-3} * \left\{ [-4I - \tau L + e^{\tau L} * (4I - 3\tau L + (\tau L)^2)] * N(A_n) \right. \\
&\quad + 2 [2I + \tau L + e^{\tau L} * (-2I + \tau L)] * (N(a_n) + N(b_n)) \\
&\quad \left. + [-4I - 3\tau L - (\tau L)^2 + e^{\tau L} * (4I - \tau L)] * N(c_n) \right\},
\end{aligned}$$

where τ is the time step, and all arithmetics are element-by-element, including exponent arithmetic and inverse arithmetic. For the nonlinear term $N(\cdot)$ handled explicitly, we use the pseudo-spectral method to compute it by 2D FFT. Hence, the total computation cost is dominated by $\mathcal{O}(MN \log(MN))$.

4.3 Applications to nonlocal models

In this part, we will combine the hybrid algorithm and ETDRK4 to simulate some nonlocal models, including nonlocal Allen–Cahn (NAC) equation, nonlocal Cahn–Hilliard (NCH) equation, and nonlocal phase-field crystal (NPFC) model. For related studies, we refer to [14, 17, 18, 20, 21] and references cited therein. We start with two typical free energy functionals, namely Ginzburg–Landau free energy functional

$$\mathcal{E}(u) = \int_{\Omega} \left\{ \frac{\epsilon^2}{2} |\nabla u|^2 + \frac{1}{4} (u^2 - 1)^2 \right\} dx, \quad (4.1)$$

and Swift–Hohenberg free energy functional

$$\mathcal{E}(u) = \int_{\Omega} \left\{ \frac{1}{4} u^4 + \frac{1-\epsilon}{2} u^2 - |\nabla u|^2 + \frac{1}{2} (\Delta u)^2 \right\} dx. \quad (4.2)$$

Thus, the local Allen–Cahn (LAC) equation and the local Cahn–Hilliard (LCH) equation can be viewed as an L^2 and H^{-1} gradient flow of (4.1) respectively, given as below

$$\begin{aligned}
\text{LAC: } \quad & \frac{\partial u}{\partial t} = \epsilon^2 \Delta u + u - u^3, \\
\text{LCH: } \quad & \frac{\partial u}{\partial t} = -\Delta(\epsilon^2 \Delta u + u - u^3).
\end{aligned}$$

On the other hand, the local phase-field crystal (LPFC) model [17, 18] can be viewed as an H^{-1} gradient flow of (4.2)

$$\frac{\partial u}{\partial t} = \Delta(\Delta^2 u + 2\Delta u + u^3 + (1 - \epsilon)u).$$

If we replace the Laplace operator by the nonlocal diffusion operator in above equations, we obtain the NAC equation, NCH equation and NPFC model respectively [14, 20].

Example 2. NAC *We consider the two-dimensional NAC equation given by*

$$\frac{\partial u}{\partial t} = \epsilon^2 \mathcal{L}_\delta u + u - u^3,$$

in $[0, 4\pi] \times [0, 4\pi]$ with periodic boundary conditions.

To apply the ETDRK4, we set the linear part as $Lu = \epsilon^2 \mathcal{L}_\delta u - \beta u$ and the remaining part involving nonlinearity is given as $N(u) = (1 + \beta)u - u^3$. In this example, we fix $\beta = 1$.

The first part of this example is designed to verify the spectral convergence of the spatial discretization. We take the smooth initial value as $u_0(x) = 0.05 \sin(0.5x) \sin(0.5y)$, $\epsilon = 0.1$, $\delta = 0.2$, and the fractional kernel with power $\alpha = 3$. The time step size is fixed small enough as $\tau = 0.001$. The reference solution is obtained on a very fine mesh as $M = N = 128$. The logarithm scale plot of errors at $T = 2$ and $T = 5$ are shown in Figure 2, in which the exponential convergence is observed.

Figure 2: (Example 2) The log scale plot of errors for the NAC equation.

The second part aims to further confirm an observation given in [14] for the 2D case. In [14], an condition is given to determine whether the steady states of NAC equations are continuous or not.

Proposition 1. (Proposition 7 in [14]) *Under certain assumptions, if $\epsilon^2 C_\delta < 1$, the locally increasing u^* has a discontinuity at x_* . Moreover,*

$$\lim_{x \rightarrow x_*^+} u^*(x) = \sqrt{1 - \epsilon^2 C_\delta}, \quad \lim_{x \rightarrow x_*^-} u^*(x) = -\sqrt{1 - \epsilon^2 C_\delta}. \quad (4.3)$$

Here C_δ is the integral of the kernel

$$C_\delta = \int_{\mathcal{B}(0, \delta)} \rho_\delta(|\mathbf{y}|) d\mathbf{y} = \frac{4(4 - \alpha)}{(2 - \alpha)\delta^2}.$$

The above result is proved for 1D case in [14], but it is equally applicable for 2D case. We fix $\epsilon = 0.15$, and take the fractional kernel with power $\alpha = 1$. In these settings, $\delta_0 = 2\sqrt{3}\epsilon$ is the critical value to satisfy $\epsilon^2 C_\delta = 1$. Hence, for NAC equation, we choose $\delta_1 = 3\epsilon$ ($\delta_1 < \delta_0$) and $\delta_2 = 4\epsilon$ ($\delta_2 > \delta_0$).

We also simulate the LAC model in comparison. Figure 3 demonstrates the numerical evolutions in all three simulations. We see that the NAC equation with a smaller δ has more similar dynamics with LAC equation. We also observe that LAC equation and the NAC equation with δ_1 have wider (more diffusive) interface than the the NAC equation with δ_2 . We further present the 3D plots of the interfaces around the left bottom corner at $t = 200$ for three cases in Figure 4. Clearly, we can see the smooth diffusive interface in the local model, continuous interface for the case $\delta = 3\epsilon$, however, sharp and discontinuous interface for $\delta = 4\epsilon$. Some oscillations are seen around the interface in the case $\delta = 4\epsilon$, in which the condition $\epsilon^2 C_\delta < 1$ in Proposition 1 holds. Therefore, these oscillations are no surprise since the steady state is discontinuous in these settings, leading to the Gibbs phenomenon observed in Figure 4.

Example 3. NCH *We consider the two-dimensional NCH equation given below*

$$\frac{\partial u}{\partial t} = \mathcal{L}_\delta (-\epsilon^2 \mathcal{L}_\delta^2 u + u^3 - u),$$

in $[0, 4\pi] \times [0, 4\pi]$ with periodic boundary conditions. We fix $\epsilon = 0.1$, $M = N = 128$, and the fractional kernel with power $\alpha = 2$.

We solve NCH by ETDRK4 with the linear part given by $Lu = -\epsilon^2 \mathcal{L}_\delta^2 u + \beta \mathcal{L}_\delta u$, and the nonlinear part $N(u) = -(1 + \beta) \mathcal{L}_\delta u + \mathcal{L}_\delta u^3$. Note that the NCH describes a conserved dynamics, we thus modify the zero eigenvalue in $\mathcal{L}_\delta$ to 1 when we need to invert the linear operator L in ETDRK4. This technique can guarantee the mass conservation without affecting other frequency modes.

Figure 3: (Example 2) Numerical evolutions of both LAC and NAC equations.

In the first part of this example, we test the numerical convergence rate of the temporal discretization. We take the smooth initial value as $u_0(x) = 0.01 + 0.1 \sin(x) \cos(y) + 0.04 \cos(2x) \sin(4y)$ and $\delta = 0.1$. From Table 4 where τ is time step size, it is observed that the numerical convergence rates are very close to fourth order.

The second part of this example is designed to investigate differences between the dynamics of

Figure 4: (Example 2) Interfaces around the left bottom corner of LAC and NAC equations at $t = 200$.

LCH equations and NCH equations. We do three numerical experiments, including LCH equation, NCH equation with small δ ($= 0.1$), and NCH equation with large δ ($= 1$). All three simulations start from same random initial values and with same time step size $\tau = 0.01$. The snapshots of numerical dynamics at $T = 0.4, 2, 10, 40$ are shown in Figure 5 and the energy evolutions are shown in Figure 6. It is seen that NCH equation with a small δ has nearly the same numerical solutions as local model. This also confirms that Fourier spectral methods are asymptotically compatible for NCH equation. However, NCH equation with a larger δ differs from LCH equation in spatial and temporal morphology, showing a slower phase separation and coarsening processes, although the energy evolution behaves more or less the same. We also observe that the larger δ leads to sharper interfaces than those allowed in LCH for more fragmented bulk regions, thus displaying a much more heterogeneous phase structure.

	T=1		T=10	
τ	$\ u_{MN}^\tau - u_{MN}^{\frac{\tau}{2}}\ _2$	Rate	$\ u_{MN}^\tau - u_{MN}^{\frac{\tau}{2}}\ _2$	Rate
0.02	2.06e-3	-	3.68e-4	-
0.01	1.71e-4	3.60	3.12e-5	3.56
0.005	1.22e-5	3.81	2.20e-6	3.83
0.0025	8.06e-7	3.92	1.60e-7	3.78

Table 4: Numerical convergence rates for NCH equations.

Figure 5: (Example 3) Numerical evolutions of both LCH and NCH models.

Example 4. NPFC We consider the two-dimensional NPFC model given below

$$\frac{\partial u}{\partial t} = \mathcal{L}_\delta(\mathcal{L}_\delta^2 u + 2\mathcal{L}_\delta u + (1 - \epsilon)u + u^3),$$

Figure 6: (Example 3) Energy evolutions starting from $T = 1$ for LCH and NCH equations.

in $[0, 50] \times [0, 50]$ with periodic boundary conditions. We fix $\epsilon = 0.025$, $M = N = 64$, and $\delta = 2$.

In this example, we consider sign changing kernels for NPFC models with the following mixing form of two fractional kernels with fractional power α_1 and α_2 as

$$\rho_\delta^{mix}(r) = c_1 \frac{2(4 - \alpha_1)}{\pi} \frac{1}{\delta^{4-\alpha_1} r^{\alpha_1}} - c_2 \frac{2(4 - \alpha_2)}{\pi} \frac{1}{\delta^{4-\alpha_2} r^{\alpha_2}}, \quad r \in (0, \delta) \quad \alpha_1, \alpha_2 \in [0, 4). \quad (4.4)$$

To satisfy the normalized condition (1.3), we require

$$c_1 - c_2 = 1.$$

Furthermore, if we assume that $\alpha_1 > \alpha_2$ and $c_1(4 - \alpha_1) < c_2(4 - \alpha_2)$, then the mixing kernel is positive around the origin but negative at $r = \delta$, thus leading to a sign-changing kernel. On the other hand, the corresponding (m, n) -th eigenvalue is the combination of the ones corresponding α_1 and α_2 as

$$\lambda_\delta^{mix}(m, n) = c_1 \lambda_\delta^{\alpha_1}(m, n) - c_2 \lambda_\delta^{\alpha_2}(m, n).$$

As we can compute both $\lambda_\delta^{\alpha_1}(m, n)$ and $\lambda_\delta^{\alpha_2}(m, n)$ by the hybrid algorithm, we can obtain $\lambda_\delta^{mix}(m, n)$ accurately and efficiently.

In the simulations, three c_1 s are chosen as 1, 6, and 20, and two α s are chosen as $\alpha_1 = 3$ and $\alpha_2 = 0$. For all c_1 s, numerical computation shows that the nonlocal eigenvalues are all negative (except for zero eigenvalue), providing the necessary diffusive effect. In all experiments, the NPFC models start from the same random initial values with mean value 0.07. Figure 7 shows steady states, energy evolutions, and residual evolutions for NPFC models. All three experiments lead to

Figure 7: (Example 4) Steady states, energy evolutions, and residual evolutions for NPFC models.

the typical hexagonal lattice structure. It is observed that as c_1 increases, the size of cells become larger. All energy curves are below the energy for the constant solution in the end, which means the steady states are physical meaningful solutions. The residual evolutions shown in the bottom figures indicate that the simulations are almost at the steady states.

5 Concluding remarks

The main objective of this paper is to present a hybrid algorithm to compute the Fourier symbols of the linear nonlocal diffusion (peridynamic) operators so that effective Fourier spectral methods can be adopted to solve both linear and nonlinear nonlocal equations. A key observation made in

the discussion is that each (l, m, n) th nonlocal eigenvalue can be viewed as a function in term of a unit-less parameter $\delta\sqrt{l^2 + m^2 + n^2}$ (denoted as a). We carefully derived two different forms of this function, namely, the series expansion form and the ODE form. Each has distinct advantages for different parameter regimes. This leads naturally to the proposed hybrid algorithm: that is to get $\lambda_\delta(m, n)$ by the truncated series expansion form for small a , while for large a , we obtain the Fourier symbols by solving the ODE with RK4. We then efficiently implemented this hybrid algorithm to get all desirable eigenvalues by doing a two-phase RK4 time-stepping procedures. This can reduce the computational significantly in comparison with the brutal force computation of the eigenvalues.

Utilizing the newly developed hybrid algorithm, we further simulated several nonlocal problems, including NAC equations, NCH equations, and NPFC models. In these numerical experiments, we showed the accuracy and effectiveness of the hybrid algorithm, as well as revealed some interesting results generated by nonlocal models, such as those allowing discontinuous solutions, sharpening the interfaces, slowing down phase coarsening process, and etc. We also showed that our hybrid algorithm can be valid not only for special fractional power kernels but also some mixing form sign changing kernels. Hence, extending this hybrid algorithm to more general kernels will be an meaningful future work. Meanwhile, eliminating the Gibbs phenomena is also an interesting work, while we have developed suitable strategies for the steady state problems, the extension to time-dependent cases remains to be investigated. We notice that there have been much development in the context of spectral methods for PDEs on effective singularity detection algorithms and high order recovery of solution information near and away from singularities [34]. Thus, it is natural to pursue further studies on how to adopt and extend those techniques to nonlocal models in connection with the techniques developed here.

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