

Implementation of Exponential Time Differencing Methods for Allen–Cahn Equations in Programming

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Abstract

In this note, the utilization of the Fast Fourier Transform (FFT) and its variations to implement Exponential Time Differencing (ETD) methods for Allen–Cahn equations on a regular mesh in \mathbb{R}^d for $d = 1, 2, 3$ is demonstrated. Three types of boundary conditions will be discussed: Dirichlet boundary conditions, periodic conditions, and Neumann conditions. This note builds upon previous preliminary codes for ETDRK methods for the Allen–Cahn equations and is inspired by [1].

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1 Introduction

Consider an open rectangular domain $\Omega \in \mathbb{R}^d$ for $d = 1, 2, 3$ and a given time interval $T > 0$. We aim to solve numerically the semilinear parabolic equations of the following form:

$$u_t = D\Delta u + f(u), \quad \mathbf{x} \in \Omega, t \in [t_0, t_0 + T],$$

where D denotes the diffusion coefficient. Equations of this type are of broad interest as they model various physical phenomena. To illustrate, consider the widely used phase-field model, the Allen–Cahn equation:

$$\begin{cases} u_t = \varepsilon^2 \Delta u + f(u), & \mathbf{x} \in \Omega, t \in (0, T], \\ u(\mathbf{x}, 0) = u^0(\mathbf{x}), & \mathbf{x} \in \bar{\Omega}, \end{cases} \quad (1)$$

equipped with dirichlet, periodic or Neumann boundary conditions. Here, Δ representing the Laplacian operator over d dimensions, the unknown function u denotes the phase variable, and the parameter $\varepsilon > 0$ represents the interfacial width. The nonlinear term $f(u) = -F'(u)$, where F is a double-well potential with two wells at $\pm\beta$ for some $\beta > 0$. More precisely, $f : \mathbb{R} \rightarrow \mathbb{R}$ is a continuously differentiable function satisfying:

$$\exists \text{ a constant } \beta > 0, \text{ such that } f(\beta) \leq 0 \leq f(-\beta). \quad (2)$$

A notable feature of the Allen–Cahn equation is the *maximum bound principle* (MBP), i.e., if the initial values are within β in absolute value, the solution remains bounded by β at all times. Furthermore, this model satisfies the so-called *energy dissipation law*, because (1) can be viewed as an L^2 gradient flow with respect to the energy functional:

$$E(u) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + F(u) \right) dx. \quad (3)$$

The energy dissipation law is more precisely formulated as:

$$\frac{d}{dt} E(u) = \left(\frac{\delta E(u)}{\delta u}, \frac{\partial u}{\partial t} \right) = - \|\partial_t u\|^2 \leq 0, \quad \forall t > 0, \quad (4)$$

where (\cdot, \cdot) and $\|\cdot\|$ represent the standard L^2 inner product and norm.

Assume that f satisfies the Lipschitz condition with a Lipschitz constant C_l , i.e.,

$$|f(u) - f(v)| \leq C_l |u - v| \quad \forall u, v \in \mathbb{R}. \quad (5)$$

Following this, we introduce a stabilizing constant κ , satisfying:

$$\kappa \geq C_l. \quad (6)$$

By adding and subtracting a stabilization term κu to the Allen–Cahn equation (1), we derive an equivalent form of (1)

$$u_t = \mathcal{L}u + \mathcal{N}(u), \quad \mathbf{x} \in \Omega, \quad t \in (0, T], \quad (7)$$

where the linear operator \mathcal{L} and nonlinear operator \mathcal{N} are defined as

$$\mathcal{L} := \varepsilon^2 \Delta - \kappa \mathcal{I}, \quad \mathcal{N} := f + \kappa \mathcal{I}, \quad (8)$$

and \mathcal{I} denotes the identity operator.

Given a positive integer N_t , let the time interval $[0, T]$ be divided into N_t subintervals with a uniform time step $\tau = T/N_t$, and define $t_n = n\tau, n = 0, 1, \dots, N$. To solve the Allen–Cahn equation (1), we focus on the equivalent equation (7) over the interval $[t_n, t_{n+1}]$, or equivalently $w^n(x, s) = u(x, t_n + s)$ satisfying the system

$$\begin{cases} \partial_s w^n = \mathcal{L}w^n + \mathcal{N}(w^n), & \mathbf{x} \in \Omega, \quad s \in (0, \tau], \\ w^n(\mathbf{x}, 0) = u(\mathbf{x}, t_n), & \mathbf{x} \in \bar{\Omega}. \end{cases} \quad (9)$$

The central concept of ETD involves applying Duhamel’s principle to the system, which leads to the following formulation:

$$w^n(\mathbf{x}, \tau) = e^{\tau \mathcal{L}} w^n(\mathbf{x}, 0) + \int_0^\tau e^{(\tau-s)\mathcal{L}} \mathcal{N}[w^n(\mathbf{x}, s)] \, ds \quad (10)$$

and then approximating the nonlinear function $\mathcal{N}[u(t_n + s)]$ in the integral. Employing interpolation to approximate $\mathcal{N}[u(t_n + s)]$ leads to the development of ETD Runge–Kutta (ETDRK) methods.

2 FFT-based Numerical Methods in One Dimensions

Fast explicit numerical methods are derived for the model in one dimension. Suppose $\Omega = \{x_b < x < x_e\}$. The spatial domain is discretized using a uniform rectangular mesh as follows: $x_i = x_b + ih_x$ for $0 \leq i \leq N_x$, where $h_x = (x_e - x_b)/N_x$. The numerical solution at each mesh point is denoted by $u_i = u_i(t) \approx u(x_i, t)$ for $0 \leq i \leq N_x$. A second-order accurate central difference discretization scheme is employed for approximating the Laplace operator.

2.1 The Problem with Periodic Boundary Conditions

Suppose that the model (1) is equipped with a periodic boundary condition as

$$u(x_b, t) = u(x_e, t), \quad \frac{\partial u}{\partial x}(x_b, t) = \frac{\partial u}{\partial x}(x_e, t), \quad t \in [0, T],$$

is imposed, then the set of unknowns is given as

$$\mathbf{u} = \{u_i\}_{(N_x-1) \times 1} = \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N_x-1} \end{pmatrix}.$$

Let

$$(\Delta_h^P)_{n \times n} := \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 1 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 1 & \cdots & 0 & 0 & 1 & -2 \end{pmatrix}_{n \times n}$$

for $n \in \mathbb{N}^+$.

Then we can write the semi-discretization of (9) in space in the following compact representation:

$$\frac{d\mathbf{u}}{dt} = \mathbf{L}\mathbf{u} - \kappa\mathbf{u} + \mathcal{N}(\mathbf{u}),$$

where $\mathbf{L}^P := \frac{\varepsilon^2}{h_x^2} (\Delta_h^P)_{N_x \times N_x}$. The corresponding Duhamel's principle is

$$\mathbf{u}^{n+1} = e^{\tau \mathbf{L}_\kappa} \mathbf{u}^n + \int_0^\tau e^{(\tau-s) \mathbf{L}_\kappa} \mathcal{N}[\mathbf{u}(t_n + s)] ds, \quad (11)$$

where $\mathbf{L}_\kappa := \mathbf{L}^P - \kappa \mathbf{I}$. Applying the theory of circular matrices, the following lemma presents the eigen-pairs of the circular matrix Δ_h^D of dimensions $n \times n$.

Lemma 2.1. *The eigen-pairs of the circular matrix $(\Delta_h^P)_{n \times n}$ is*

$$\begin{aligned} \lambda_k &= -2 + w^k + w^{k(n-1)} = 2(\cos \frac{2k\pi}{n} - 1), \\ \vec{\phi}_k &= (1, w^k, w^{2k}, \dots, w^{(n-1)k})^T, \end{aligned} \quad (12)$$

where $w := e^{-i\frac{2\pi}{n}}$ is the principal n -th root of unity, and $k = 0, 1, \dots, n-1$.

Since $\Phi\Phi^H = \Phi^H\Phi = nI$, the eigen-decomposition of Δ_h^P is

$$(\Delta_h^P)_{n \times n} = \frac{1}{\sqrt{n}}\Phi(\Lambda^P)_{n \times n}\frac{1}{\sqrt{n}}\Phi^H,$$

where $\Phi = [\vec{\phi}_0, \vec{\phi}_1, \dots, \vec{\phi}_{n-1}]$. Please note that Φ is the matrix of the discrete Fourier transform (DFT) and $\frac{1}{n}\Phi^H$ is the matrix of the discrete Fourier transform (iDFT).

Lemma 2.2. *For two matrices A, P , if P is invertible, then $e^{PAP^{-1}} = Pe^AP^{-1}$.*

This lemma can be proved directly by using the definition of matrix exponential, i.e. the series form. To compute (11), the most challenging aspect involves computing the products of $\exp(\mathbf{L})$ and \mathbf{L}^k with vectors. When the spatial domain of the problem is regular and the matrix \mathbf{L} possesses specific structural properties, such as being a circular matrix, algorithms based on the Fast Fourier Transform (FFT) are particularly effective for calculating these products.

Define $\gamma(z) = ce^z + \sum c_k z^k$ for $c, c_k \in \mathbb{R}$. For $\mathbf{L}^P \in \mathbb{R}^{n \times n}$ and any vector $\mathbf{v} \in \mathbb{R}^{n \times 1}$, the FFT can be used to compute $\gamma(a\mathbf{L}^P + b\mathbf{I})\mathbf{v}$. More precisely,

$$\begin{aligned} \phi(a\mathbf{L}^P + b\mathbf{I})\mathbf{v} &= \gamma\left(\frac{1}{\sqrt{n}}\Phi\Lambda_1\frac{1}{\sqrt{n}}\Phi^H\right)\mathbf{v} \\ &= \frac{1}{\sqrt{n}}\Phi\gamma(\Lambda_1)\frac{1}{\sqrt{n}}\Phi^H\mathbf{v} \\ &= \Phi\gamma(\Lambda_1)\left(\frac{1}{n}\Phi^H\right)\mathbf{v} \\ &= \text{DFT}[\gamma(\text{diag}(\Lambda_1)) \odot \text{iDFT}(\mathbf{v})], \end{aligned} \tag{13}$$

where $\text{diag}(A)$ denotes the diagonal vector of A , and \odot denotes element by element multiplication between two arrays of same sizes. The computational complexity of (13) is $2O(n \log_2 n) + O(n) = O(n \log_2 n)$, while the complexity of direct computation of $\mathbf{L}^P\mathbf{v}$ is $O(n^2)$.

2.2 The Problem with Dirichlet Boundary Conditions

Suppose that the model (1) is equipped with a Dirichlet boundary condition

$$u(\mathbf{x}, t) = \alpha(\mathbf{x}, t), \quad \mathbf{x} \in \partial\Omega, \quad t \in [0, T].$$

In this case, the set of unknowns is given as

$$\mathbf{u} = \{u_i\}_{(N_x-1) \times 1} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{N_x-1} \end{pmatrix}.$$

Let

$$\mathbf{b}^D := \frac{\varepsilon^2}{h_x^2} \begin{pmatrix} \alpha(x_0, t) \\ 0 \\ \vdots \\ 0 \\ \alpha(x_{N_x}, t) \end{pmatrix}_{(N_x-1) \times 1},$$

and

$$(\Delta_h^D)_{n \times n} := \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & 0 & 0 & 1 & -2 \end{pmatrix}_{n \times n}$$

for $n \in \mathbb{N}^+$.

Then we can write the semi-discretization of (9) in space in the following compact representation:

$$\frac{d\mathbf{u}}{dt} = \mathbf{L}\mathbf{u} - \kappa\mathbf{u} + \mathbf{b}^D + \mathcal{N}(\mathbf{u}),$$

where $\mathbf{L}^D := \frac{\varepsilon^2}{h_x^2} (\Delta_h^D)_{(N_x-1) \times (N_x-1)}$. The corresponding Duhamel's principle is

$$\mathbf{u}^{n+1} = e^{\tau \mathbf{L}_\kappa} \mathbf{u}^n + \int_0^\tau e^{(\tau-s)\mathbf{L}_\kappa} \{ \mathbf{b}^D(t_n + s) + \mathcal{N}[\mathbf{u}(t_n + s)] \} ds, \quad (14)$$

where $\mathbf{L}_\kappa := \mathbf{L}^D - \kappa \mathbf{I}$.

In this case, \mathbf{L}^D is not a circular matrix, but a topeliz matrix. The DFT will become discrete sine transform (DST). We have similar lemma:

Lemma 2.3. *The eigen-pairs of the circular matrix $(\Delta_h^D)_{n \times n}$ is*

$$\begin{aligned} \lambda_k &= 2(\cos \frac{k\pi}{n+1} - 1), \\ \vec{\phi}_k &= \left(\sin \frac{k\pi}{n+1}, \sin \frac{2k\pi}{n+1}, \dots, \sin \frac{nk\pi}{n+1} \right)^T, \end{aligned} \quad (15)$$

where $k = 1, 2, \dots, n$.

Since $\Phi\Phi^H = \Phi^H\Phi = \frac{n+1}{2}I$, the eigen-decomposition of Δ_h^D is

$$(\Delta_h^D)_{n \times n} = \sqrt{\frac{2}{n+1}}\Phi(\Lambda^D)_{n \times n}\sqrt{\frac{2}{n+1}}\Phi^H,$$

where $\Phi = [\vec{\phi}_1, \vec{\phi}_2, \dots, \vec{\phi}_n]$. Please note that Φ is the matrix of the discrete Sine transform (DST) and $\frac{2}{n+1}\Phi^H$ is the matrix of the discrete Sine transform (iDST).

Define $\gamma(z) = ce^z + \sum c_k z^k$ for $c, c_k \in \mathbb{R}$. For $\mathbf{L}^D \in \mathbb{R}^{n \times n}$ and any vector $\mathbf{v} \in \mathbb{R}^{n \times 1}$, the fast DST can be used to compute $\gamma(a\mathbf{L}^D + b\mathbf{I})\mathbf{v}$. More precisely,

$$\begin{aligned} \phi(a\mathbf{L}^D + b\mathbf{I})\mathbf{v} &= \gamma\left(\sqrt{\frac{2}{n+1}}\Phi\Lambda_1\sqrt{\frac{2}{n+1}}\Phi^H\right)\mathbf{v} \\ &= \sqrt{\frac{2}{n+1}}\Phi\gamma(\Lambda_1)\sqrt{\frac{2}{n+1}}\Phi^H\mathbf{v} \\ &= \Phi\gamma(\Lambda_1)\left(\frac{2}{n+1}\Phi^H\right)\mathbf{v} \\ &= \text{DST}(\gamma(\text{diag}(\Lambda_1)) \odot \text{iDST}(\mathbf{v})), \end{aligned} \tag{16}$$

where $\text{diag}(A)$ denotes the diagonal vector of A , and \odot denotes element by element multiplication between two arrays of same sizes. The computational complexity of (13) is $2O(n \log_2 n) + O(n) = O(n \log_2 n)$, whereas the complexity of directly computing $\mathbf{L}^D\mathbf{v}$ is $O(n^2)$. There are multiple methods to achieve fast DST via FFT. Please read [2] and the Signal Processing Stack Exchange for more information. One convenient approach involves using $2n$ FFT padding as described in [2]:

$$\left[\left(\begin{array}{ccc|ccc} -2 & 1 & & & & \\ & 1 & -2 & 1 & & \\ & & & \ddots & & \\ & & & & 1 & -2 \\ \hline & & & & 1 & \\ & & & & & -2 & 1 \\ & & & & & & \ddots \\ & & & & & & 1 & -2 & 1 \\ & & & & & & & 1 & -2 \\ 1 & & & & & & & & \end{array} \right) \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \frac{u_{N_x-1}}{0} \\ \vdots \\ 0 \\ 0 \end{pmatrix} \right] (1 : N_x - 1).$$

2.3 The Problem with Neumann Boundary Conditions

Suppose that the model (1) is equipped with a Neumann boundary condition

$$\frac{\partial u}{\partial \mathbf{x}} = \beta(\mathbf{x}, t), \quad \mathbf{x} \in \partial\Omega, \quad t \in [0, T].$$

In this case, the set of unknowns is given as

$$\mathbf{u} = \{u_i\}_{(N_x-1) \times 1} = \begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N_x} \end{pmatrix}.$$

Let

$$\mathbf{b}^N := \frac{2\varepsilon}{h_x} \begin{pmatrix} \beta(x_0, t) \\ 0 \\ \vdots \\ 0 \\ \beta(x_{N_x}, t) \end{pmatrix}_{(N_x+1) \times 1},$$

and

$$(\Delta_h^N)_{n \times n} := \begin{pmatrix} -2 & 2 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & 0 & 0 & 2 & -2 \end{pmatrix}_{n \times n}$$

for $n \in \mathbb{N}^+$.

Then we can write the semi-discretization of (9) in space in the following compact representation:

$$\frac{d\mathbf{u}}{dt} = \mathbf{L}^N \mathbf{u} - \kappa \mathbf{u} + \mathbf{b}^N + \mathcal{N}(\mathbf{u}),$$

where $\mathbf{L}^N := \frac{\varepsilon^2}{h_x^2} (\Delta_h^N)_{(N_x+1) \times (N_x+1)}$. The corresponding Duhamel's principle is

$$\mathbf{u}^{n+1} = e^{\tau \mathbf{L}_\kappa} \mathbf{u}^n + \int_0^\tau e^{(\tau-s) \mathbf{L}_\kappa} \{ \mathbf{b}^N(t_n + s) + \mathcal{N}[\mathbf{u}(t_n + s)] \} ds, \quad (17)$$

where $\mathbf{L}_\kappa := \mathbf{L}^N - \kappa \mathbf{I}$. In this case, \mathbf{L}^N is neither a circular matrix nor a Toeplitz matrix. To employ a FFT-based fast algorithm, we must make

In fact, $I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x$ represents the 2D DFT. Using $(AB) \otimes (CD) = (A \otimes C)(B \otimes D)$, we have

$$\begin{aligned} I \otimes A &= (QIQ^H) \otimes (Q\Lambda Q^H) \\ &= (Q \otimes Q)(I \otimes \Lambda)(Q^H \otimes Q^H). \end{aligned} \quad (20)$$

Note that $(Q \otimes Q)(Q^H \otimes Q^H) = (Q^H \otimes Q^H)(Q \otimes Q) = I$, so by lemma 2.2, we have the 2D eigen decomposition.

$$I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x = (Q^y \otimes Q^x)(I^y \otimes \Lambda^x + \Lambda^y \otimes I^x)(Q^y \otimes Q^x)^H$$

$$I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x = ((Q^y)^H \otimes Q^x)(I^y \otimes \Lambda^x + \Lambda^y \otimes I^x)(Q^y \otimes (Q^x)^H)$$

$$I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x = (Q^y \otimes (Q^x)^H)(I^y \otimes \Lambda^x + \Lambda^y \otimes I^x)((Q^y)^H \otimes Q^x)$$

$$I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x = ((Q^y)^H \otimes (Q^x)^H)(I^y \otimes \Lambda^x + \Lambda^y \otimes I^x)(Q^y \otimes Q^x)$$

This is the separability of 2D DFT.

Since $\text{vec}(AXB) = (B^T \otimes A)\text{vec}(X)$ and $(Q$ is symmetric), we have

$$\begin{aligned} (Q^H \otimes Q^H)\text{vec}(M) &= \text{vec}(Q^H M Q^H), \\ (Q \otimes Q)\text{vec}(M) &= \text{vec}(Q M Q). \end{aligned} \quad (21)$$

Then we can compute $Q^H M Q^H$ in this way,

$$Q^H M Q^H = \frac{1}{n} \Phi^H M \Phi^H = \frac{1}{n} \Phi^H (\Phi M^H)^H \quad (22)$$

and compute $Q M Q$ similarly,

$$Q M Q = \Phi M (\frac{1}{n} \Phi) = \Phi [(\frac{1}{n} \Phi^H) M^H]^H. \quad (23)$$

Note that Φ is DFT, $\frac{1}{n} \Phi^H$ is iDFT.

4 FFT-based Numerical Methods in Three Dimensions

Let $\Omega = \{x_b < x < x_e, y_b < y < y_e, z_b < z < z_e\}$. We present the case with a Dirichlet boundary condition as $u = g$ on $\partial\Omega$ and discussions on other boundary condition cases simply follow. Similar to solving the two-dimensional system, we denote h_x, h_y, h_z as the spatial step size, and N_x, N_y, N_z as the number of grid intervals in x, y, z direction, respectively.

Set $u_{i,j,k} = u_{i,j,k}(t) \approx u(t, x_i, y_j, z_k)$ for $0 \leq i \leq N_x, 0 \leq j \leq N_y$ and $0 \leq k \leq N_z$. Denote the unknowns as a three-dimensional array $\mathbf{U} = (u_{i,j,k})_{(N_x-1) \times (N_y-1) \times (N_z-1)}$. Define the vector of \mathbf{U} :

$$\text{vec}_2(\mathbf{U}) = \begin{pmatrix} \text{vec}(\mathbf{U}(:, :, 1)) \\ \text{vec}(\mathbf{U}(:, :, 2)) \\ \vdots \\ \text{vec}(\mathbf{U}(:, :, n_3)) \end{pmatrix}.$$

Then it is easy to check

$$(I^z \otimes (I^y \otimes \Delta_h^x + \Delta_h^y \otimes I^x) + \Delta_h^z \otimes (I^y \otimes I^x)) \text{vec}(\mathbf{U}) \approx \Delta(\text{vec}\mathbf{U}). \quad (24)$$

Then

$$\begin{aligned} I \otimes I \otimes A &= (QIQ^H) \otimes [(Q \otimes Q)(I \otimes \Lambda)(Q^H \otimes Q^H)] \\ &= (Q \otimes Q \otimes Q)(I \otimes I \otimes \Lambda)(Q^H \otimes Q^H \otimes Q^H). \end{aligned} \quad (25)$$

Then

$$\text{vec}_2^{-1}[(Q \otimes Q \otimes Q)\text{vec}_2(\mathbf{U})](r, s, t) = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^{n_3} u_{i,j,k} \cdot e^{-2\pi i \left(\frac{ri}{n_1} + \frac{sj}{n_2} + \frac{tk}{n_3} \right)}$$

is a 3D FFT.

$$\begin{aligned} &I^z \otimes I^y \otimes \Delta_h^x + I^z \otimes \Delta_h^y \otimes I^x + \Delta_h^z \otimes I^y \otimes I^x \\ &= (Q^z I^z (Q^z)^H) [(Q^y \otimes Q^x)(I^y \otimes \Lambda^x + \Lambda^y \otimes I^x)(Q^y \otimes Q^x)^H] \\ &\quad + \Delta_h^z \otimes I^y \otimes I^x \\ &= (Q^z \otimes Q^y \otimes Q^x)(I^z \otimes I^y \otimes \Lambda^x + I^z \otimes \Lambda^y \otimes I^x)(Q^z \otimes Q^y \otimes Q^x)^H \\ &\quad + (Q^z \otimes Q^y \otimes Q^x)(\Lambda^z \otimes I^y \otimes I^x)(Q^z \otimes Q^y \otimes Q^x)^H \end{aligned} \quad (26)$$

$$\begin{aligned}
& (Q^z \otimes Q^y \otimes Q^x) \text{vec}_2(\mathbf{U}) \\
&= (Q^z \otimes (Q^y \otimes Q^x)) \text{vec}(\text{vec}(\mathbf{U}(:, :, 1)), \text{vec}(\mathbf{U}(:, :, 2)), \dots, \text{vec}(\mathbf{U}(:, :, n_3))) \\
&= \text{vec} \{ (Q^y \otimes Q^x) (\text{vec}(\mathbf{U}(:, :, 1)), \text{vec}(\mathbf{U}(:, :, 2)), \dots, \text{vec}(\mathbf{U}(:, :, n_3))) Q^z \} \\
&= \text{vec} \left\{ (Q^y \otimes Q^x) \left[(Q^z)^H (\text{vec}(\mathbf{U}(:, :, 1)), \text{vec}(\mathbf{U}(:, :, 2)), \dots, \text{vec}(\mathbf{U}(:, :, n_3)))^H \right]^H \right\}
\end{aligned} \tag{27}$$

Maybe the matrix form is not the best.

5 Circular Matrix and FFT

Definition 5.1. A circular matrix is like

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-1} \\ a_{n-1} & a_0 & a_1 & \cdots & a_{n-2} \\ a_{n-2} & a_{n-1} & a_0 & \cdots & a_{n-3} \\ \vdots & \vdots & \vdots & & \vdots \\ a_1 & a_2 & a_3 & \cdots & a_0 \end{pmatrix}. \tag{28}$$

A special circular matrix is

$$J = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}. \tag{29}$$

It is easy to know that J^k is also a circular matrix.

$$J^k = \begin{pmatrix} 0 & I_{n-k} \\ I_k & 0 \end{pmatrix} (1 \leq k \leq n). \tag{30}$$

Thus, $A = a_0 I + a_1 J + \dots + a_{n-1} J^{n-1}$. If we define a polynomial $g(x) := a_0 + a_1 x + a_2 x^2 + \dots + a_{n-1} x^{n-1}$, then $A = g(J)$.

It is easy to know that the eigenvalues of J are principal roots of order n of unity $w^k = e^{-\frac{k}{n} 2\pi i}$ ($k = 0, 1, 2, \dots, n-1$) because $|\lambda I - J| = \lambda^n - 1$. And it is easy to compute that the corresponding eigenvectors are

$$\vec{\phi}_k = (1, w^k, w^{2k}, \dots, w^{(n-1)k})^T, k = 0, 1, 2, \dots, n-1. \tag{31}$$

Therefore, we have the next threorem:

Theorem 5.2. *The eigen-pairs of the circular matrix A is*

$$\begin{aligned}\lambda_k &= g(w^k), & k &= 0, 1, 2, \dots, n-1, \\ \vec{\phi}_k &= (1, w^k, w^{2k}, \dots, w^{(n-1)k})^T, & k &= 0, 1, 2, \dots, n-1.\end{aligned}\quad (32)$$

Note that $\vec{\phi}_k (k = 0, 1, 2, \dots, n-1)$ form the matrix of discrete Fourier transformation (DFT).

Definition 5.3. *For a continuous Fourier transformation $F(w) = \int_{-\infty}^{+\infty} f(t)e^{-iwt}dt$, its discrete transformation is*

$$F(w_n) = \sum_{m=0}^{N-1} f(t_m) e^{-i\frac{2\pi mn}{N}}, \quad (33)$$

and the inverse discrete Fourier transformation is

$$f(t_m) = \frac{1}{N} \sum_{n=0}^{N-1} F(w_n) e^{i\frac{2\pi mn}{N}}. \quad (34)$$

By this definition, the DFT can be written as

$$\begin{bmatrix} F(t_0) \\ F(t_1) \\ \vdots \\ F(t_{N-1}) \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & w_N^1 & w_N^2 & \cdots & w_N^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & w_N^{(n-1)} & w_N^{2(n-1)} & \cdots & w_N^{(n-1)^2} \end{bmatrix} \begin{bmatrix} f(w_0) \\ f(w_1) \\ \vdots \\ f(w_{N-1}) \end{bmatrix}, \quad (35)$$

where $w := e^{-i\frac{2\pi}{n}}$ is the principal n -th root of unity.

As we all know, the computation can be fasten by FFT. Here is a simple discussion. The starting point is to examine the block structure of an even-order DFT matrix after its columns are reordered so that the odd-indexed columns come first. Consider the case

$$F_8 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & w & w^2 & w^3 & w^4 & w^5 & w^6 & w^7 \\ 1 & w^2 & w^4 & w^6 & 1 & w^2 & w^4 & w^6 \\ 1 & w^3 & w^6 & w & w^4 & w^7 & w^2 & w^5 \\ 1 & w^4 & 1 & w^4 & 1 & w^4 & 1 & w^4 \\ 1 & w^5 & w^2 & w^7 & w^4 & w & w^6 & w^3 \\ 1 & w^6 & w^4 & w^2 & 1 & w^6 & w^4 & w^2 \\ 1 & w^7 & w^6 & w^5 & w^4 & w^3 & w^2 & w \end{bmatrix} \quad (w = w_8)$$

(Note that w_8 is a root of unity so that high powers simplify.) If $cols = [1, 3, 5, 7, 2, 4, 6, 8]$, then

$$F_8(:, cols) = \left[\begin{array}{cccc|cccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & w^2 & w^4 & w^6 & w & w^3 & w^5 & w^7 \\ 1 & w^4 & 1 & w^4 & w^2 & w^6 & w^2 & w^6 \\ 1 & w^6 & w^4 & w^2 & w^3 & w & w^7 & w^5 \\ \hline 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & w^2 & w^4 & w^6 & -w & -w^3 & -w^5 & -w^7 \\ 1 & w^4 & 1 & w^4 & -w^2 & -w^6 & -w^2 & -w^6 \\ 1 & w^6 & w^4 & w^2 & -w^3 & -w & -w^7 & -w^5 \end{array} \right].$$

The lines through the matrix are there to help us think of $F_8(:, cols)$ as a 2-by-2 matrix with 4-by-4 blocks. Noting that $w^2 = w_8^2 = w_4$, we see that

$$F_8(:, cols) = \left[\begin{array}{c|c} F_4 & \Omega_4 F_4 \\ \hline F_4 & -\Omega_4 F_4 \end{array} \right],$$

where $\Omega_4 = \text{diag}(1, w_8, w_8^2, w_8^3)$. It follows that if $x \in \mathbb{R}^8$, then

$$F_8 x = F_8(:, cols) \cdot x(cols) = \left[\begin{array}{c|c} F_4 & \Omega_4 F_4 \\ \hline F_4 & -\Omega_4 F_4 \end{array} \right] \begin{bmatrix} x(1:2:8) \\ x(2:2:8) \end{bmatrix} = \left[\begin{array}{c|c} I_4 & \Omega_4 \\ \hline I_4 & -\Omega_4 \end{array} \right] \begin{bmatrix} F_4 x(1:2:8) \\ F_4 x(2:2:8) \end{bmatrix}$$

Thus, if $N = 2^k$, then the complexity of k -step is $T(k) = 2T(\frac{k}{2}) + O(N)$, so the all complexity is $O(N \log_2 N)$. We can use FFT to compute the eigen decomposition of circular matrix. Firstly, let us see a lemma:

Lemma 5.4. *For principal roots of order n of unity $w^k = e^{-ik/n}$ ($k = 0, 1, 2, \dots, n-1$), if $w^k \neq 1$, then*

$$1 + w^k + w^{2k} + \dots + w^{(n-1)k} = 0.$$

It is very simple to prove because

$$0 = (w^k)^n - 1 = (w^k - 1)(1 + w^k + w^{2k} + \dots + w^{(n-1)k}).$$

Using this lemma, we have

Corollary 5.5. $\vec{\phi}_k = (1, w^k, w^{2k}, \dots, w^{(n-1)k})^T$, ($k = 0, 1, 2, \dots, n-1$) are conjugate orthogonal.

Because

$$\vec{\phi}_k^H \vec{\phi}_l = 1 + w^{l-k} + w^{2(l-k)} + \dots + w^{(n-1)(l-k)} = n\delta_{k,l}.$$

Theorem 5.6. *If we note the DFT matrix as Φ , then the eigen decomposition of the circular matrix C is*

$$C = \frac{1}{\sqrt{n}} \Phi \cdot \Lambda \cdot \frac{1}{\sqrt{n}} \Phi^H = \frac{1}{n} \Phi \Lambda \Phi^H.$$

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