

Space-time Spectral Methods for PDEs on Irregular Domains

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Spectral Methods

- Numerical methods for solving ODEs, PDEs, integral equations, eigenvalue problems of differential/integral operators, etc.
- Use global basis functions.

Pros

- + Error decreases exponentially for an analytic solution.
- + Spectral collocation is easy to implement for variable coef and nonlinear problems.

Cons

- Collocation generates dense and ill-conditioned matrices.
- Difficult to implement on irregularly shaped domains.

Space-time Spectral Methods

- Traditionally, apply low-order finite difference temporal discretization and spectral discretization in space. Error in temporal discretization reduces overall convergence rate.
- Space-time spectral method applies spectral discretization in both space and time.

Pros

- + Spectral convergence in both space and time.
- + Far fewer unknowns compared to FDM/FEM.
- + Easy implementation (no CFL, matrix exponentials).
- + Extremely robust (parabolic, hyperbolic, dispersive, higher order PDEs, all standard BC's).

Cons

- Collocation leads to dense ill-conditioned matrices.
- Basic version of method is only suitable for regular domains (rectangles/disks).
- Time stepping cannot be implemented - solve for all unknowns over all times simultaneously; hence larger system to solve.

Fast Solvers for Space-time Systems

- Multiple Shooting (Brugnano, Keller, Lions, Maday, Nievergelt, Turinici, ...)
- Parallel-in-Time Diagonalization (Gander, Maday, Ng, Rønquist, Wathen, Wu, ...)
- Parallel Full Approximation Scheme in Space and Time (Emmett, Götschel, Minion, Ruprecht, Speck, ...)
- Space-time Multigrid (De Sterck, Falgout, Gander, Hackbusch, Horton, Langer, Manteuffel, McCormick, Neumuller, Olson, Schroder, Steinbach, Vandewalle, ...)
- Spectral Deferred Correction (Dutt, Greengard, Minion, Rokhlin, Ruprecht, Speck, Spiteri, ...)
- Waveform Relaxation (Gander, Halpern, Jackiewicz, Nataf, Vandewalle, ...)
- etc.

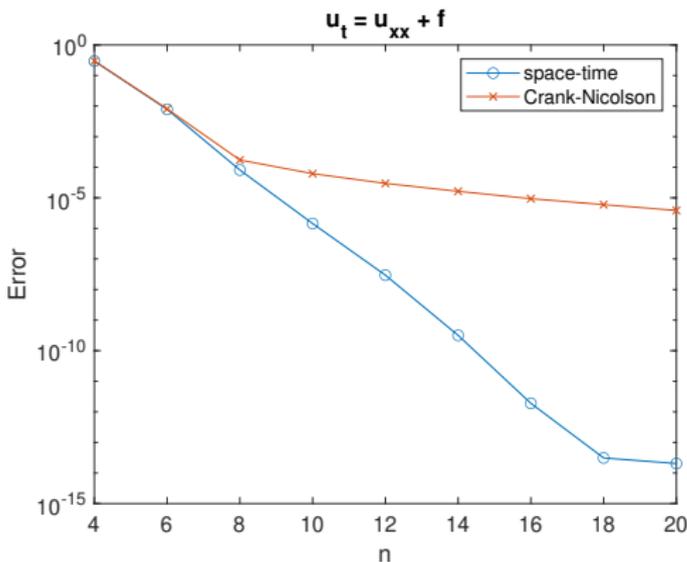


Figure: Comparison of convergence of space-time Legendre collocation vs CN scheme in time and Legendre scheme in space for 1D heat equation.

Space-time spectral discretization of heat equation

$$u_t = u_{xx} + f, \quad (x, t) \in (-1, 1)^2$$

$u(\pm 1, t) = 0$ and $u(x, -1) = u_0(x)$. Assume soln analytic. Define $u_h \in P_n$ by

$$u_h(t) = \begin{bmatrix} u_h(x_1, t) \\ \vdots \\ u_h(x_{n-1}, t) \end{bmatrix}, \quad f_h(t) = \begin{bmatrix} f(x_1, t) \\ \vdots \\ f(x_{n-1}, t) \end{bmatrix}.$$

Let $\{\ell_k, 1 \leq k \leq n-1\}$ denote the Lagrange polynomials ($\in P_n$) so that $\ell_k(x_j) = \delta_{jk}$.

Semi-discrete approx (Tang and Xu)

$$u'_h(t) = \sum_{k=0}^n (A u_h(t_k) + f_h(t_k)) \ell_k(t),$$

with $u_h(-1) = u_{0h}$, where $A = [[D^2]]$ is pseudospectral second derivative matrix. Note

$$u'_h(t_j) = A u_h(t_j) + f_h(t_j), \quad 0 \leq j \leq n-1.$$

Above are precisely the collocation equations.

Discrete system is $A_h \hat{u}_h = \hat{f}_h - (u_{0h} \otimes d_h)$, where

$$A_h = (I_{n-1} \otimes [D]) - (A \otimes I_n).$$

$[D]$ is discrete **time derivative**.

Theorem 1 (Lui and Nataj)

Let A_h be global space-time Chebyshev/Legendre operator for heat equation. For $n \geq 2$,

$$c \leq |\lambda(A_h)| \leq cn^4, \quad \kappa(A_h) \leq cn^4.$$

Proof: Recall $A_h = (I_{n-1} \otimes [D]) - (A \otimes I_n)$. Therefore

$$\lambda(A_h) = \lambda_j([D]) - \lambda_k(A), \quad \forall j, k.$$

Result holds since $\text{Re } \lambda_j([D]), \lambda_k(-A) \geq c > 0$ and $|\lambda_j([D])| \leq cn^2, |\lambda_k(A)| \leq cn^4, \forall j, k$.

Theorem 2 (Lui and Nataj)

Let E_h be error vector at collocation points. For $n \geq 2$,

$$|W^{1/2} E_h| \leq cn^{3.5} e^{-Cn}.$$

Condition number estimates for space-time spectral discretizations of other linear PDEs (Lui and Nataj):

- Schrodinger: $u_t = iu_{xx} + f$, $c \leq |\lambda| \leq Cn^4$;
- wave: $u_{tt} = u_{xx} + f$, $c \leq |\lambda| \leq Cn^4$;
- Airy: $u_t + u_{xxx} = f$, $c \leq |\lambda| \leq Cn^6$;
- beam: $u_{tt} + u_{xxxx} = f$, $c \leq |\lambda| \leq Cn^8$.

Proofs required eigval estimates of spectral deriv operators (25 year old conjectures).

(Lui and Nataj) Numerical results space-time spectral discretizations for standard nonlinear PDEs (nonlinear diffusion, Burgers, kdV, Allen–Cahn, Cahn–Hilliard, Kuramoto–Sivashinsky, nonlinear Schrodinger, Sine–Gordon).

2D Stokes Equations in primitive variables

$$\begin{aligned}
 u_t - \Delta u + \nabla p &= f \quad \text{in } \Omega = (-1, 1)^2, \\
 \nabla \cdot u &= 0 \quad \text{in } \Omega, \\
 u &= 0 \quad \text{on } \partial\Omega, \\
 u(x, y, -1) &= u_0(x, y) \quad \text{in } \Omega.
 \end{aligned}$$

Theorem 3 (Kaur and Lui)

For a $P_n - P_{n-2}$ Legendre discretization of A_h , the steady Stokes operator (sym saddle point matrix), $\kappa(A_h) \leq cn^4$.

Results for space-time spectral discretization of unsteady case (Kaur and Lui):

- Condition number estimate for spectral operator
- Proof of full spectral convergence
- Numerical results for Navier–Stokes

Space-time Spectral Stokes Equations

- Stream function formulation: $(\psi_{xx})_t = \psi_{xxxx} + f$ with initial condition $\psi(x, -1) = \psi_0(x)$ and boundary conditions $\psi(\pm 1, t) = 0 = \psi_x(\pm 1, t)$.
Chebyshev space-time discretization:

$$A_h \hat{\psi}_h = \hat{f}_h - (\psi_{0h} \otimes d_h),$$

where

$$A_h = (B_2 \otimes [D]) - (B_4 \otimes I_N).$$

Theorem 4 (Lui and Willegoda Liyanage)

Let $n \geq 2$ and λ be an eigenvalue of A_h . Then

$$c \leq |\lambda| \leq Cn^8,$$

where c and C are positive and independent of n .

Theorem 5 (Lui and Willegoda Liyanage)

Let ψ be the solution of the 1D unsteady Stokes equation in the stream function formulation, assumed to be analytic. Let $n \geq 2$ and $\hat{\psi}_h$ be soln of Chebyshev space-time collocation scheme. Define $E_h = \psi(\cdot, \cdot) - \hat{\psi}_h$. Then

$$|W^{1/2} E_h| \leq cn^{7.5} e^{-Cn}.$$

Space-time Spectral Methods for PDEs on Irregular Domains

- One major drawback of classical spectral methods is their inability to handle irregularly shaped domains.
- Previous work on spectral methods for elliptic PDEs on irregular domains: [Boyd](#), [Bruno](#), [Bueno-Orovio](#), [Glowinski](#), [Griffith](#), [Guidotti](#), [Lui](#), [Lyon](#), [Nave](#), [Orszag](#), [Shen](#), [Stein](#),
- Far fewer studies on spectral collocation methods for time-dependent PDEs in complex geometries.
- **Goal: Space-time spectral collocation method for time-dep PDEs on irregular domains.**

Techniques

- Spectral element methods ([Karniadakis, Maday, Patera, Sherwin, ...](#))
- Coordinate transformations
- **Domain embedding/Fictitious domains**
- Penalty methods ([Nave](#))
- Smooth extension embedding method ([Agress and Guidotti](#))
- ...

Periodic and Non-periodic 2D Extensions in Domain Embedding

- Assume source term is only known in physical domain; perform a periodic or non-periodic extension to extended regular domain.
- Apply Huybrechts' method to extend periodically the source term from physical domain to extended domain with exponential accuracy.
- Implemented 2D Fourier extension - *Alternating Fourier Extension*.
- Implemented 2D non-periodic extension - *Alternating Non-Periodic Extension*.

Fourier Extension - Huybrechs' Method

Problem 1. For $T > 1$, let G_n be $2T$ -periodic functions of the form

$$G_n = \left\{ \frac{a_0}{2} + \sum_{k=1}^n a_k \cos \frac{\pi kx}{T} + b_k \sin \frac{\pi kx}{T}, a_k, b_k \in \mathbb{R} \right\}.$$

The Fourier extension of f , defined on $[-1, 1]$, to $[-T, T]$ is the soln of:

$$g_n := \arg \min_{g \in G_n} \|f - g\|_{L^2(-1,1)}.$$

$T = 2$ uses half-range Chebyshev polynomials of first and second kinds.

Theorem 6 (Huybrechs)

Given $f \in L^2[-1, 1]$, soln to problem 1 is

$$g_n(x) = \sum_{k=0}^n a_k T_k^h \left(\cos \frac{\pi x}{2} \right) + \sum_{k=0}^{n-1} b_k U_k^h \left(\cos \frac{\pi x}{2} \right) \sin \left(\frac{\pi x}{2} \right),$$

where

$$a_k = \int_{-1}^1 f(x) T_k^h \left(\cos \frac{\pi x}{2} \right) dx,$$

$$b_k = \int_{-1}^1 f(x) U_k^h \left(\cos \frac{\pi x}{2} \right) \sin \left(\frac{\pi x}{2} \right) dx,$$

T_k^h and U_k^h are half-range Chebyshev polyns of first and second kinds.

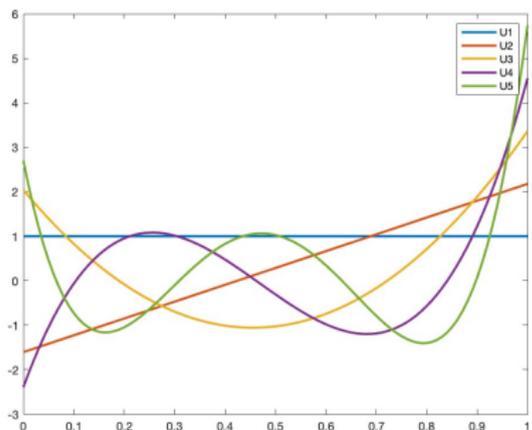
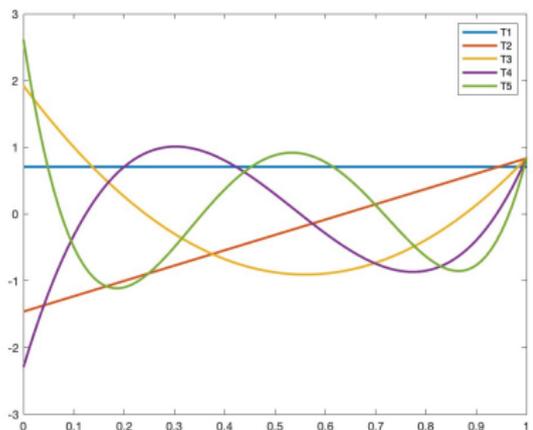


Figure: First five half-range Chebyshev polyns of first (left) and second (right) kind.

2D Alternating Fourier Extension

2D Fourier Extension - Algorithm

- Fix y_i , $1 \leq i \leq n+1$. Identify $[x_{i,1}, x_{i,n+1}]$. Extend periodically in x to $[-2, 2]$ using Huybrechts' method.

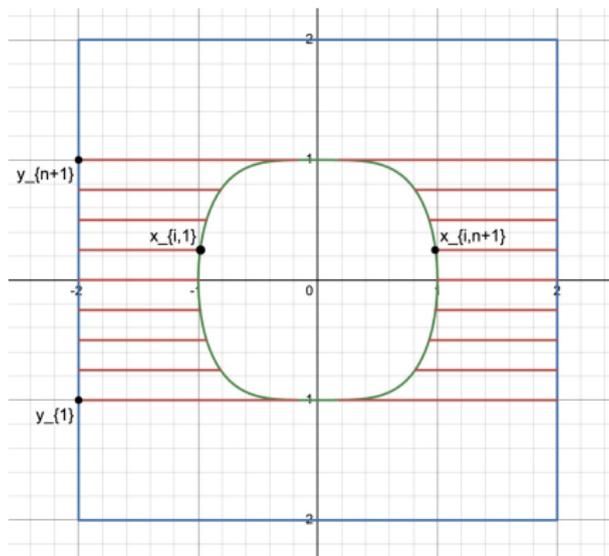
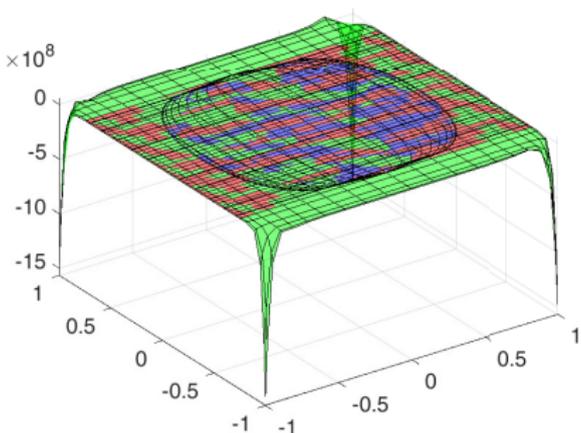


Figure: Periodic extension in the x-direction.

- Do periodic extension in y direction.
- Iterate until extensions converge.
- Solve PDE on extended square domain, imposing physical BC as constraints. **No BC on boundary of square** and **no extension in time**.
- Not suitable for non-rectangular physical domains since extension results in spikes at corners of extended domain.



Alternating Non-Periodic Extension

- Essentially same as Alternating Fourier extension except do only one x -extension and one y -extension - **no iteration**: $O(n^3)$ complexity.
- Solve PDE on extended square domain, imposing physical BC as constraints.
- $O(n^3 \log n)$ complexity assuming soln of linear system by FFT (constant coef PDEs), and $O(n^6)$ using direct solver (Hessenberg-Schur) for $O(n^3)$ unknowns.
- Works well for various types of complex geometries, including non-convex domains and non-simply-connected domains.
- More efficient than Alternating Fourier Extension and resolves issue of latter with spikes at corners of extended domain.

Spectral Convergence

Theorem 7 (Lui and Willegoda Liyange)

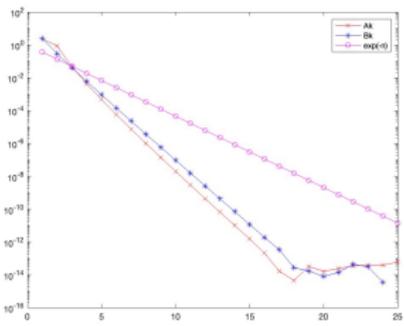
Let u and f be the soln and source term, both analytic, of 2D heat equation on (irregular) domain Ω . Suppose v and g are the soln and source term on extended domain $\tilde{\Omega}$.

For any positive integer n , define v_n as soln of $(v_n)_t = \Delta v_n + g_n$ on $\tilde{\Omega} \times (-1, 1)$, where g_n is the n -term truncation of g . Let $e_n = u - v_n|_{\Omega}$.

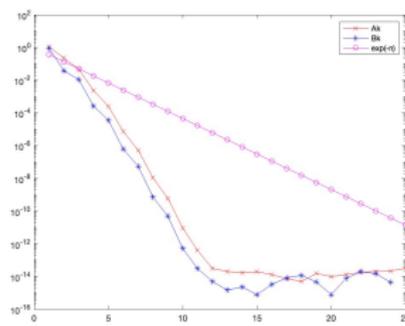
Then $\|e_n(\cdot, \cdot, t)\| \leq Ce^{-cn}$, $t \in [-1, 1]$.

Note same convergence rate holds for 2D Poisson equation.

Huybrechs' Method: source term only known in physical domain

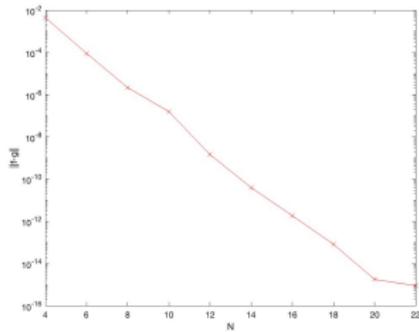


(a) $f(x) = 2x^2 + 3x + 1$



(b) $f(x) = \cos \cos \frac{\pi x}{2} + \sin \sin \frac{\pi x}{2}$

Figure: Logarithmic plots of the a_k and b_k coefficients of extension g of f .



Periodic Extensions:

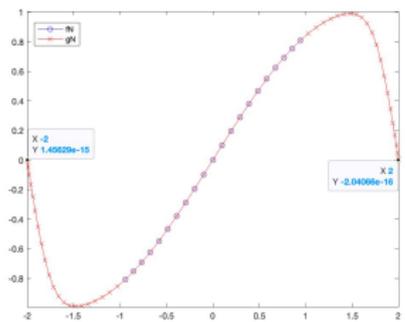
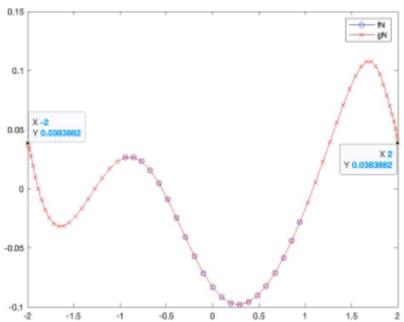


Figure: Periodic extensions from $[-1, 1]$ to $[-2, 2]$ for two different functions.

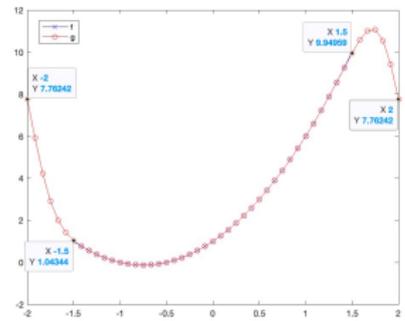
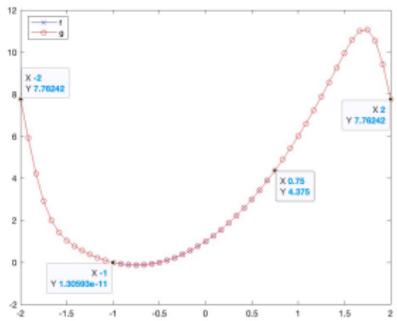


Figure: Periodic extensions from arbitrary physical domain $[-a, b]$ to $[-2, 2]$.

1D Heat Equation

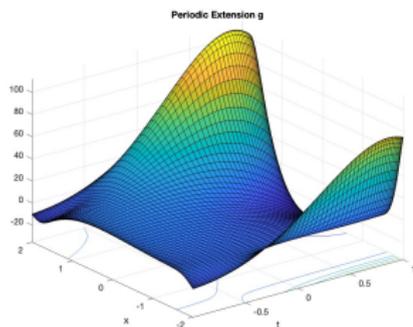
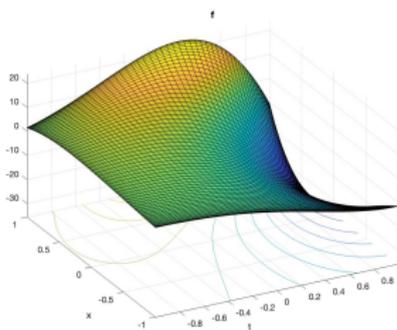


Figure: Fourier extension for the soln of 1D heat equation.

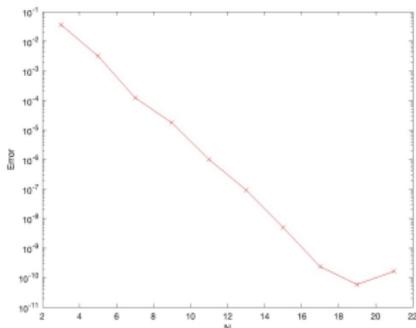


Figure: Spectral error convergence for 1D heat equation.

Non-periodic Extension:

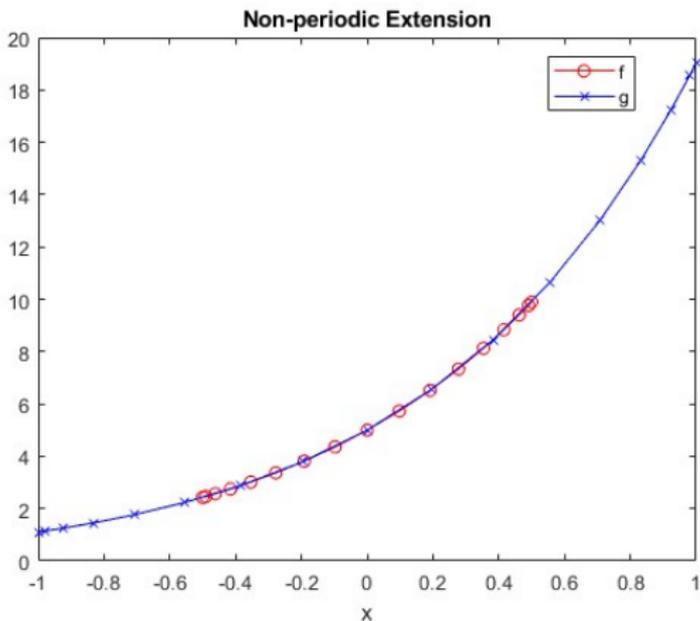


Figure: Non-periodic extension of function $f(x) = e^x(5 + 2x)$ from $[-0.5, 0.5]$ to $[-1, 1]$.

Examples of convex domains for Alternating Non-periodic Extension

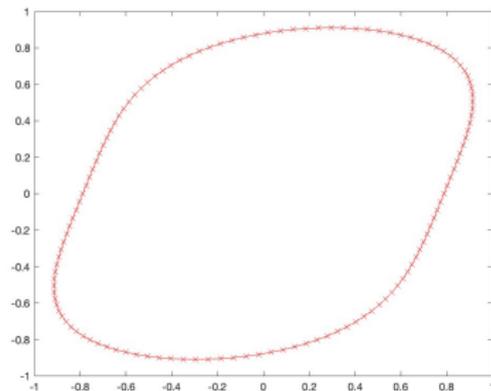
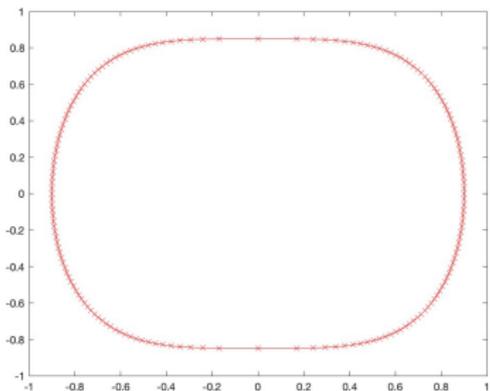


Figure: First and second domains.

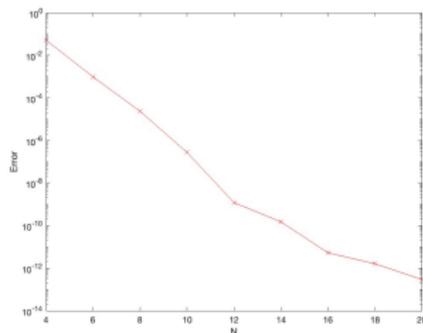
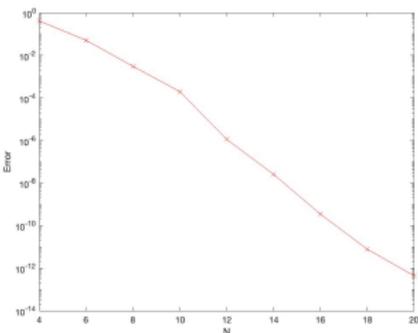


Figure: Wave: first and second domains.

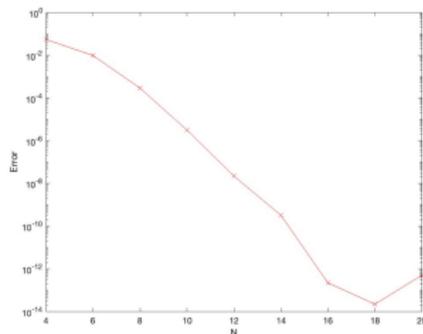
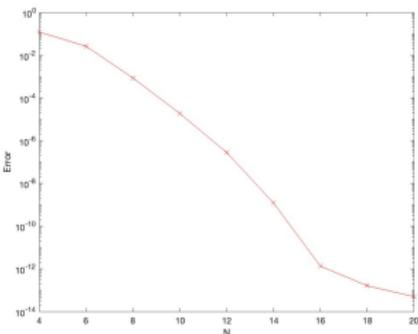


Figure: Unsteady Stokes ($Re = 1000$): first and second domains.

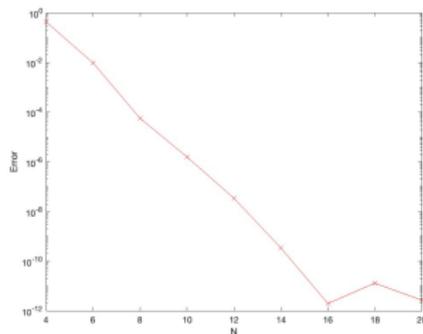
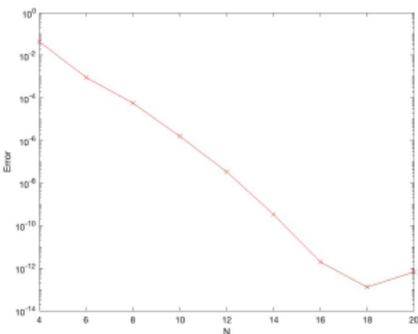


Figure: Allen-Cahn: first and second domains.

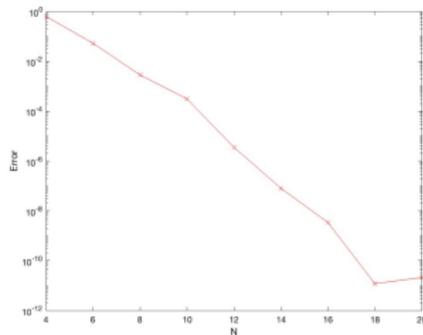
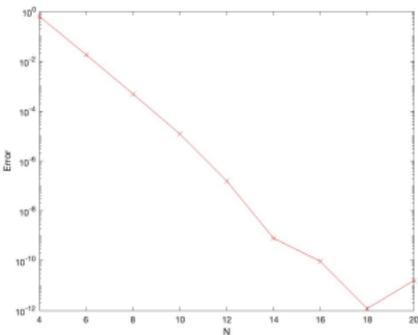


Figure: Nonlinear Schrodinger: first and second domains.

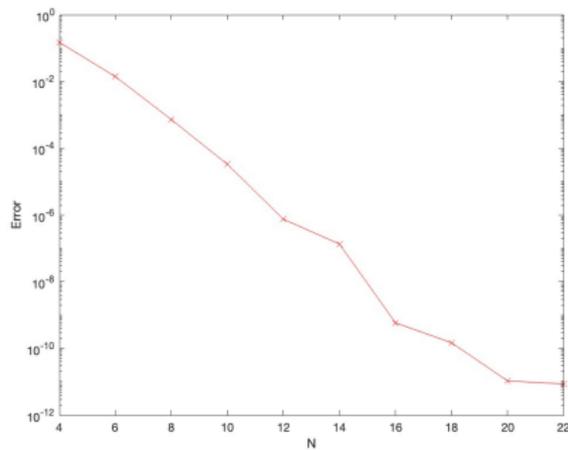
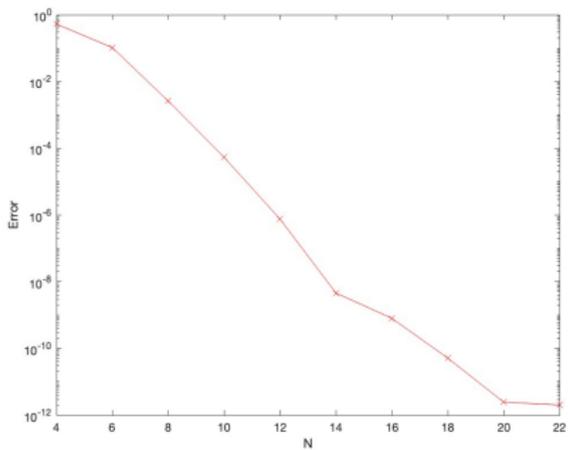


Figure: Unsteady NS ($Re = 10$): first and second domains.

Examples of non-convex domains for Alternating Non-periodic Extension

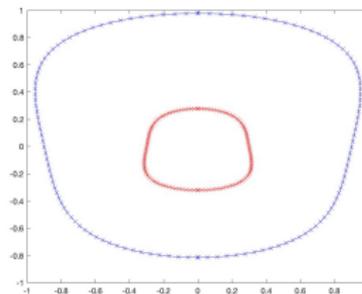
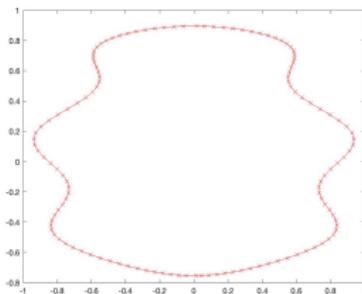


Figure: Third and Fourth domains.

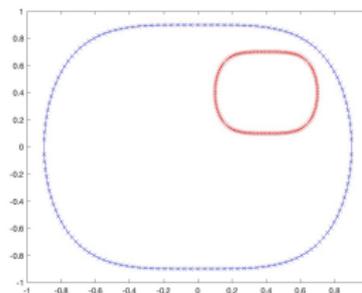
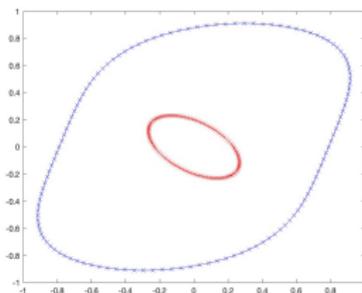


Figure: Fifth and Sixth domains.

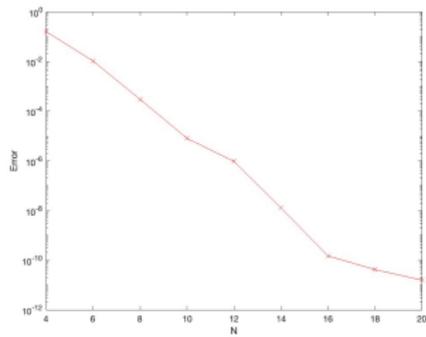
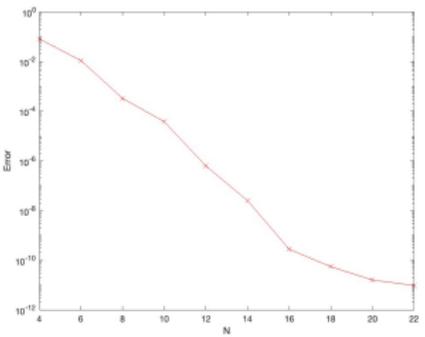


Figure: Unsteady NS ($Re = 10$): third and fourth domains.

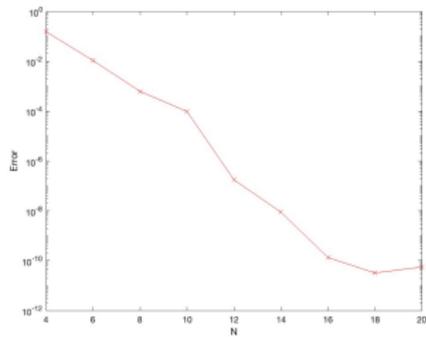
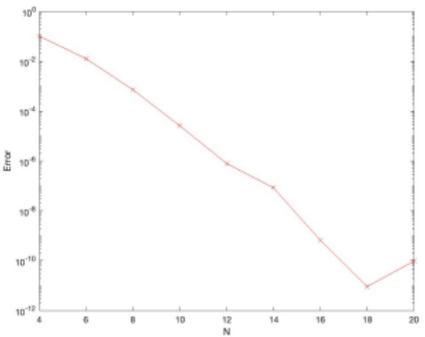


Figure: Unsteady NS ($Re = 10$): fifth and sixth domains.

Conclusions

- Condition number estimate of matrix in space-time Chebyshev collocation scheme for stream function formulation of unsteady Stokes equation.
- Proof of spectral convergence of scheme.
- Introduced space-time Chebyshev collocation scheme with Alternating Non-Periodic Extension (modifying Huybrechs' 1D Fourier extension) to solve PDEs on 2D irregular domains.
- Observed spectral convergence for 2D Poisson, heat, wave, unsteady Stokes, Allen-Cahn, nonlinear Schrödinger and Navier-Stokes equations.
- Proved spectral convergence of the Non-Periodic Extension scheme for 2D Poisson and heat equations.

Future Work

- Prove spectral convergence of Alternating Non-periodic Extension scheme for wave and Stokes equations.
- Derive condition number estimates.
- Implement RASPEN to solve Navier-Stokes and MHD equations at high Re .
- Delay DE.

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Thank You!