UNIVERSITY OF NOTRE DAME: DEPARTMENT OF APPLIED AND COMPUTATIONAL MATHEMATICS AND STATISTICS

THE LIGHTNING METHOD FOR THE HEAT EQUATION

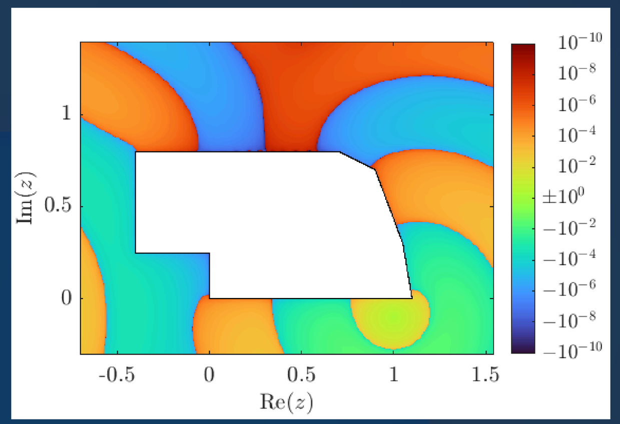
HUNTER LA CROIX AND ALAN LINDSAY

INTRODUCTION

We wish to numerically solve the planar heat equation given by

$$\begin{aligned} \frac{\partial u}{\partial t} &= D\Delta u, && x \in \mathbb{R}^2 \setminus \Omega; \\ u &= f(x), && x \in \partial\Omega^a; \\ D\frac{\partial u}{\partial n} &= g(x), && x \in \partial\Omega^r; \\ u &= u_0(x), && x \in \mathbb{R}^2 \setminus \Omega. \end{aligned}$$

Ex: Modified Helmholtz Solution



The Laplace transformed problem is then the Modified Helmholtz equation

We are able to decompose the solution of the Laplace transformed problem into a particular solution solved by Green's function, and a homogeneous solution whose problem is given below, which we solve numerically.

$$\hat{u}(z;s) = \hat{u}_p(z;s) + \hat{u}_h(z;s), \qquad \hat{u}_p(z;s) = \int_{\mathbb{C}\setminus\Omega} G(z,\xi;s)u_0(\xi)d\xi.$$

$$\begin{aligned} D\Delta\hat{u}_h - s\hat{u}_h &= 0, && z \in \mathbb{C}\setminus\Omega; \\ \hat{u}_h &= \hat{f}(z;s), && z \in \partial\Omega^a; \\ D\partial_n\hat{u}_h &= \hat{g}(z;s), && z \in \partial\Omega^r, \end{aligned}$$

Where

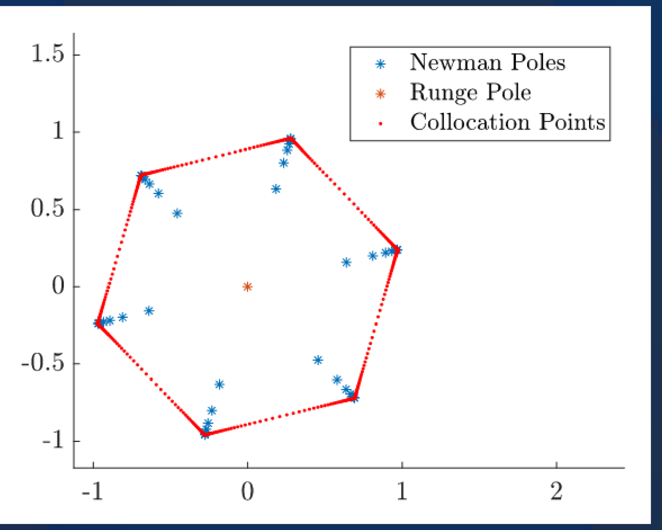
$$G(z,\xi;s) = \frac{1}{2\pi D}K_0(\alpha(s)|z-\xi|) \qquad \alpha(s) = \sqrt{\frac{s}{D}}$$

$$\hat{f}(z;s) = \frac{f(z)}{s} - \int_{\mathbb{C}\setminus\Omega} G(z,\xi;s)u_0(\xi)d\xi\,, \qquad \hat{g}(z;s) = \frac{g(z)}{s} - D\int_{\mathbb{C}\setminus\Omega} \partial_n G(z,\xi;s)u_0(\xi)d\xi$$

The homogenous problem is solved via the **Lightning Method** which sums a series of fundamental solutions (poles) to approximate the boundary condition via collocation (we solve for the coefficients via least-squares.)

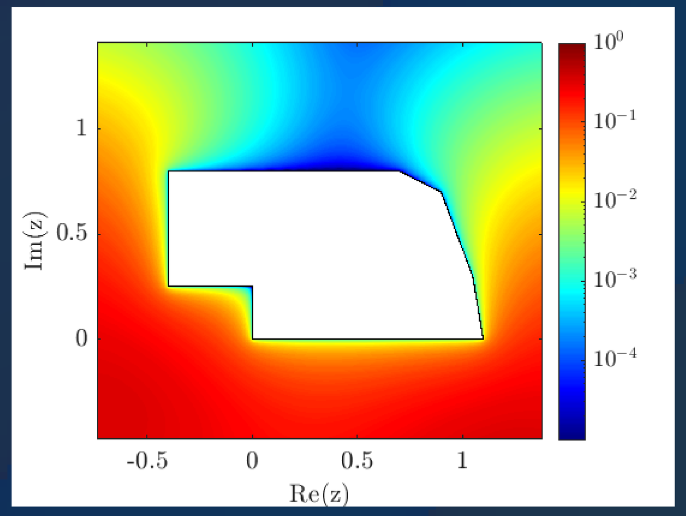
$$\phi_n(z,\xi;s) = \frac{1}{2\pi D}K_{|n|}(\alpha|z-\xi|)\frac{(z-\xi)^n}{|z-\xi|^n}, \qquad \alpha = \sqrt{\frac{s}{D}}$$

$$\hat{u}_h(z;s) = \underbrace{\sum_{j=1}^{N_1}\left(a_j\phi_{-1}(z,z_j;s) + b_j\phi_0(z,z_j;s) + c_j\phi_1(z,z_j;s)\right)}_{\text{(Newman Expansion)}} + \underbrace{\sum_{k=-N_2}^{N_2} d_k\phi_k(z,z_*;s)}_{\text{(Runge Expansion)}}$$



The LM approximation is then numerically integrated in the inverse Laplace transform to yield the solution to the heat problem.

Ex: Heat Solution



Interdisciplinary Application:

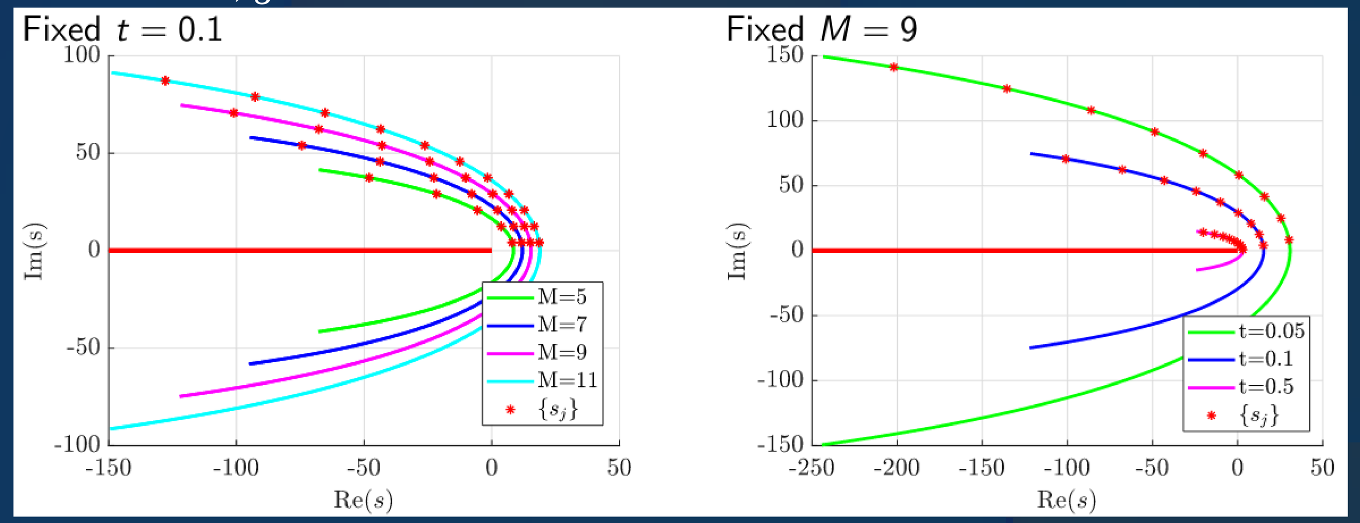
The Lightning Method is specifically formulated to be solved in/on shapes with corners. Corners are generally difficult for numerical solvers; mathematically we consider them "singular," as in singularity.

The heat equation is key in many biological models (chemo-receptivity, forager/prey dynamics) as it generally models diffusion of nutrients/stimuli or random movement.

While organisms in biology do not tend to have 'corners,' the environment they are embedded in may, and some biological problems pose singularities of their own.

We hope the resolution of corner singularities yielded by the Lightning Method may be similar in principle to future methods we can use to resolve other singularities in biological modeling.

The inverse Laplace transform uses a deformation of the Bromwich contour, the Talbot contour, given below



$$B_T = \left\{\frac{2M}{t}\rho(\theta) \,\middle|\, -\pi < \theta < \pi\right\}, \qquad \rho(\theta) = \left(-\sigma + \mu\theta\cot(\alpha\theta) + \nu i\theta\right)$$

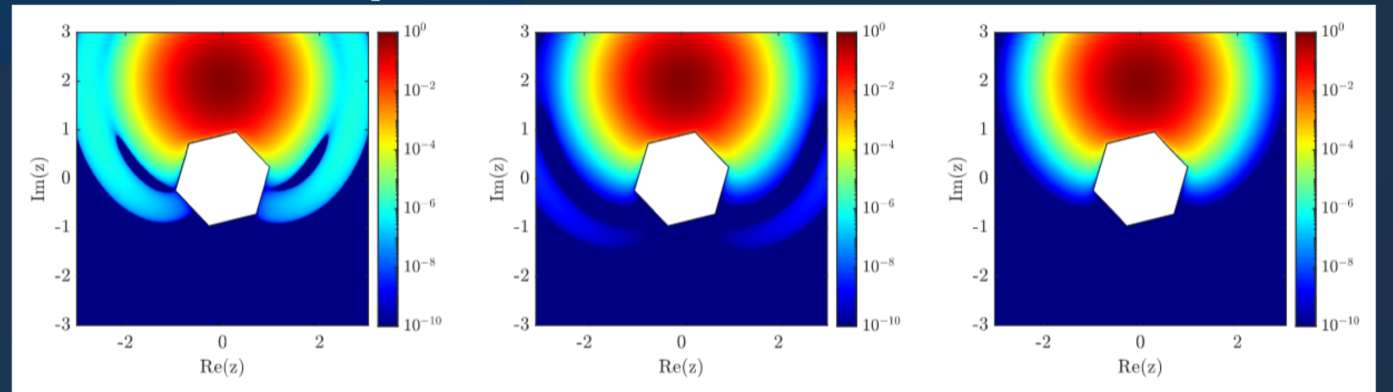
We simply numerically integrate the curve using midpoint rule. Each point on the contour is one Modified Helmholtz problem to solve. We find M=9 a good number of points.

Pros: **1.** Can evaluate the solution for single points of time without needing to iterate from earlier times, 2. Root exponential convergence wrt. d.o.f. can give fair accuracy with a non-taxing number of terms, 3. Not a large number of Talbot points needed for accuracy.

Cons: 1. The matrix in the least-squares solver can get quite large (scales with number of bodies & corners) and must be repeated for each point in the Talbot quadrature, 2. Some s values in the Talbot quadrature can be quite difficult on the solver (more oscillatory, more difficulty).

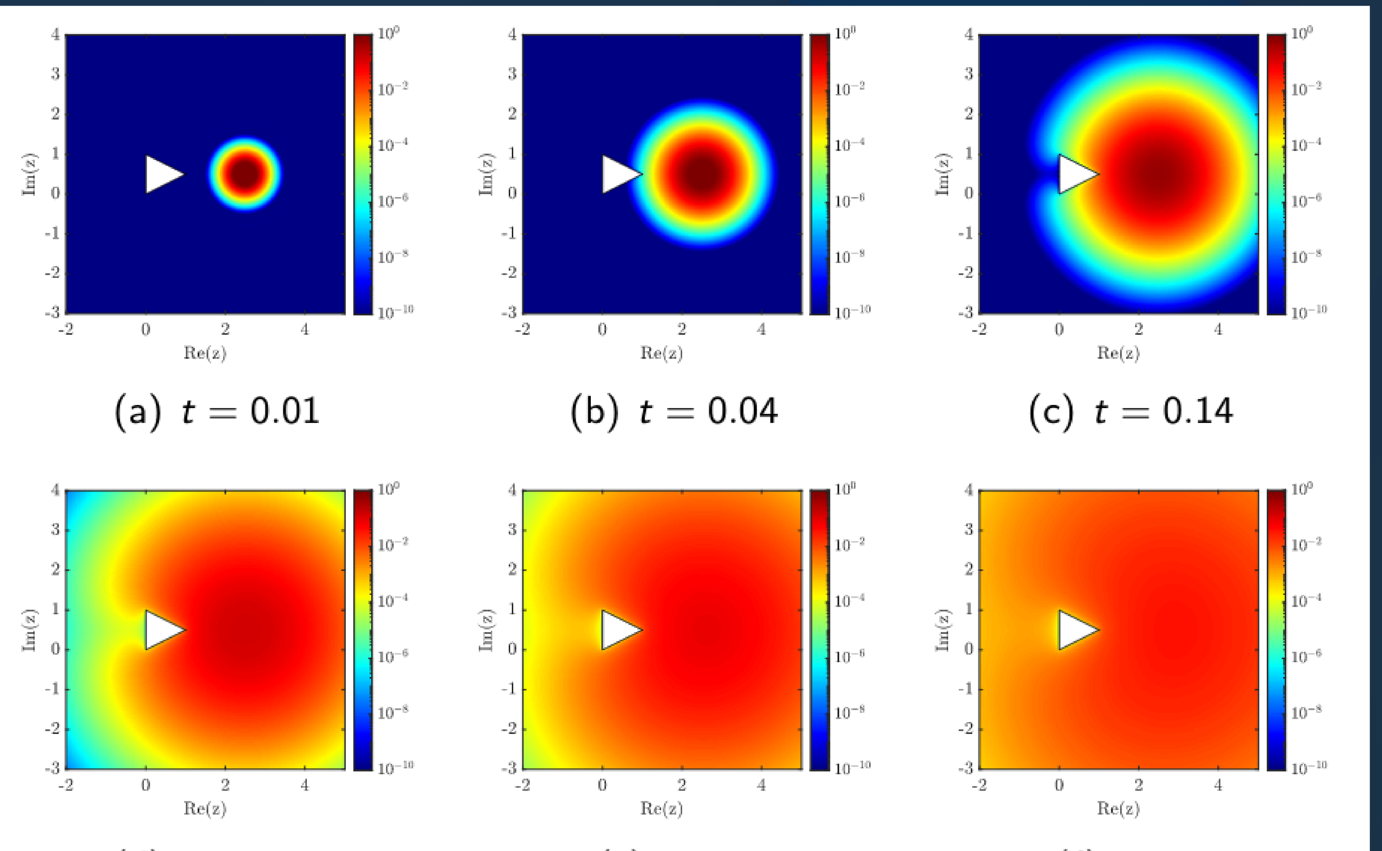
NUMERICAL RESULTS

Accuracy of solution (even further in the bulk) depends on accuracy of numerical inverse Laplace transform



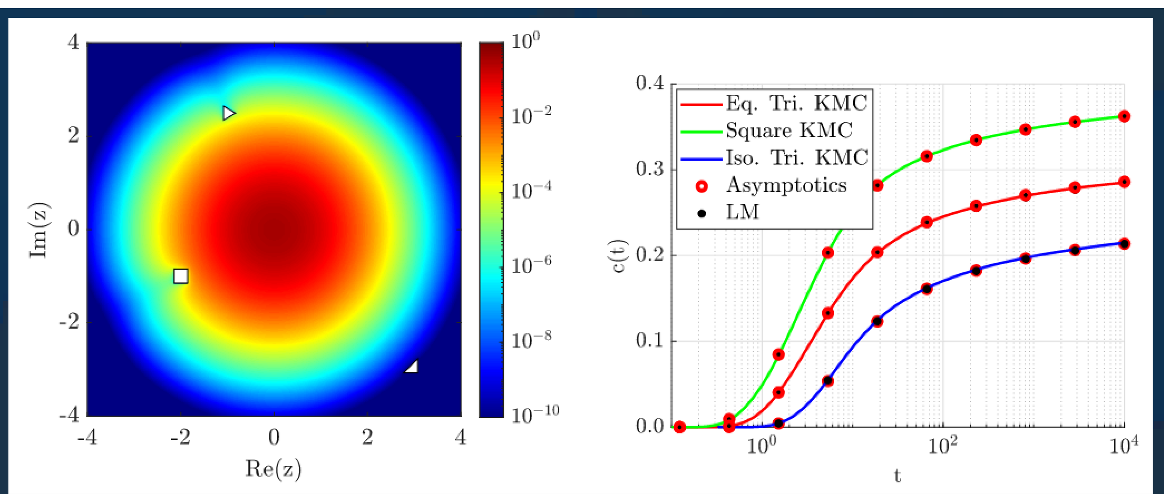
(a) $M = 5$. (b) $M = 7$. (c) $M = 9$.

Chronological solution with M=9 and validation with other methods:

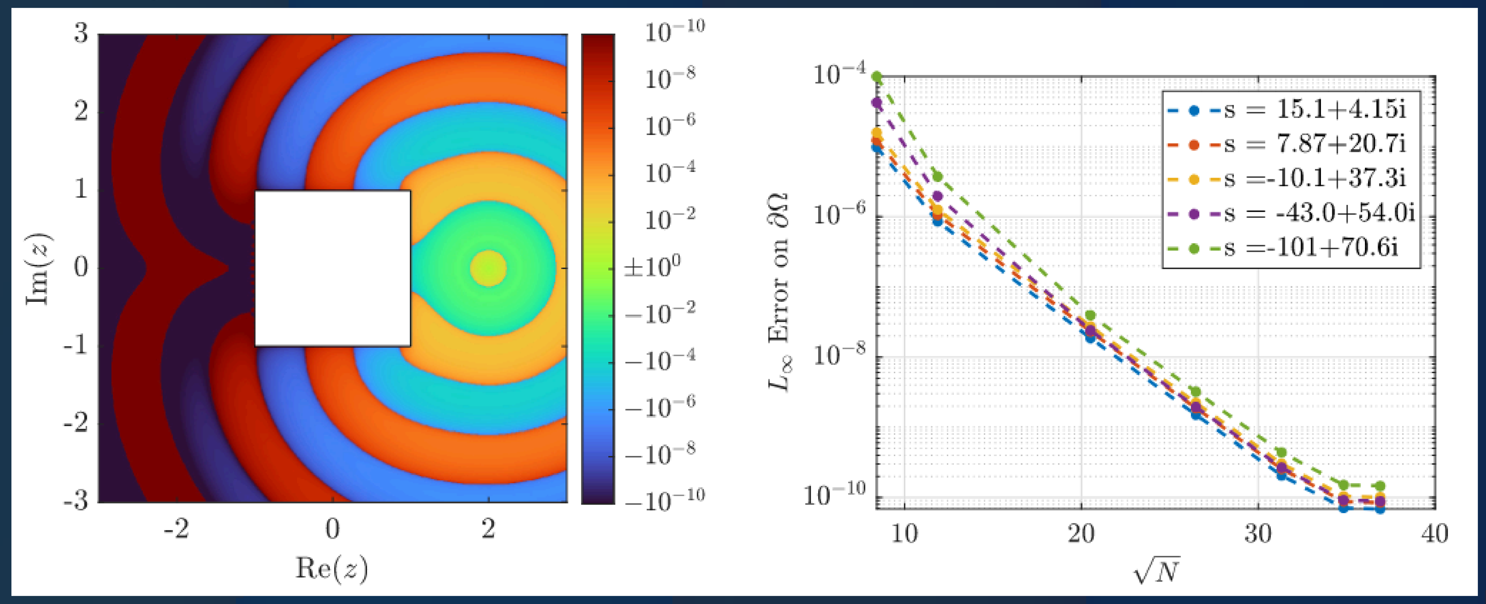


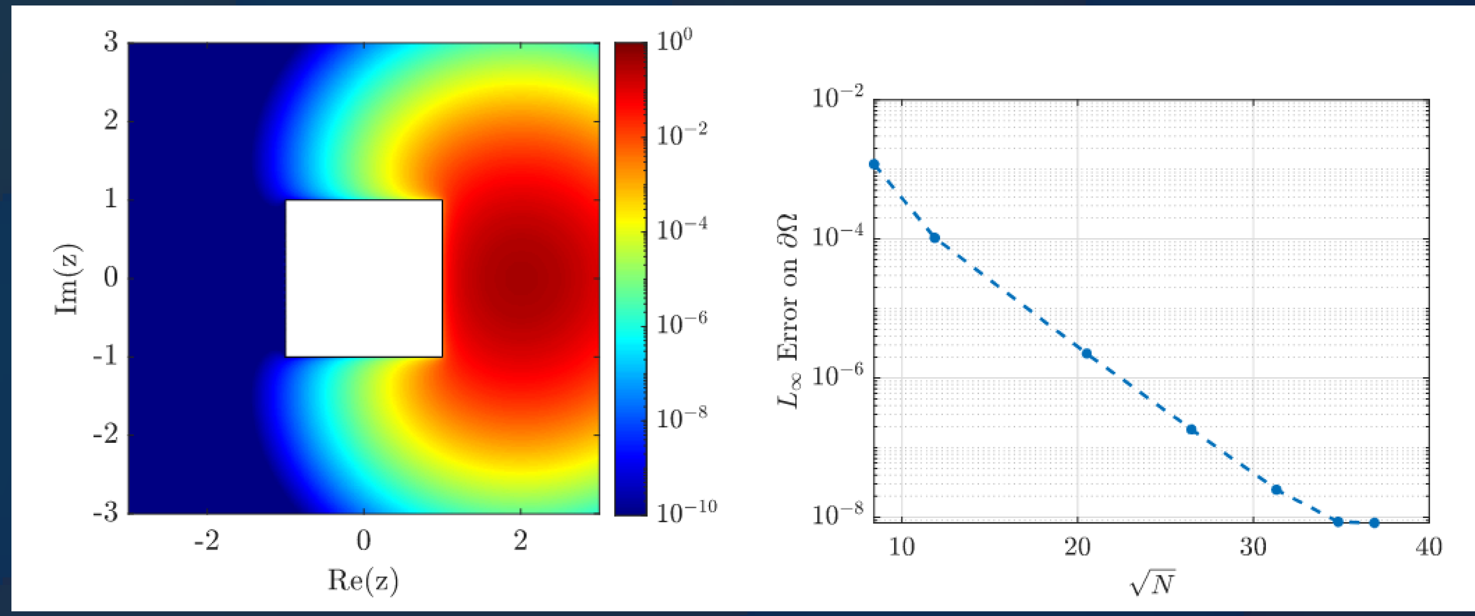
(a) $t = 0.01$ (b) $t = 0.04$ (c) $t = 0.14$

(d) $t = 0.53$ (e) $t = 1$ (f) $t = 2$

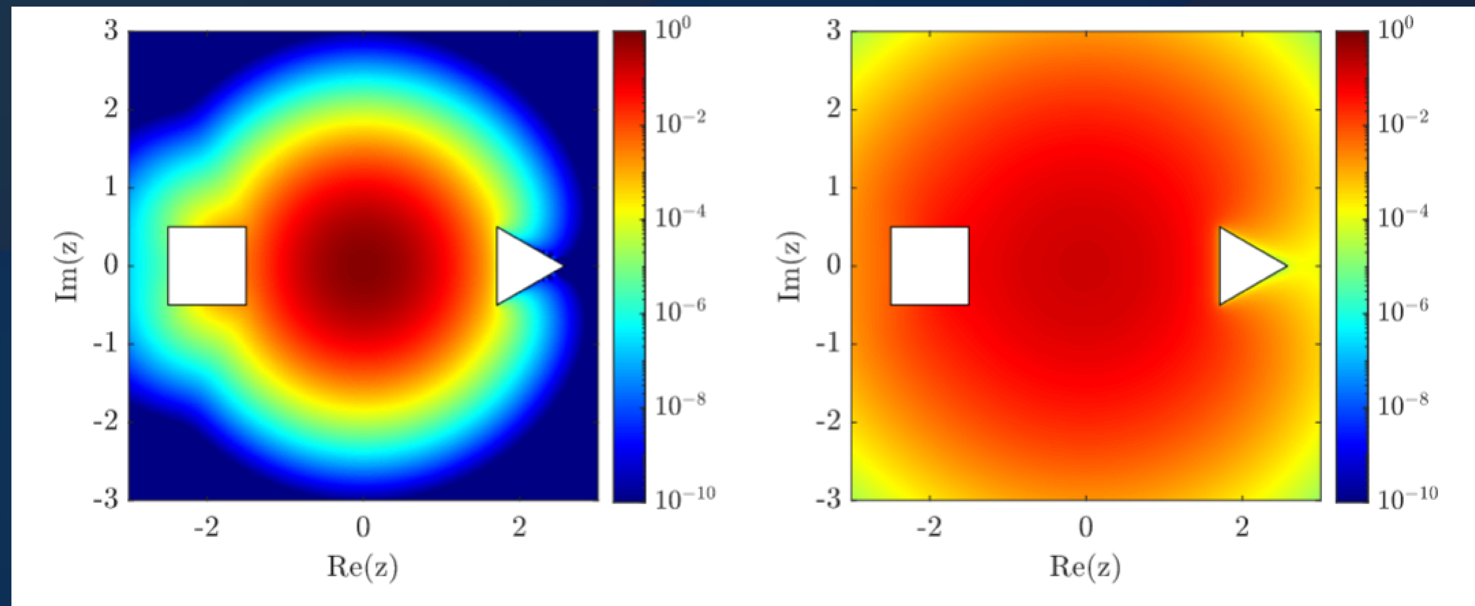


Convergence Study for Helmholtz s values and Heat at t=0.2, with # of terms N



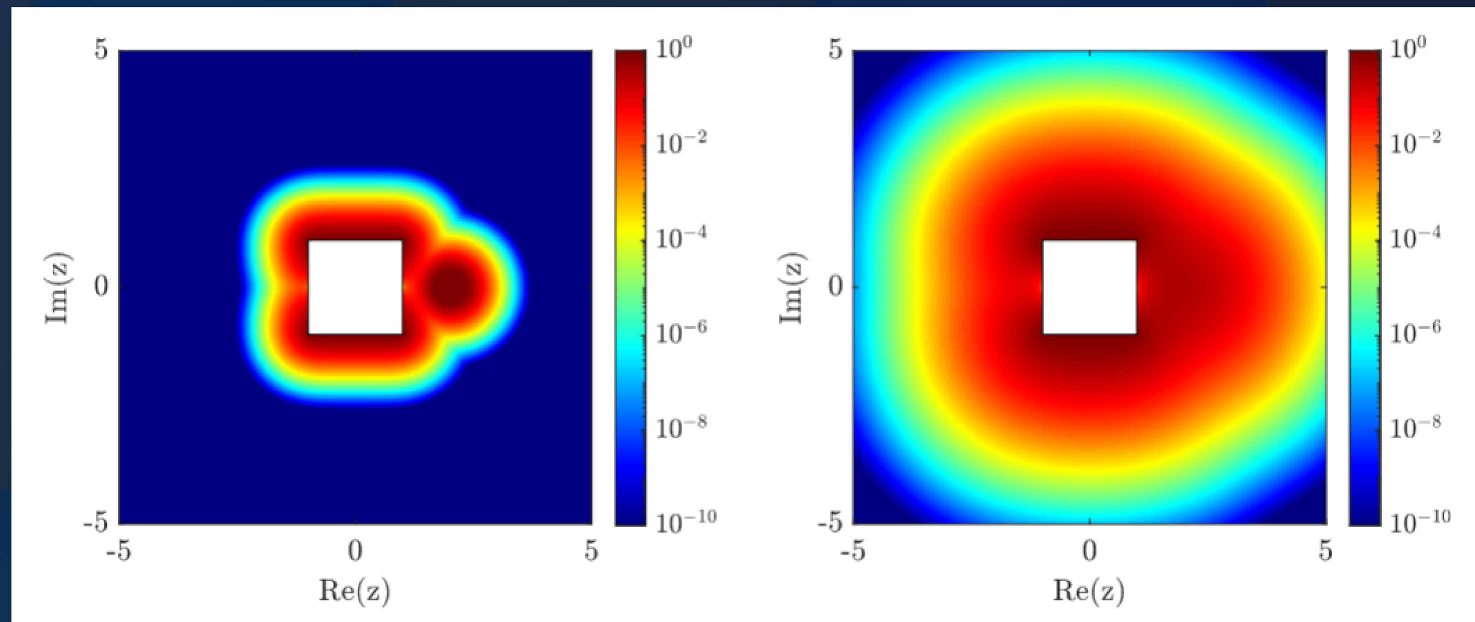


Neumann condition on square boundary, Dirichlet on triangle:



(m) $t = 0.1$ (n) $t = 0.5$

Easy implementation of arbitrary boundary conditions: $f(z) = [\mathrm{Im}(z)]^2$



(o) $t = 0.03$ (p) $t = 0.3$

CITATIONS

Abate, J. and Whitt, W., 2006. A unified framework for numerically inverting Laplace transforms. INFORMS Journal on Computing, 18(4), pp.408-421.

Jake Cherry, Alan E. Lindsay, Adrian Navarro Hernandez, and Bryan Quaife, Trapping of Planar Brownian Motion, Full First Passage Time Distributions by Kinetic Monte-Carlo, Asymptotic and Boundary Integral Equations, SIAM Journal on Multiscale Modelling and Simulation, 20 (2022), pp. 1284–1314.

Benedict Dingfelder and J. A. C. Weideman, An improved talbot method for numerical laplace transform inversion, Numerical Algorithms, 68 (2015), pp. 167–183.

Ginn, H. and Trefethen, L.N., 2023. Lightning Helmholtz Solver. arXiv preprint arXiv:2310.01665.

Abinand Gopal and L.N. Trefethen, Solving laplace problems with corner singularities via rational functions, SIAM Journal of Numerical Analysis, 57 (2019), pp. 2074–2094.

Abinand Gopal and Lloyd N. Trefethen, New laplace and helmholtz solvers, Proceedings of the National Academy of Sciences, 116 (2019), pp. 10223–10225.