A novel solver for diffusive processes in exterior domains

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Abstract

To describe transport of quantities such as heat or chemical concentrations, the diffusion equation must be solved in complex unbounded geometries. Since closed-form solutions rarely exist, we must resort to numerical methods. Three major challenges that numerical methods must address include (i) computing high-order accurate solutions in both space and time, (ii) accurately capturing far-field conditions, and (iii) computing long-time behaviors. I will describe a numerical method that recasts the time-dependent heat equation into an elliptic PDE by applying a Laplace transform. By using the Laplace transform, the solution of the PDE can be found at any time without the need to time step. This elliptic PDE is solved with high-order methods that accurately capture the far-field conditions. After solving the elliptic PDE, an inverse Laplace transform must be performed. This is done by carefully choosing a Bromwich contour that results in an integrand that is not oscillatory and rapidly decays to zero. By combining these techniques, high-order accuracy in both space and time are achieved.

Introduction

The diffusion equation describes the density $c(\mathbf{x}, t)$ of many diffusive particles with constant diffusion coefficient D. We let Ω be the two-dimensional unbounded domain, with Dirichlet boundary condition, and a point-source initial condition located at $\mathbf{x}^*$:

$$\begin{aligned} \frac{\partial c}{\partial t} &= D\Delta c, && \mathbf{x} \in \Omega,\ t > 0, \\ c(\mathbf{x}, t) &= 0, && \mathbf{x} \in \partial\Omega,\ t > 0, \\ c(\mathbf{x}, 0) &= \delta(\mathbf{x} - \mathbf{x}^*), && \mathbf{x} \in \Omega,\ t = 0. \end{aligned}$$

The solution of this PDE describes a diffusing point source.

Transforming the PDE

Applying the Laplace transform to the diffusion equation yields a time-independent elliptic PDE with a single parameter $s \in \mathbb{C}$. Letting $C(\mathbf{x}, s) = \mathcal{L}[c(\mathbf{x}, t)](s)$,

$$\begin{aligned} (s - \Delta)C(\mathbf{x}, s) &= \delta(\mathbf{x} - \mathbf{x}^*), && \mathbf{x} \in \Omega, \\ C(\mathbf{x}, s) &= 0, && \mathbf{x} \in \partial\Omega. \end{aligned}$$

We write the solution as

$$C(\mathbf{x}, s) = C^h(\mathbf{x}, s) - \frac{1}{2\pi} K_0(\sqrt{s}\|\mathbf{x} - \mathbf{x}^*\|)$$

where K_0 is the modified Bessel function of the second kind which satisfies

$$(s - \Delta)\left(-\frac{1}{2\pi} K_0(\sqrt{s}\|\mathbf{x} - \mathbf{x}^*\|)\right) = \delta(\mathbf{x} - \mathbf{x}^*).$$

The homogeneous solution $C^h(\mathbf{x}, s)$ is chosen to satisfy

$$\begin{aligned} (s - \Delta)C^h(\mathbf{x}, s) &= 0, && \mathbf{x} \in \Omega, \\ C^h(\mathbf{x}, s) &= \frac{1}{2\pi} K_0(\sqrt{s}\|\mathbf{x} - \mathbf{x}^*\|), && \mathbf{x} \in \partial\Omega, \end{aligned}$$

so that $C(\mathbf{x}, s)$ satisfies both the PDE and the boundary condition.

Numerical Methods

We focus on the domain $\Omega = \mathbb{R}^2 \backslash B(0, 1)$ so that $C^h(\mathbf{x}, s)$ can be solved accurately with Fourier methods. After a change of variables to polar coordinates, discretizing the boundary at N points and applying an FFT yields a system of N ODEs

$$\begin{aligned} \left(s + \frac{n^2}{r^2}\right)\hat{C}_n^h(r) - \hat{C}_n^h(r)'' - \frac{1}{r}\hat{C}_n^h(r)' &= 0, && r \in (1, \infty), n = 1, \ldots, N, \\ \hat{C}_n^h(r) &= \mathcal{F}\left(\frac{1}{2\pi} K_0(\sqrt{s}\|\mathbf{x} - \mathbf{x}^*\|)\right), && r = 1, \\ \hat{C}_n^h(r) &= 0, && r \to \infty. \end{aligned}$$

The solution of these ODEs involves Hankel functions of the second kind. Then, an IFFT is used to compute $\hat{C}_n^h(r)$. This method of solving $\hat{C}_n^h(r)$ does not apply for non-circular or multiply-connected domains, however, an integral equation method is proposed in the Discussion section that will allow us to consider more general unbounded domains.

Inverting a Laplace transform requires evaluating a contour integral (Bromwich integral) along a vertical line in the complex plane which lies to the right of all singularities of the integrand. In the case of the diffusion equation, all singularities lie on the negative real axis. To compute the Bromwich integral numerically, we integrate along a Talbot contour (Figure 1) instead of along a vertical line.

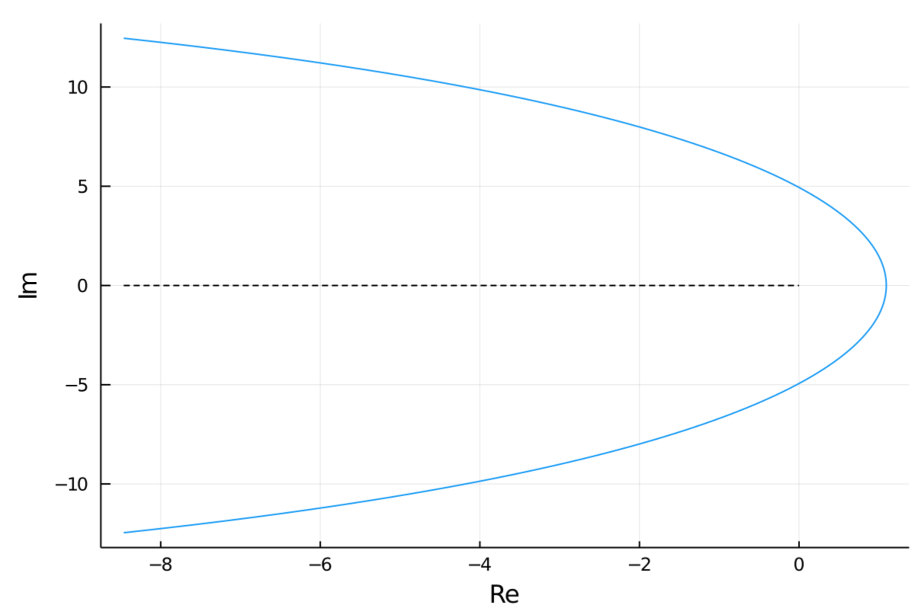

Figure 1: *Example of a sufficient Talbot contour (blue curve) for inverting $C(\mathbf{x}, s)$. All singularities of the integrand lie along the negative real axis, shown as a dashed line.*

Evaluating the inverse Laplace transform using a Talbot contour rather than a vertical Bromwich contour results in an integrand that is much less oscillatory (Figure 2), and because the midpoint rule is spectrally accurate on Talbot contours, we require very few quadrature points.

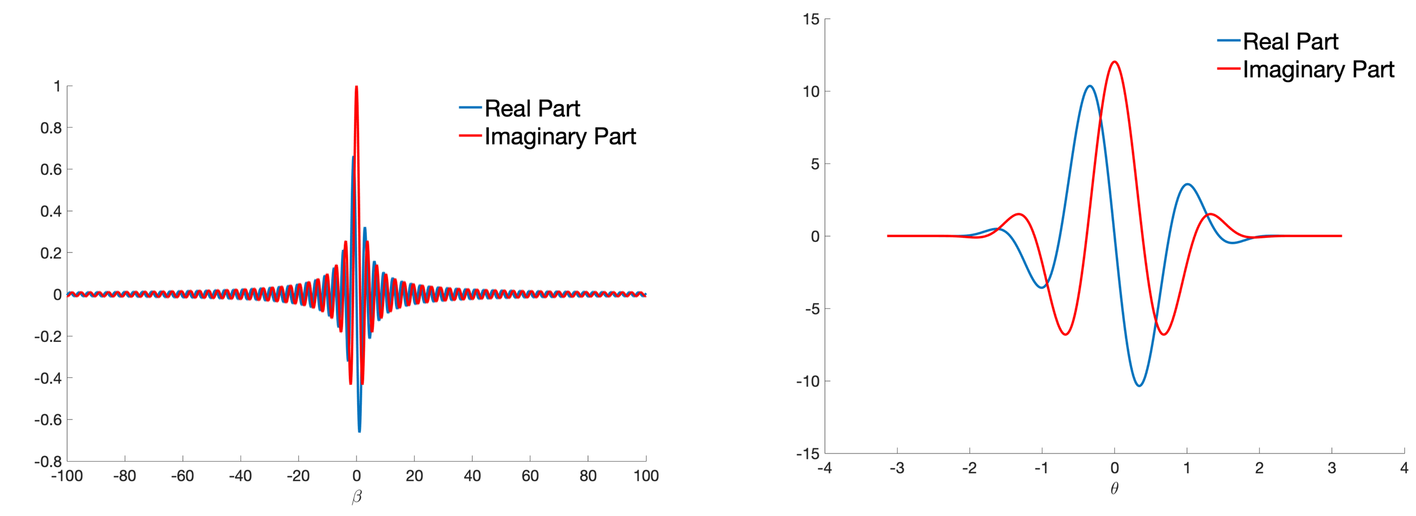

Figure 2: *The Bromwich integrand when using a vertical contour (left) and when using a Talbot contour (right).*

Example

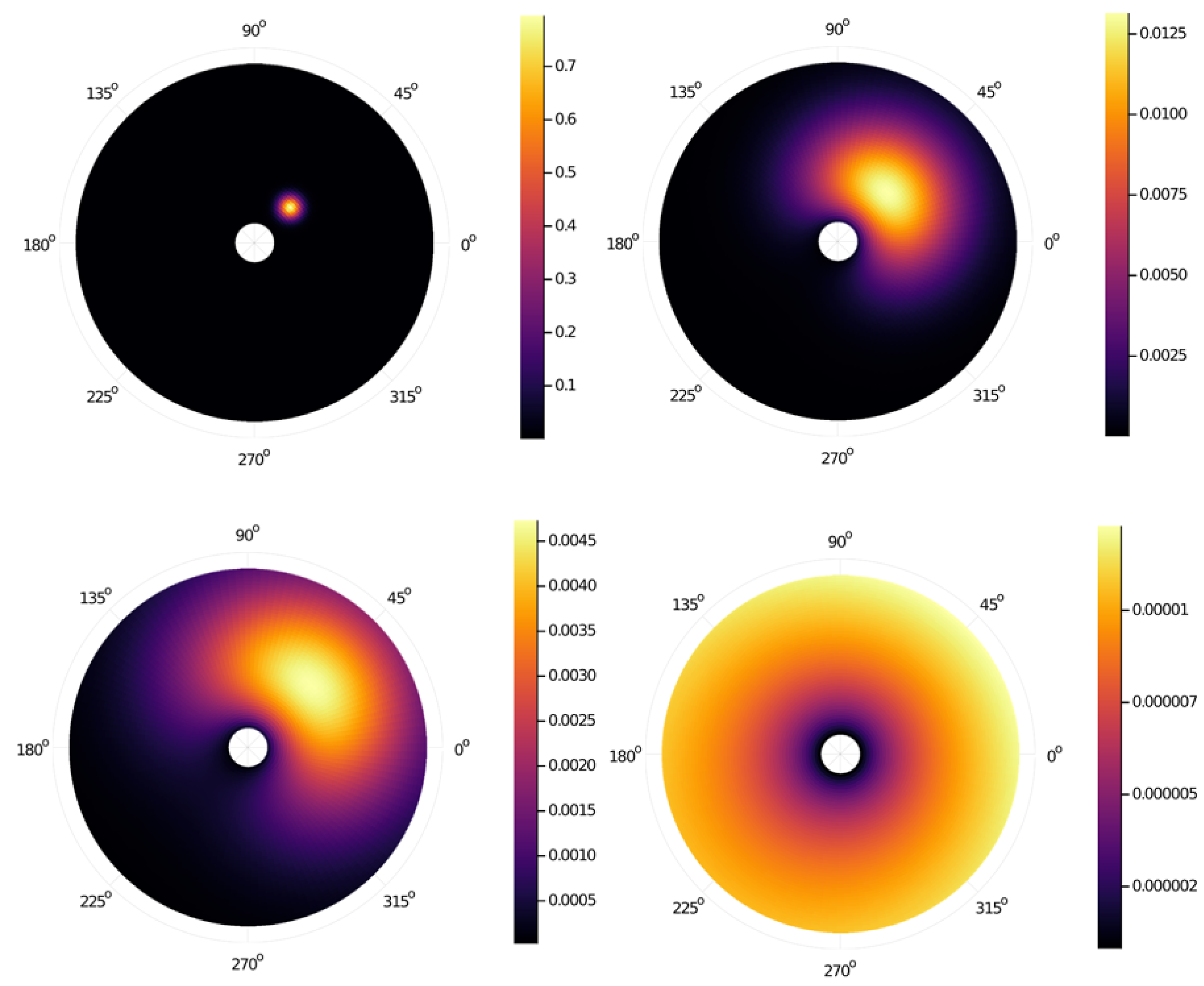

Figure 3: *Diffusion of a point source at $\mathbf{x}^* = (2, 2)$ in a domain exterior to the unit circle. The solution is plotted at times $t = 0.1$, $t = 5$, $t = 10$, and $t = 1000$.*

Discussion

- Using this method, the diffusion equation is solved without stepping through time. Therefore, the cost of evaluating the solution at late times is far less expensive compared to standard time stepping methods.
- This method is spectrally accurate in both space and time, and accurately captures far-field conditions.
- Future work will extend the method to handle more general domains, where a Fourier method is not applicable. The homogeneous solution $C^h(\mathbf{x}, s)$ will instead be solved using boundary integral equation methods.

References

[1] Milton Abramowitz and Irene A Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables.* Vol. 55. US Government printing office, 1964.

[2] Tracy L Stepien et al. "Moth Mating: Modeling Female Pheromone Calling and Male Navigational Strategies to Optimize Reproductive Success". In: *Applied Sciences* 10.18 (2020), p. 6543.

[3] Lloyd N Trefethen, J André C Weideman, and Thomas Schmelzer. "Talbot quadratures and rational approximations". In: *BIT Numerical Mathematics* 46.3 (2006), pp. 653–670.