

Rothe's Method with Neumann Conditions

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1 Introduction

In this document, we implement Rothe's method to solve the 1D heat equation on the unit interval, with large diffusion coefficient, $1/\epsilon$, $\epsilon \ll 1$, and non-zero Neumann BCs. We use order 2 accurate centered finite-differences to discretize in space and BDF2 formula to discretize in time.

We present a numerical example where the time-step is $\Delta t \gg \epsilon$ and perform a grid refinement study to check whether Rothe's method remains order 2 accurate as $\epsilon \rightarrow 0$.

2 The problem

Let $u(x, t)$ solve the following heat equation problem on the domain $\Omega = [0, 1]$,

$$\begin{cases} \epsilon u_t - \Delta u = 0, & x \in \Omega \times (0, T], \\ \partial_n u = f, & x \in \partial\Omega \times (0, T], \\ u(x, 0) = 0, & x \in \Omega. \end{cases} \quad (2.1)$$

Here, $\epsilon \ll 1$, T is a final time, and f represents known Neumann data. The notation $\partial_n u$ represents the derivatives in the direction of the normal vector at the boundary.

3 Rothe's method

Rothe's method applies a temporal discretization to the differential equation in (2.1) to arrive at a sequence of elliptic equations which are then solved using boundary integral methods.

Leaving the space variable continuous, we discretize the heat equation in (2.1) in time using BDF2. Let $t^n = n\Delta t$, with $n = 0, \dots, N_t$, $u^n \approx u(\cdot, t^n)$. Here, N_t represents the number of time steps. We have

$$u^{n+1} - \frac{4}{3}u^n + \frac{1}{3}u^{n-1} = \frac{2}{3}\frac{\Delta t}{\epsilon}(u_{xx})^{n+1},$$

so that

$$(u_{xx})^{n+1} - \frac{3\epsilon}{2\Delta t}u^{n+1} = \frac{-2\epsilon}{\Delta t}u^n + \frac{\epsilon}{2\Delta t}u^{n-1}. \quad (3.1)$$

At each time-step, we solve an elliptic equation to find u^{n+1} , a total of N_t elliptic solves.

We approximate the solution at the first time-step $t = \Delta t$ using

$$u(x, \Delta t) = u_0(x) + \frac{\Delta t}{\epsilon \Delta x^2}(u_0(x + \Delta x) - 2u_0(x) + u_0(x - \Delta x)) + \mathcal{O}(\Delta t^2), \quad \text{as } \Delta t \rightarrow 0, \quad (3.2)$$

where Δx is the spatial step size.

4 Treatment of Neumann BCs

Let $x_i = i\Delta x$ represent the discretization in space with $i = -1, 0, \dots, N_x, N_x + 1$. Here we introduce two *ghost* grid points to treat the Neumann conditions using a centered discretization. Let $u_i^n \approx u(x_i, t^n)$. The discretization of the Neumann conditions at $x = 0$ and $x = 1$, takes the form

$$\begin{aligned} -D_{0x}u_0^n &= f_l(t^n), \\ D_{0x}u_{N_x}^n &= f_r(t^n), \end{aligned}$$

where $D_{0x}u_i^n = (u_{i+1}^n - u_{i-1}^n)/(2\Delta x)$, f_l and f_r represent given Neumann data on the left and right boundaries respectively. We can then evaluate the solution at the ghost grid points using the following

$$\begin{aligned} u_{-1}^n &= u_1^n + 2\Delta x f_l(t^n), \\ u_{N_x+1}^n &= u_{N_x-1}^n + 2\Delta x f_r(t^n). \end{aligned}$$

5 Implementation

For the implementation, we use the exact solution

$$u_e(x, t) = A \cos(\sqrt{\epsilon}x + a)e^{-t} + B \sin(\sqrt{\epsilon}x + a)e^{-t}, \quad x \in [0, 1], t \in [0, T], \quad (5.1)$$

for testing. We set $A = 200$, $B = 100$, $a = -1.123$, and $T = 1$. We use second-order centered finite-differences to solve the elliptic equations in (3.1) rather than boundary integral methods (at least for this preliminary test), and perform a grid refinement study. We measure the error using the maximum norm

For $\epsilon = 10^{-4}$, we obtain the following results

```
Using the Rothe method with Neumann BC and eps = 1.0e-04
t=1.0000e+00: Nx= 10 Nt= 10 dt=1.000e-01 maxErr=2.19e-02
t=1.0000e+00: Nx= 20 Nt= 20 dt=5.000e-02 maxErr=5.65e-03 order=1.95e+00
t=1.0000e+00: Nx= 40 Nt= 40 dt=2.500e-02 maxErr=1.43e-03 order=1.98e+00
t=1.0000e+00: Nx= 80 Nt= 80 dt=1.250e-02 maxErr=3.61e-04 order=1.99e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=9.07e-05 order=1.99e+00
t=1.0000e+00: Nx=320 Nt= 320 dt=3.125e-03 maxErr=2.30e-05 order=1.98e+00
t=1.0000e+00: Nx=640 Nt= 640 dt=1.563e-03 maxErr=6.35e-06 order=1.85e+00
t=1.0000e+00: Nx=1280 Nt=1280 dt=7.813e-04 maxErr=1.05e-07 order=5.91e+00
```

In the output table above, **Nx** refers to the number of grid points, **Nt** denotes the number of time-steps, **dt** corresponds to the time step Δt , **maxErr** is the error in the maximum norm and **order** denotes the overall order of accuracy. The same follows for the other tables presented in this section.

For $\epsilon = 10^{-6}$, we obtain the following results

```
Using the Rothe method with Neumann BC and eps = 1.0e-06
eps=1.0e-06, t=1.0e+00: Nx= 10 Nt= 10 dt=1.0e-01 maxErr=3.10e-02, condNum=3.5e+08
eps=1.0e-06, t=1.0e+00: Nx= 20 Nt= 20 dt=5.0e-02 maxErr=7.99e-03, condNum=1.2e+09 order=1.95e+00
eps=1.0e-06, t=1.0e+00: Nx= 40 Nt= 40 dt=2.5e-02 maxErr=2.03e-03, condNum=4.6e+09 order=1.98e+00
eps=1.0e-06, t=1.0e+00: Nx= 80 Nt= 80 dt=1.3e-02 maxErr=5.14e-04, condNum=1.8e+10 order=1.98e+00
eps=1.0e-06, t=1.0e+00: Nx= 160 Nt= 160 dt=6.3e-03 maxErr=1.35e-04, condNum=7.0e+10 order=1.93e+00
eps=1.0e-06, t=1.0e+00: Nx= 320 Nt= 320 dt=3.1e-03 maxErr=1.92e-05, condNum=2.8e+11 order=2.81e+00
eps=1.0e-06, t=1.0e+00: Nx= 640 Nt= 640 dt=1.6e-03 maxErr=1.49e-05, condNum=1.1e+12 order=3.69e+01
eps=1.0e-06, t=1.0e+00: Nx=1280 Nt=1280 dt=7.8e-04 maxErr=6.13e-04, condNum=4.4e+12 order=-5.37e+00
eps=1.0e-06, t=1.0e+00: Nx=2560 Nt=2560 dt=3.9e-04 maxErr=3.24e-04, condNum=1.7e+13 order=9.22e-01
```

In the above results, `condNum` refers to the condition number of the implicit matrix used to solve the elliptic equations numerically. As expected the condition number worsens as we increase the resolution, and thus the error worsens at the finer resolutions.

For $\epsilon = 10^{-8}$, we obtain the following results

```
Using the Rothe method with Neumann BC and eps = 1.0e-08
eps=1.0e-08, t=1.0e+00: Nx= 10 Nt= 10 dt=1.0e-01 maxErr=3.19e-02, condNum=3.5e+10
eps=1.0e-08, t=1.0e+00: Nx= 20 Nt= 20 dt=5.0e-02 maxErr=8.24e-03, condNum=1.2e+11 order=1.95e+00
eps=1.0e-08, t=1.0e+00: Nx= 40 Nt= 40 dt=2.5e-02 maxErr=2.11e-03, condNum=4.6e+11 order=1.96e+00
eps=1.0e-08, t=1.0e+00: Nx= 80 Nt= 80 dt=1.3e-02 maxErr=5.82e-04, condNum=1.8e+12 order=1.86e+00
eps=1.0e-08, t=1.0e+00: Nx= 160 Nt= 160 dt=6.3e-03 maxErr=2.70e-04, condNum=7.0e+12 order=1.11e+00
eps=1.0e-08, t=1.0e+00: Nx= 320 Nt= 320 dt=3.1e-03 maxErr=3.24e-03, condNum=2.8e+13 order=-3.58e+00
eps=1.0e-08, t=1.0e+00: Nx= 640 Nt= 640 dt=1.6e-03 maxErr=3.89e-03, condNum=1.1e+14 order=-2.63e-01
eps=1.0e-08, t=1.0e+00: Nx=1280 Nt=1280 dt=7.8e-04 maxErr=4.92e-02, condNum=4.4e+14 order=-3.66e+00
eps=1.0e-08, t=1.0e+00: Nx=2560 Nt=2560 dt=3.9e-04 maxErr=1.66e-01, condNum=1.7e+15 order=-1.75e+00
```

We fix $N_x = 100$, $\Delta t = 0.1$, vary ϵ and measure the error

```
Using the Rothe method with Neumann BC
eps=1.0e-02, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=6.89e-02
eps=1.0e-03, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=8.08e-05
eps=1.0e-04, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=2.19e-02
eps=1.0e-05, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=2.88e-02
eps=1.0e-06, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=3.10e-02
eps=1.0e-07, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=3.17e-02
eps=1.0e-08, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=3.21e-02
eps=1.0e-09, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=3.19e-02
eps=1.0e-10, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=1.61e-02
eps=1.0e-11, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=4.73e-02
eps=1.0e-12, t=1.0000e+00: Nx=100 Nt= 10 dt=1.000e-01 maxErr=6.26e-01
```

6 Conclusion and remarks

Using a simple 1D test case, we test the effectiveness of Rothe's method when the diffusion coefficient becomes very large, i.e. $1/\epsilon$, $\epsilon \ll 1$. We find that the performance of the Rothe's method becomes worse as ϵ decreases and this may be due to the worsening of the condition number of the implicit matrix used in the solve.

References

- [1] Alex H. Barnett. Quasistatic correction in powers of reciprocal diffusivity for heat initial boundary value problems. unpublished, September 21 2023.