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 $\epsilon \to 0$.

2 The problem

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

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

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 $n = 0, \ldots, N_t$, $u^n \approx u(\cdot, t^n)$. 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

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

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

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

where Δx is the spatial step size.

4 Treatment of Neumann BCs

Let $x_i = i\Delta x$ represent the discretization in space with $i = -1, 0, \ldots, N_x, N_x+1$. Here we introduce one *ghost* grid point at each end of the interval 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

$$\begin{aligned} -D_{0x}u_0^n &= f_l(x, t^n), \quad x = 0, \\ D_{0x}u_{N_x}^n &= f_r(x, t^n), \quad x = 1, \end{aligned}$$

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

$$\begin{aligned} u_{-1}^n &= u_1^n + 2\Delta x f_l(x, t^n), \quad x = 0, \\ u_{N_x+1}^n &= u_{N_x-1}^n + 2\Delta x f_r(x, t^n), \quad x = 1. \end{aligned}$$

5 Implementation

For the implementation, we use the exact solution

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

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), 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.

The results confirm the expected order 2 accuracy of the scheme.

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.

We see order 2 accurate convergence at coarse resolutions. The condition number increases as we increase the resolution, and thus the error increases 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
```

Decreasing the value of ϵ appears to cause the condition number of the matrix used in the solve to become worse at the finer resolutions.

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
```

Unlike the case with Dirichlet boundary conditions where the error decreases as ϵ decreases, the case with a Neumann condition appears to settle at an error of order 10^{-2} as we decrease the value of ϵ.

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.

6.1 Next steps:

- Use boundary integral equations methods to solve the resulting equations after the time discretization in Rothe's method (3.1) instead of finite differences. Would that improve the convergence as ϵ becomes small?
- Implement the Quasi-static asymptotic method with a Neumann boundary condition and see if there is an improvement in the error for small epsilon.

References

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