Implementation of a High-Diffusivity Heat Equation Scheme

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1 Introduction

In this document, we implement the scheme presented in [1] to second order accuracy using the 1D domain $\Omega = [0, 1]$. We compare this implementation to one that uses Rothe's method and second-order accurate centered finite-differences in space.

After presenting the problem, we give the order 2 accurate scheme using quasistatic corrections. We then discuss Rothe's method. We finally present numerical examples and a comparison.

2 The problem

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

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

Here, $\epsilon \ll 1$, T is a final time, and f represents known Dirichlet data.

3 The high-order accurate scheme using quasistatic corrections

The notes in [1] develop an $\mathcal{O}(\epsilon^p)$ accurate solution to the IBVP in (2.1) given by

$$u_p = \sum_{k=0}^{p-1} \epsilon^k \Delta_0^{-k} \mathrm{Lap}_D \partial_t^k f, \tag{3.1}$$

where the operators $\mathrm{Lap}_D f$ and $\Delta_0^{-1} g$ solve the problems

$$\begin{cases} \Delta u = 0, & x \in \Omega \times (0, T], \\ u = f, & x \in \partial\Omega \times (0, T], \\ u(x, 0) = 0, & x \in \Omega, \end{cases} \qquad \text{and} \qquad \begin{cases} \Delta u = g, & x \in \Omega \times (0, T], \\ u = 0, & x \in \partial\Omega \times (0, T], \\ u(x, 0) = 0, & x \in \Omega, \end{cases}$$

respectively.

4 The second-order accurate solution

Consider the order-two-accurate solution to the IBVP in (2.1) using quasi-static corrections

$$u_2 = v_0 + \epsilon \Delta_0^{-1} \dot{v}_0, \tag{4.1}$$

where $v_0 \equiv \text{Lap}_D f$ and $\dot{v}_0 \equiv \text{Lap}_D \partial_t f$.

To implement (4.1), we use the algorithm proposed in [1] as follows

1. For each time step j, fill $w_0(\cdot, t_j) = \text{Lap}_D f(\cdot, t_j)$ and $w_1(\cdot, t_j) = \Delta_0^{-1} w_0(\cdot, t_j)$.
2. Compute $v_0(\cdot, t_j) = w_0(\cdot, t_j)$ and $v_1(\cdot, t_j) = \partial_t w_1(\cdot, t_j)$ using an order 2 accurate finite-difference formula.
3. Compute $u_2 = v_0 + \epsilon v_1$ at each node and each time-step.

In the algorithm above, we approximate $\partial_t w_1 \approx (w_1(t+\Delta t) - w_1(t-\Delta t))/2\Delta t$; we need to choose an appropriate value for the time step Δt in the finite-difference formula. For an implementation at a final time T, we need two elliptic solves at each of $t = T$, $T - \Delta t$ and $T + \Delta t$, a total of 6 elliptic solves.

5 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

$$(u_{xx})^{n+1} - \frac{3\epsilon}{2\Delta t}u^{n+1} = \frac{-2\epsilon}{\Delta t}u^n + \frac{\epsilon}{2\Delta t}u^{n-1}. \tag{5.1}$$

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

$$u(x, \Delta t) = u_0(x) + \frac{\Delta t}{\epsilon \Delta x^2}(u_0(x + \Delta x) - 2u_0(x) + u_0(x - \Delta x)) + \mathcal{O}(\Delta t^2), \qquad \text{as } \Delta t \to 0. \tag{5.2}$$

6 Implementation

We carry out numerical implementations of Rothe's Method and the Quasistatic asymptotic method using three exact solutions of (2.1) as test cases.

6.1 Example 1

For this implementation, we use the exact solution

$$u_e(x,t) = A\cos(\sqrt{\epsilon}x + a)e^{-t}, \qquad x \in [0,1], t \in [0,T], \tag{6.1}$$

for testing. We set $A = 200$, $a = -1.123$ and $T = 1$. We use second-order centered finite-differences to solve the elliptic equations in (5.1) 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 Rothe's method

```
Using Rothe method for epsilon = 1.0e-04
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=1.45e-06
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=3.48e-07 order=2.05e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=8.54e-08 order=2.03e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=2.12e-08 order=2.01e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=5.27e-09 order=2.01e+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 the Quasistatic asymptotic method, we obatin

```
Using Quasistatic method for epsilon = 1.0e-04
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=6.67e-07
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=1.63e-07 order=2.03e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=3.77e-08 order=2.12e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=6.29e-09 order=2.59e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=1.58e-09 order=1.99e+00
```

For $\epsilon = 10^{-6}$, and using Rothe's method, we find

```
Using Rothe method for epsilon = 1.0e-06
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=1.43e-08
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=3.45e-09 order=2.05e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=8.46e-10 order=2.03e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=2.16e-10 order=1.97e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=6.72e-11 order=1.69e+00
```

while the quasistatic approach yields the following results

```
Using Quasistatic method for epsilon = 1.0e-06
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=6.65e-09
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=1.66e-09 order=2.00e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=4.14e-10 order=2.00e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=1.03e-10 order=2.01e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=2.03e-11 order=2.34e+00
```

Fixing the number of grid point to 100 and setting $\Delta t = 0.1$, we also generate the following results for Rothe's method

```
Using Rothe method
eps = 1.0000e-02, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.58e-04
eps = 1.0000e-03, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.48e-05
eps = 1.0000e-04, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.45e-06
eps = 1.0000e-05, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.44e-07
eps = 1.0000e-06, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.43e-08
eps = 1.0000e-07, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.44e-09
eps = 1.0000e-08, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.53e-10
eps = 1.0000e-09, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.16e-11
eps = 1.0000e-10, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.91e-12
eps = 1.0000e-11, t=1.0000e+00, Nx=100 Nt=  10 dt=1.000e-01 maxErr=1.10e-11
```

It appears that Rothe's method remains accurate as ϵ becomes smaller and $\Delta t \gg \epsilon$.

6.2 Example 2

For this example, we use the exact solution

$$u_e(x,t) = ax^2 + bx + c + \frac{2a}{\epsilon}t, \qquad x \in [0,1], t \in [0,T], \tag{6.2}$$

with $a = \epsilon/2$, $b = 23$ and $C = 123$. For $\epsilon = 10^{-4}$ we obtain

```
Using Rothe method for epsilon = 1.0e-04
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=1.71e-13
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=2.74e-12 order=-4.01e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=6.17e-12 order=-1.17e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=2.73e-11 order=-2.14e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=1.15e-10 order=-2.08e+00
```

```
Using Quasistatic method for epsilon = 1.0e-04
t=1.0000e+00: Nx= 10 Nt=  10 dt=1.000e-01 maxErr=4.97e-13
t=1.0000e+00: Nx= 20 Nt=  20 dt=5.000e-02 maxErr=1.96e-12 order=-1.98e+00
t=1.0000e+00: Nx= 40 Nt=  40 dt=2.500e-02 maxErr=4.48e-12 order=-1.19e+00
t=1.0000e+00: Nx= 80 Nt=  80 dt=1.250e-02 maxErr=9.66e-12 order=-1.11e+00
t=1.0000e+00: Nx=160 Nt= 160 dt=6.250e-03 maxErr=4.60e-11 order=-2.25e+00
```

This solution is a linear combination of a degree 2 polynomial in x and degree 1 polynomial in t. We expect the numerical solution to be accurate to machine precision times the condition number of the underlying matrix system being inverted.

6.3 Example 3

Work in progress...

In this example, we plan to find a test solution of (2.1) for which the boundary conditions are oscillatory functions. That is, we find a solution to the problem

$$\begin{cases} \epsilon u_t - u_{xx} = 0, & x \in (0,1), \\ u(0,t) = A(t), \\ u(1,t) = B(t), \\ u(x,0) = u_0(x), & x \in [0,1], \end{cases} \tag{6.3}$$

where $A(t)$ and $B(t)$ may be of the form $\alpha \cos(\beta t)$, for example.

We solve (6.3) by setting $u(x,t) = U(x,t) + K(x,t)$, so that U solves the following problem

$$\begin{cases} \epsilon U_t - U_{xx} = \underbrace{-\epsilon K_t + K_{xx}}_{q(x,t)}, & x \in (0,1), \\ U(0,t) = 0, \\ U(1,t) = 0, \\ U(x,0) = \underbrace{u_0(x) - K(x,0)}_{U_0(x)}, & x \in [0,1]. \end{cases} \tag{6.4}$$

The simplest function K for which the (6.4) holds takes the form

$$K(x,t) = (B(t) - A(t))x + A(t). \tag{6.5}$$

We seek a solution of $U(x,t)$ to (6.4) as the series

$$U(x,t) = \sum_{n=1}^{\infty} T_n(t) F_n(x), \tag{6.6}$$

where

$$F_n(x) = \sin \omega_n x, \quad \lambda_n = \omega_n^2 = n^2\pi^2, \tag{6.7}$$

and for $D = 1/\epsilon$,

$$T_n(t) = T_n(0)e^{-\lambda_n Dt} + \int_0^t \hat{q}_n(\tau)e^{-\lambda_n D(t-\tau)}d\tau. \tag{6.8}$$

Here,

$$T_n(0) = 2\int_0^1 U_0(x)F_n(x)dx, \tag{6.9}$$

and

$$\hat{q}_n(t) = 2\int_0^1 q(x,t)F_n(x). \tag{6.10}$$

7 Conclusion and remarks

Using examples of exact solutions to (2.1), we implemented the quasistatic asymptotic scheme developed in [1] and compared it to an implementation using Rothe's method. Based on the results in section 6, we write down the following conclusions:

- The quasistatic asymptotic method appears to yield smaller errors than Rothe's method.
- Rothe's method remains accurate for $\Delta t \gg \epsilon$ as $\epsilon \to 0$.

References

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