

Report for Project 3

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Question 1

Answer To solve the heat equation, explicit scheme, implicit scheme and Crank–Nicolson scheme can be adopted. Denote the step of time and space by τ and h respectively. Given U^n , explicit scheme involves calculating

$$U^{n+1} = (I - \mu\Delta) U^n, \quad (1)$$

where

$$\mu = \tau/h^2 \quad (2)$$

is the grid ratio, and Δ is the discrete Laplacian

$$(\Delta U)_{j,k} = 4U_{j,k} - U_{j,k-1} - U_{j,k+1} - U_{j-1,k} - U_{j+1,k}. \quad (3)$$

Meanwhile, the implicit scheme involves solving

$$(I + \mu\Delta) U^{n+1} = U^n, \quad (4)$$

and the Crank–Nicolson scheme involves solving

$$\left(I + \frac{1}{2}\mu\Delta\right) U^{n+1} = \left(I - \frac{1}{2}\mu\Delta\right) U^n. \quad (5)$$

Denote $M = 1/\tau$ be the number of time steps. The value of $\|U^M\|_\infty$ with respect to different μ is shown in Table 1. In this experiment, h is valued $1/32$.

Table 1 Values of $\|U^M\|_\infty$ with respect to μ when $h = 1/32$

$1/\tau$	μ	Explicit	Implicit	Crank–Nicolson
32	3.20e+01	9.98914e+60	4.32021e-06	2.85218e-08
128	8.00e+00	2.53653e+214	2.19818e-07	5.32018e-08
512	2.00e+00	inf	8.01313e-08	5.51919e-08
2048	5.00e-01	inf	6.08021e-08	5.53183e-08
3072	3.33e-01	inf	5.89271e-08	5.53230e-08
3584	2.86e-01	inf	5.84007e-08	5.53240e-08
3840	2.67e-01	3.76966e+185	5.81913e-08	5.53243e-08
4096	2.50e-01	5.27528e-08	5.80086e-08	5.53246e-08
8192	1.25e-01	5.40265e-08	5.66539e-08	5.53262e-08
16384	6.25e-02	5.46733e-08	5.59869e-08	5.53266e-08
32768	3.12e-02	5.49991e-08	5.56560e-08	5.53267e-08

From the theory of numerical partial differential equations, the L^2 stability condition of the explicit scheme is

$$\mu \leq 1/4, \quad (6)$$

while the implicit scheme and Crank–Nicolson scheme are unconditionally stable. The result above clearly fits in theory.

Question 2

Answer For the implicit scheme, there are different solvers to the equation. We flatten U^n as a column vector. (Row major and Column major notion coincide here because of symmetry) Comparison of different linear system solvers is given in Table 2 and Table 3 with Python and C implementation respectively. Here τ and h are set to be $1/512$ and $1/128$ respectively.

Table 2 Comparison in efficiency of different solvers with Python implementation

Method	Time (s)	Iter.	Err. u	Rel. u	Err. u_s	Rel. u_s
SQRT	51.33407	512	6.02500e-10	4.504e-01	0.00000e+00	0.000e+00
GS	169.10408	460800	6.02520e-10	4.504e-01	1.91460e-14	9.868e-06
SD	1.16659	8280	6.02500e-10	4.504e-01	8.79253e-18	4.532e-09
CG	0.82594	4930	6.02500e-10	4.504e-01	2.26652e-18	1.168e-09
MG	9.40716	3072	6.02500e-10	4.504e-01	5.22401e-20	2.693e-11

Here the column Err. correspond to $\|u_h - u\|_2$ and Rel. correspond to $\|u_h - u\|_2 / \|u\|_2$. Note that u_s , the standard solution is selected to be the result of Cholesky decomposition solver. The rows refer to Cholesky decomposition solver, Gauss–Seidel iterations, steepest descent method, conjugate gradient method and multigrid method (with Gauss-Seidel iterations as smoother) respectively.

For details, u_h and u_s is interpolated in the bilinear manner and integration is perform using

Table 3 Comparison in efficiency of different solvers with C implementation

Method	Time (s)	Iter.	Err. u	Rel. u	Err. u_s	Rel. u_s
SQRT	1.71272	512	6.02500e-10	4.504e-01	0.00000e+00	0.000e+00
GS	95.05779	460800	6.02520e-10	4.504e-01	1.91460e-14	9.868e-06
SD	0.42192	8016	6.02500e-10	4.504e-01	1.00215e-17	5.165e-09
CG	0.32756	4939	6.02500e-10	4.504e-01	3.80416e-18	1.961e-09
MG	3.33660	3072	6.02500e-10	4.504e-01	5.23316e-20	2.697e-11

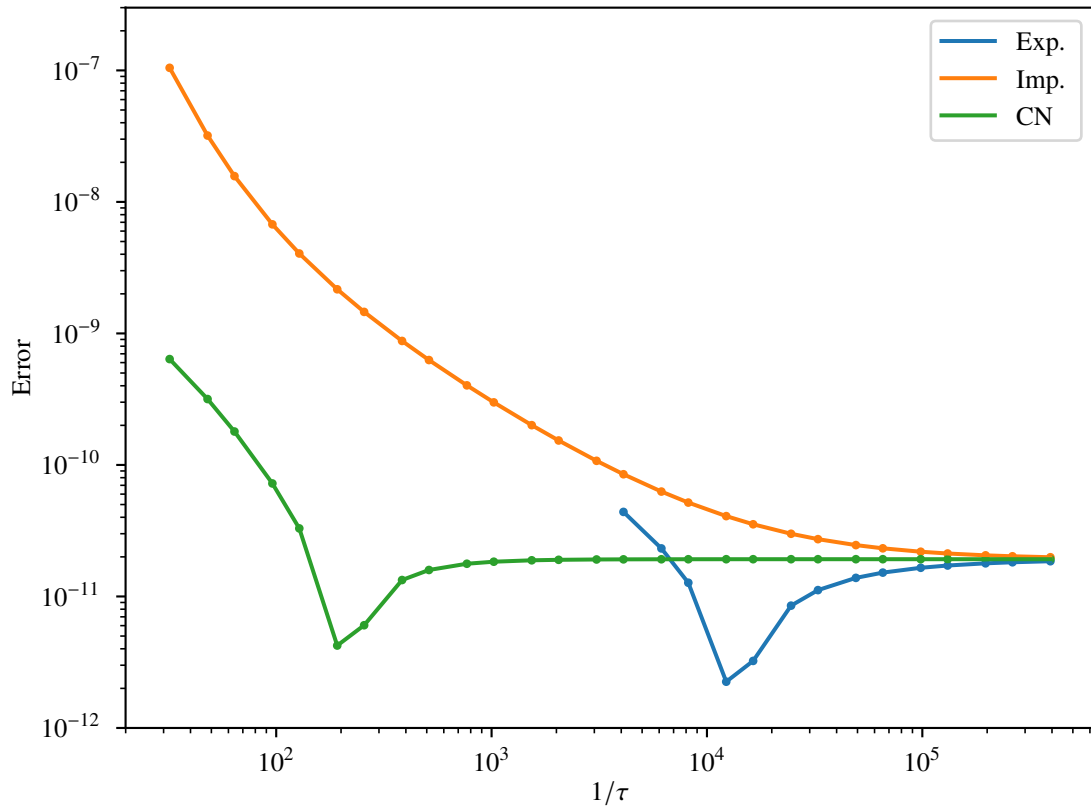
Note that the columns and rows correspond to Table 2.

Simpson's formula with interval length $1/512$. Here C implementation directly calls BLAS, LAPACK and Sparse BLAS from MKL, and time of Python interpretation is saved.

One may notice that errors to real solution u is large. This error is caused by bad grid ratio and large μ and τ . Comparisons to u_s show that solutions to systems is rather accurate.

Question 3

Answer We first investigate the influence of τ to the error $\|u - u_h\|_2^2$ as in Figure 1.


 Figure 1 Errors with respect to τ with $h = 1/32$

According to this figure, we select $\tau = h^2/4, h^2/8, h^2/12, h^2/16$ for the explicit scheme, $\tau = h, h/4, h/16$ for the implicit scheme, and $\tau = h/4, h/6, h/8$ for the Crank–Nicolson scheme. The final result is shown in Figure 2.

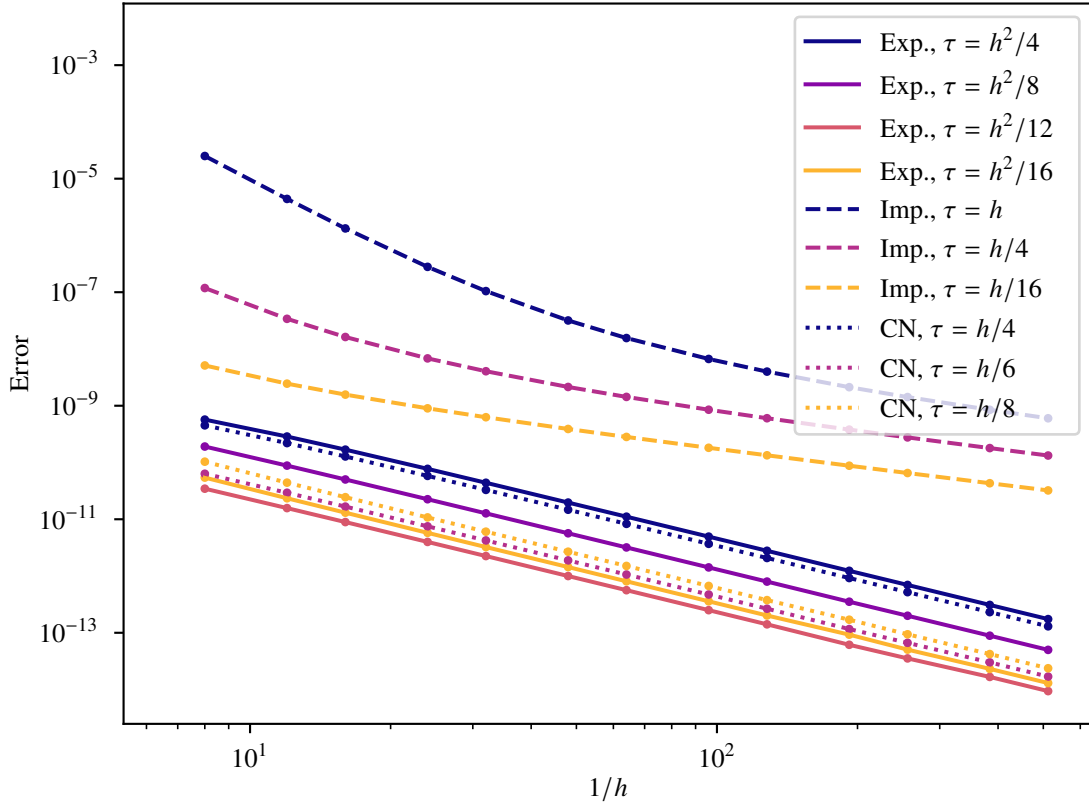


Figure 2 Errors with respect to h

For details, u_h is bilinearly interpolated from U^M , and the integral is calculated using Simpson's formula with interval length $1/512$.

It can be seen that generally the error decreases when the space grid becomes finer. The slope of curves of explicit and Crank–Nicolson schemes are approximately -2 in the logarithm scale, and this can be explained by the error $O(\tau + h^2)$ and $O(\tau^2 + h^2)$ respectively. Asymptotes of curves of the implicit scheme are approximately -1 , and this can be explained by the error term $O(\tau + h^2)$.