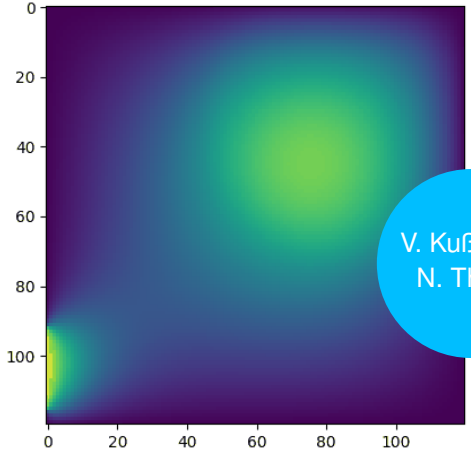
Universität Stuttgart
Department of Mathematics



Project 2: Time dependent heat equation with a source

Scientific Computing

V. Kußmaul,
N. Thorin

Introduction

We solve the **time dependent heat equation**

$$\begin{cases} \partial_t u - \Delta u = f, & \text{in} \quad (0,1)^2, \\ u = g, & \text{on} \ \partial(0,1)^2. \end{cases}$$

with a source f and boundary condition g.

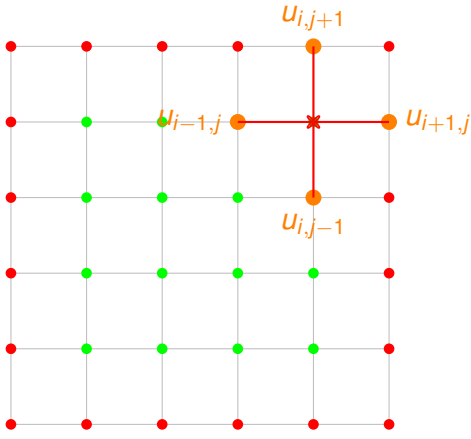
Discretization

We use finite differences for the Laplacian

$$(\Delta u)(x) \approx \big(u(x_1 - \delta x, x_2) + u(x_1 + \delta x, x_2) + u(x_1, x_2 - \delta x) + u(x_1, x_2 + \delta x) - 4u(x_1, x_2)\big)/\delta x^2$$

and the time derivative

$$\frac{u(x, t + \delta t) - u(x, t)}{\delta t} - (\Delta u)(x, t + \delta t) \approx f(x, t + \delta t)$$
$$\iff u(x, t + \delta t) - \delta t(\Delta u)(x, t + \delta t) \approx \delta t\, f(x, t + \delta t) + u(x, t)$$



Let $u_{ij}^{(\ell)} = u(x_{ij}, t_\ell)$, $0 \le i, j < N$. Then

$$u_{ij}^{(\ell+1)} - \frac{\delta t}{\delta x^2}(Lu)_{ij}^{(\ell+1)} = \delta t\, f_{ij}^{(\ell+1)} + u_{ij}^{(\ell)}$$

where

$$(Lu)_{ij} = u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}$$

and $u_{ij}^{(\ell)} = g_{ij}^{(\ell)}$ in boundary points.

Transfer to 1D by $n = iN + j$.

Discretization (summary)

Set

$$A = I - \frac{\delta t}{\delta x^2} L.$$

Want to solve

$$A u^{(\ell+1)} = u^{(\ell)} + \delta t \, f^{(\ell+1)}$$

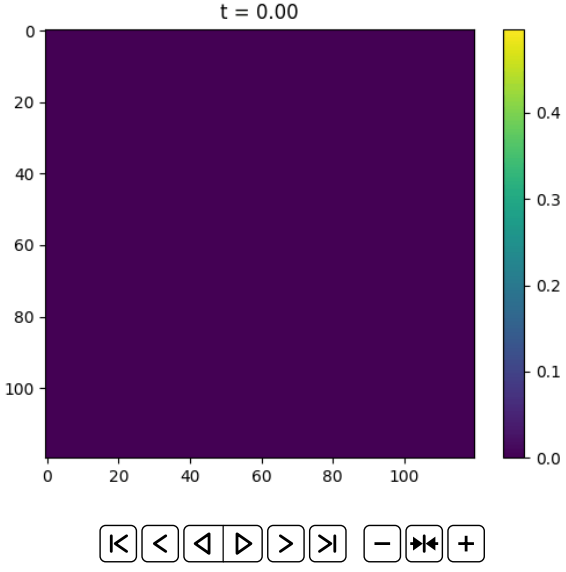
Note: A is spd! $\rightsquigarrow$ Use CG-method

Implementation details

```
def sparse_laplacian(self) -> csr_matrix:
    def in_bounds(i, j):
        return (0 <= i < self.N) and (0 <= j < self.N)

    L = lil_matrix((self.N**2, self.N**2))
    boundary_points = defaultdict(list)
    directions = [(-1, 0), (1, 0), (0, -1), (0, 1)]
    for i in range(self.N):
        for j in range(self.N):
            L[self.n(i, j), self.n(i, j)] = -4
            for dx, dy in directions:
                i_, j_ = i + dx, j + dy
                if in_bounds(i_, j_):
                    L[self.n(i, j), self.n(i_, j_)] = 1
                else:
                    boundary_points[self.n(i, j)].append(((i_+1)*self.dx, (j_+1)*self.dx))
    self.boundary_points = boundary_points
    return (1/self.dx)**2 * csr_matrix(L)
```

CG Method

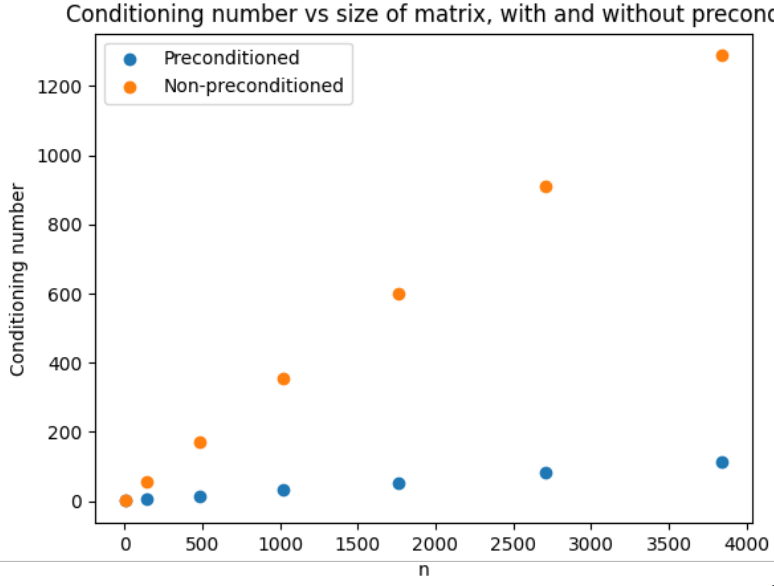
```
def unpreconditioned_solve(self, b: np.ndarray, initial_guess: np.ndarray):
 x = initial_guess
    r = p = b - self.A@x
    alpha = np.dot(r, r)

    for _ in range(self.max_iterations):
        v = self.A@p
        _lambda = alpha / np.dot(v, p)
        x = x + _lambda * p
        r = r - _lambda * v
        alpha_new = np.dot(r, r)
        p = r + (alpha_new / alpha) * p
        alpha = alpha_new

        if alpha < self.tol**2:
            return x

    return None
```


t = 0.00
0
20
40
60
80
100
0
20
40
60
80
100
0.4
0.3
0.2
0.1
0.0

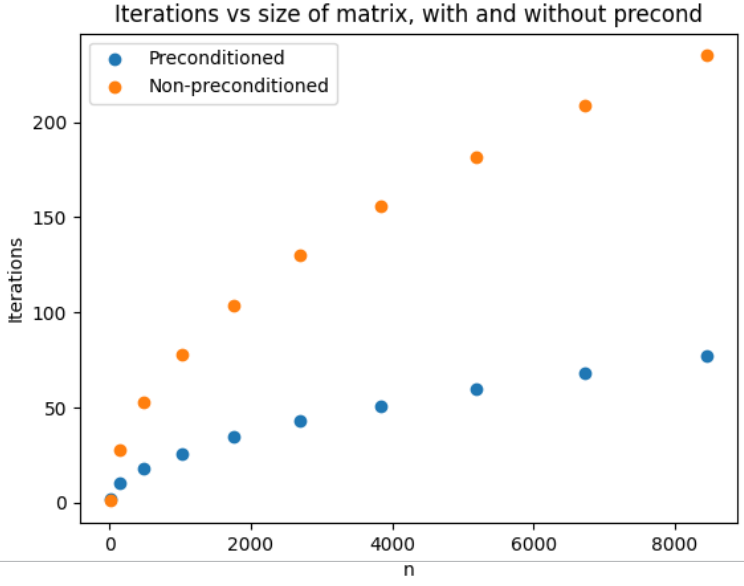
Preconditioning

- A is spd, we are doing CG $\rightsquigarrow$ Incomplete Cholesky as preconditioner.
- We use IC(0) $\rightsquigarrow$ Sparsity pattern is conserved.
- $A = L^T L \rightsquigarrow A \approx \tilde{L}^T \tilde{L} = P$
- Improvements: Smaller conditioning number $\rightsquigarrow$ Fewer iterations needed
- Downsides: Solve two sparse triangular systems $\rightsquigarrow$ More computing time per iteration

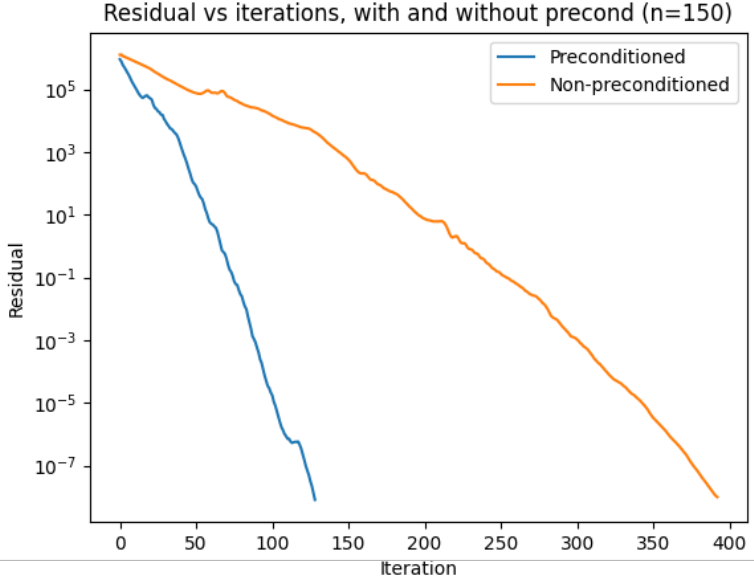
Results (conditioning number)



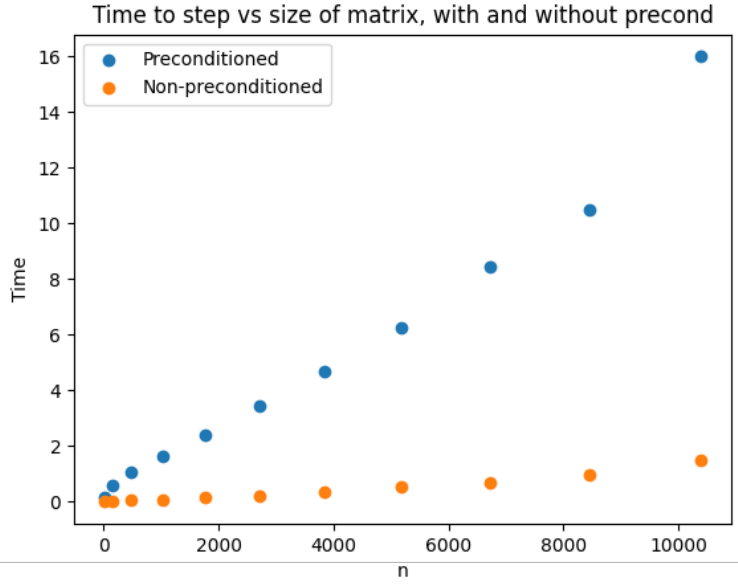
Results (iterations)



Results (residual)



Results (time)



Profiling

```
Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
   117                                           @profile
   118                                           def preconditioned_solve(self, b: np.ndarray, initial_guess: Optional[np.ndarray], testing=False) -> tuple[Optional[np.ndarray], int]:
   119                                               # Initialize variables
   120        40      13136.0    328.4      0.0      if initial_guess is not None:
   121        40      13572.0    339.3      0.0          x = initial_guess
   122                                               else:
   123                                                   x = np.zeros(b.shape[0])
   124        40    2282668.0  57066.7      0.0      r = b - self.A@x
   125        40   61470373.0   2e+06      0.7      r_hat = spsolve_triangular(self.L, r, lower=True) # r^{hat} = L^{-1} r
   126        40   48609703.0   1e+06      0.6      p = spsolve_triangular(self.L_T, r_hat, lower=False) # p = L^{-T} r
   127        40     234454.0   5861.4      0.0      alpha = np.dot(r_hat, r_hat)
   128        40      12620.0    315.5      0.0      if testing:
   129                                                   residuals = []
   130                                                   residuals.append(np.dot(r, r))
   131
   132                                               # CG method
   133      2928    1244213.0    424.9      0.0      for i in range(self.max_iterations):
   134                                                   # Compute auxilliary variables
   135      2928  143379765.0  48968.5      1.7          v = self.A@p
   136      2928   13753025.0   4697.1      0.2          _lambda = alpha / np.dot(v, p)
   137
   138                                                   # Update variables
   139      2928   27024587.0   9229.7      0.3          x = x + _lambda * p
   140      2928   23306758.0   7960.0      0.3          r = r - _lambda * v
   141      2928 4481247259.0   2e+06     53.1          r_hat = spsolve_triangular(self.L, r, lower=True)
   142                                                   # r_hat = spsolve(self.L, r)
   143      2928   15420475.0   5266.6      0.2          alpha_new = np.dot(r_hat, r_hat)
   144      2928 3592991414.0   1e+06     42.6          p = spsolve_triangular(self.L_T, r_hat, lower=False) + (alpha_new / alpha) * p
   145                                                   # p = spsolve(self.L_T, r_hat) + (alpha_new / alpha) * p
   146      2928    1580528.0    539.8      0.0          alpha = alpha_new
   147
   148      2928     706330.0    241.2      0.0          if testing:
   149                                                       residuals.append(np.dot(r, r))
   150
   151                                                   # Convergence control
   152      2928   20379428.0   6960.2      0.2          if np.dot(r, r) < self.tol**2:
   153        40       8408.0    210.2      0.0              if testing:
   154                                                           return x, i, residuals
   155                                                       else:
   156        40     580438.0  14511.0      0.0                  print(f"Preconditioned CG-method converged in {i + 1} iterations.")
   157        40      23415.0    585.4      0.0                  return x, i
   158
   159                                               # Method did not converge
   160                                               return None
```

References

[1] Dominik Göddeke.
Scientific computing.
Lecture Notes, June 2024.
Version: 25th June 2024.

ChatGPT was used for implementation details regarding sparse matrices and visualizing our numerically computed solution.