NHR FAU

Friedrich-Alexander-Universität
Erlangen-Nürnberg

PTfS Project Intro – Part 1

Modelling 2D steady-state heat equation

Sommersemester 2026

Overview

- Background
- What are your tasks
- Questions

General Outline – What the Project is About

- Learning and using concepts from the lecture in the wild
- Work with more complex codebase than in the exercises

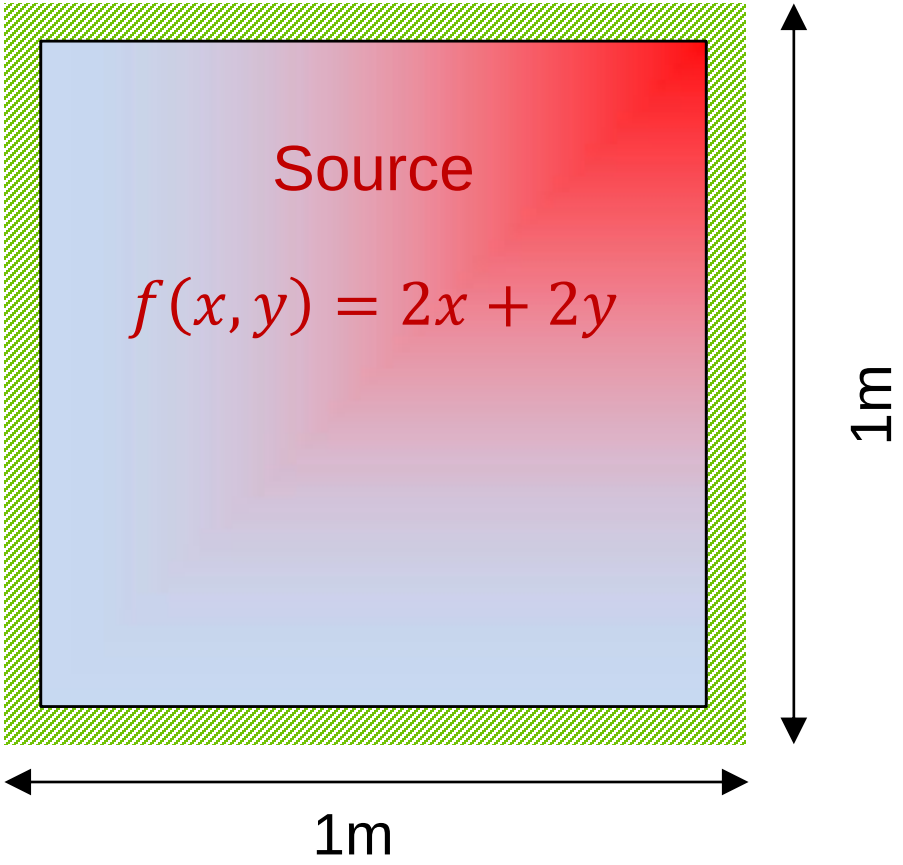
- This year: No submissions have to be made, i.e., no project report is collected and graded by us.
- Still: When working on the project it is highly encouraged to make a report in order to keep track of your changes and verify your computations/observations.

- The 10 ECTS exam will contain question(s) strongly related to/on the project.
  In order to prepare best, do the project thoroughly!

Scenario: Heat Dissipation on a Rectangular Plate

Find steady state temperature distribution inside the plate!

Boundary
$T(\varphi) = 0$



Steady-State Heat Equation

$$-k\Delta u = f \quad \forall\,(x,y) \in \Omega$$
$$\mathrm{u}(x,y) = 0 \quad \forall\,(x,y) \in \partial\Omega$$

where $\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$

Assume (w.l.o.g.) $k = 1$ (“diffusivity” or “conductivity”)

$$\Rightarrow -\Delta u = -\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f$$

But this is in the continuous world… how to solve for u with a computer?

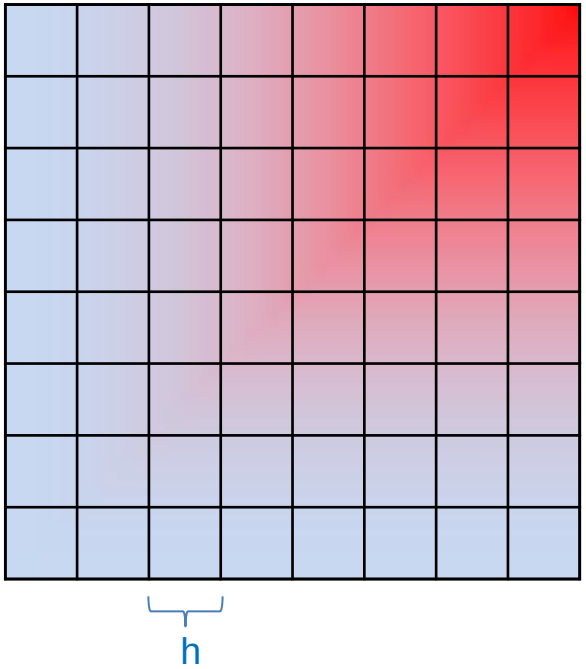
Discretization

$$-\Delta u = -\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f$$

Use Finite Difference Method (FDM) for discretization

$$\Rightarrow -\Delta u = -\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(x, y) \approx$$

$$\frac{1}{h^2}\left(4u(x, y) - u(x - h, y) - u(x + h, y) - u(x, y - h) - u(x, y + h)\right)$$

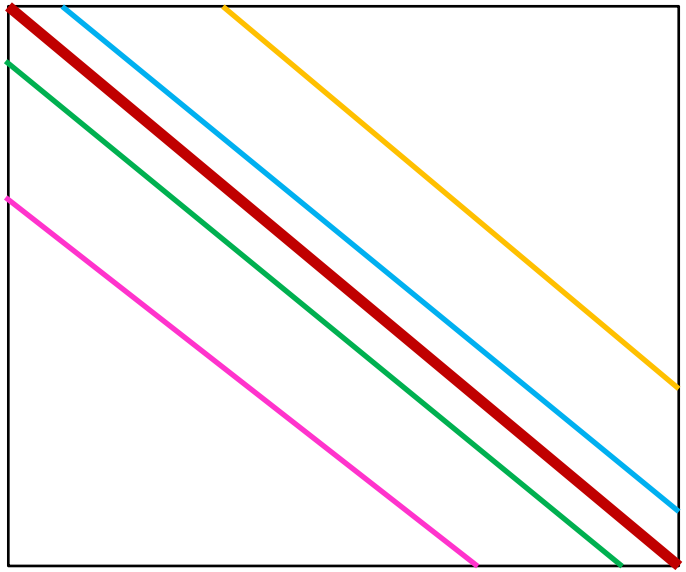


Linear System of Equations

Instead of a general point (x, y), we have one equation for every particular choice of x and y

$$\Rightarrow -\Delta u \approx \frac{1}{h^2}(4\,u(x,y) - 1\,u(x-h,y) - 1\,u(x+h,y) - 1\,u(x,y-h) - 1\,u(x,y+h)) = f$$

$$\Rightarrow A\,u = f$$

$A =$ 

$u =$

u(0,0)
u(0,h)
u(0,2h)
. . .
u(h,0)
u(h,h)
u(h,2h)
. . .

$f =$

f(0,0)
f(0,h)
f(0,2h)
. . .
f(h,0)
f(h,h)
f(h,2h)
. . .

Solving the Linear System

Solve for u : $A\,u = f$

1. Use Conjugate Gradient (CG)

2. Use Preconditioned Conjugate Gradient (PCG) with symmetric Gauss-Seidel preconditioning

Implementations of these algorithms are already given, and is not the focus of this project.

Solving the Linear System

PCG example

"Iterative method" i.e., starting with some $u = u_0$

Matrix-free implementation, i.e., stencil updates

initialization

```
r = f - A u
res_norm = <r,r>
z = P r0
α0 = <r,z>
p = z
```

iteration

```
while( (iter<niter) && (res_norm > tol*tol) )
        v  = A p
        λ  = α0 / <v,p>
        u  = u + λ p
        r  = r - λ v
        ...
```

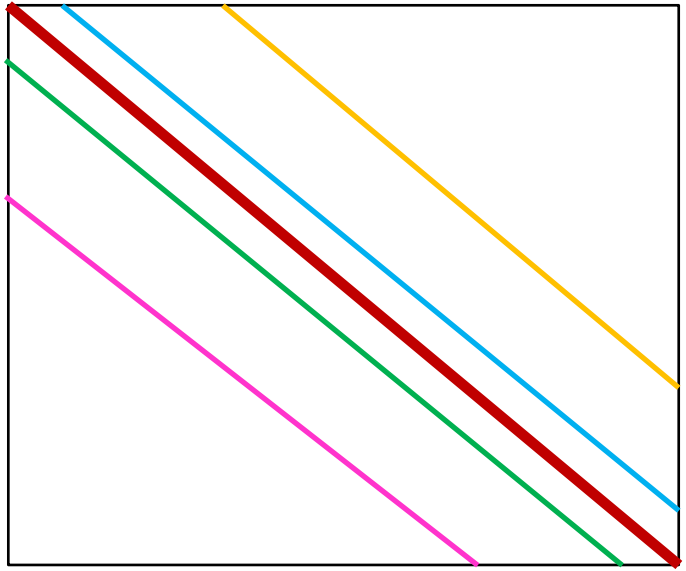
Linear System of Equations

$$\Rightarrow -\Delta u \approx \frac{1}{h^2}(4\,u(x,y) - 1\,u(x-h,y) - 1\,u(x+h,y) - 1\,u(x,y-h) - 1\,u(x,y+h)) = f$$

$$\Rightarrow\ A\,u = f$$

2d-5pt stencil

$A =$



$u =$

u(0,0)
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. . .
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f(0,h)
f(0,2h)
. . .
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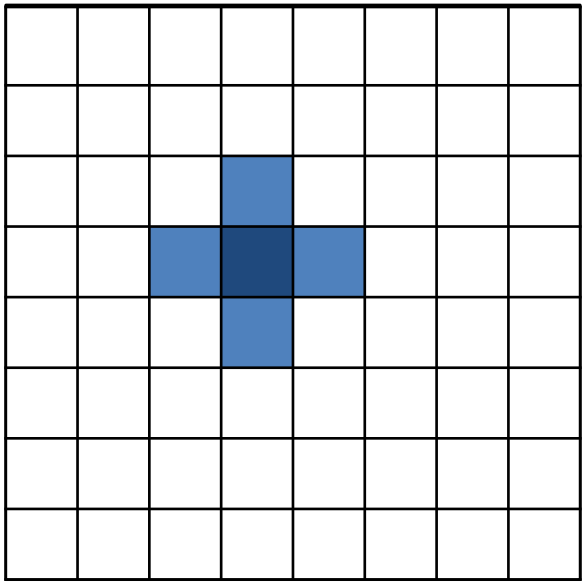
f(h,h)
f(h,2h)
. . .

2d-5pt Stencil

Computing Au efficiently:
How to take advantage of knowing the pattern of A ahead of time?



```
for j=1,jmax
  for k=1,kmax
    Au[j,k] = (1/h^2)*( 4*u[j,k] - u[j-1,k]
                      -u[j+1,k]-u[j,k-1]-u[j,k+1] )
  enddo
enddo
```

Solving the Linear System

PCG example

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```
r = f - A u
res_norm = <r,r>
z = P r0
α0 = <r,z>
p = z
```

$P = (D + U)^{-1} D (D + L)^{-1}$

Think of solving this efficiently, since also not explicitly stored! See `PDE::GS_precon` defined in PDE.cpp

iteration

```
while( (iter<niter) && (res_norm > tol*tol) )
        v   = A p
        λ   = α0 / <v,p>
        u   = u + λ p
        r   = r - λ v
        ...
```

Your Tasks

1. Clone the code from Github:
   `git clone https://github.com/RRZE-HPC/PTfS-CAM-Project.git`

2. Build the code using the given Makefile, i.e., just type **`CXX=icpx make`**

3. To switch on LIKWID measurement (for part 2) set the LIKWID flag to ‘on’, i.e.,
   `LIKWID=on CXX=icpx make`

4. Check for code correctness using the **test** executable: **`./test`**

5. To run the actual code use the **perf** executable:
   `./perf num_grids_y num_grids_x`

Do these now! Don’t wait to get familiar with code.

6. If all tests pass, **parallelize building blocks using OpenMP**. Always observe correctness!

7. Are there any possible performance optimizations that you could do in the CG and PCG solver implemented in **`SolverClass::(P)CG`** (Solver.cpp)? If so, implement them!

Walkthrough

1. No need for separate, manual compilation and linking
   - Everything can be done with a simple **`make`**

2. Important files
   - Grid.cpp (.h)
   - PDE.cpp (.h)
   - Solver.cpp (.h)

3. “./test” executable for correctness checking, “./perf” executable for… performance
   - After making optimizations, tests should always pass!
   - ./perf gives us performance w/ and w/out preconditioning
     - Also, routine specific timers (part 2). See Grid.cpp

Things to Take Care

- Think to use loop fusion wherever necessary.
- For debugging please compile code as: **`CXX=icpx make EXTRA_FLAGS=-DDEBUG`**
- Sometimes it's useful for debugging to visualize your arrays. Use the function **`writeGnuplotFile`** and plot using **`splot`** in gnuplot if needed. Additionally, when compiled with **`-DDEBUG`**, **`./test`** produces some data files that can be visualized by **`./plot.sh`**
- Take particular care with parallelizing the Gauss-Seidel preconditioner.
- Use Fritz (Ice Lake) for getting your performance results, and pin frequency to 2.4 GHz
- Check if the measurements are reproducible. (Think of pinning, scheduling, and clock frequency).
- Request a dedicated node for measuring performance.

Reminders

- Clone from git and build code sooner rather than later!

- Office hours
  - Thursdays 13:00 – 14:00
  - Blaues Hochhaus, Room 04.139
  - Starting from June 25

Scoreboard (optional)

- Submit your best run on Moodle (see “PTfS Project Leaderboard”) to see who’s the fastest!
- See instructions on the submission page
- Final submission: End of semester (Sept 30)

- The best coding project(s) win(s) a prize!

Questions?

$$\Rightarrow -\Delta u = -\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(x,y) \approx$$

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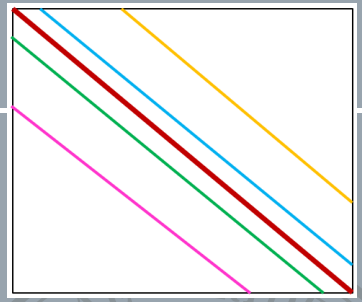

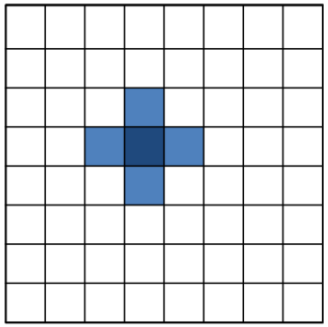

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  for k=1,kmax
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  enddo
enddo
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