PTfS-CAM

Project: Modelling 2D steady-state heat equation

Part 1

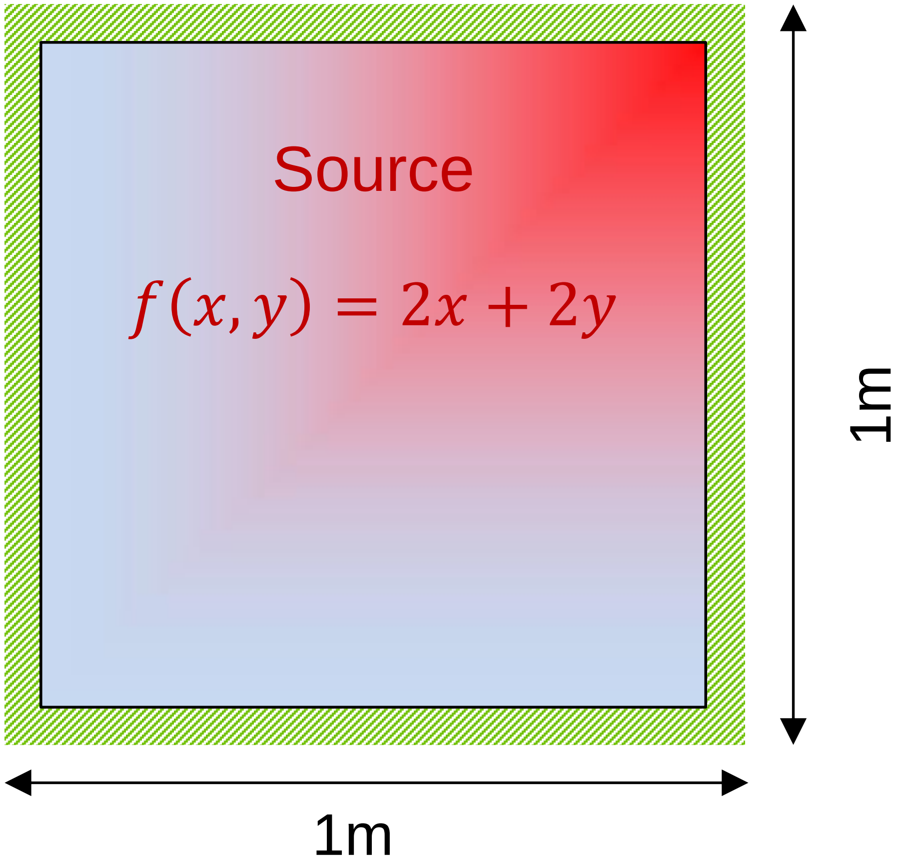
Overview

- Background
- What are your tasks
- Questions

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 $\quad \Delta u = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$

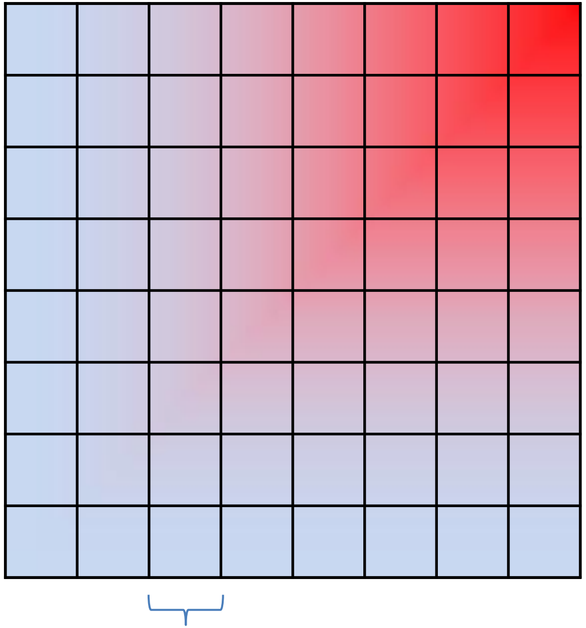
Assume (w.l.o.g.) $k = 1$ (“diffusivity” or “conductivity”)

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

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

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

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

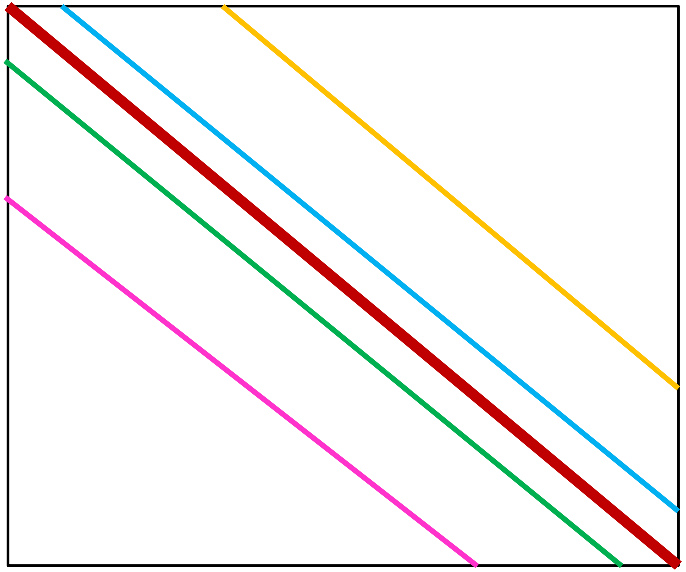
Linear system of equations

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

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

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

$A =$



$u =$

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 : $\quad A\,u = f$

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
        …
```

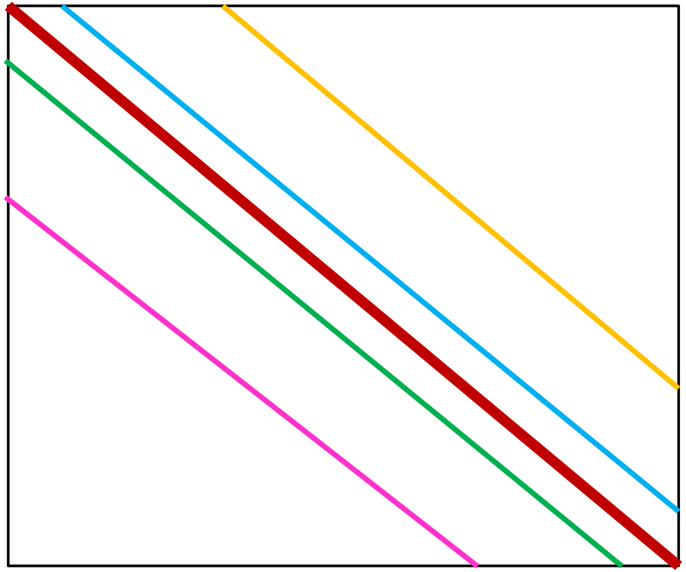
Linear system of equations

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

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

2d-5pt stencil

$A =$



$u =$

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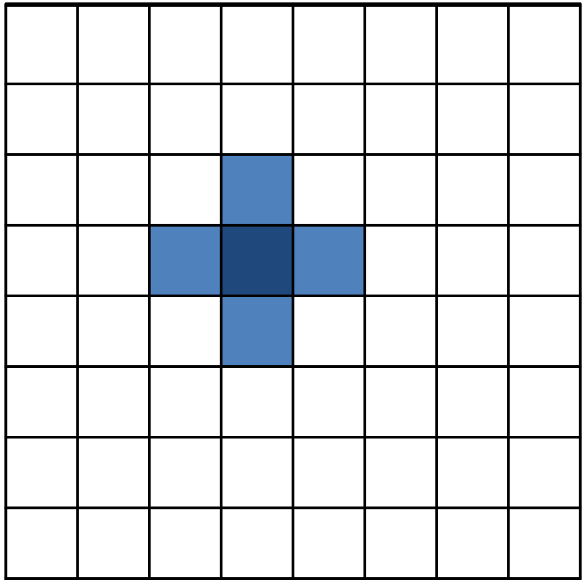
f(h,h)
f(h,2h) . . .

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/h²)*( 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
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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.
- Take particular care with parallelizing the Gauss-Seidel preconditioner.
- Use Fritz (Ice Lake) for getting your performance results.
- Fix clock frequency to 2.2 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
  - Fridays 13:00 – 14:00
  - Blaues Hochhaus, Room 04.139
  - Starting from June 6

Scoreboard (optional)

- Submit your best run on Moodle (see “PTfS-CAM 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?

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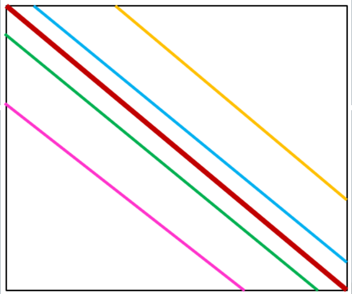

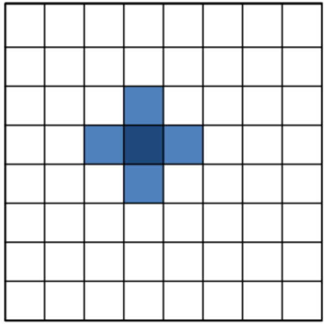

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