CSE 380 Project 2: Steady State Heat Equation Model Document

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1 Abstract

This document outlines the problem setup (governing equations and boundary conditions) as well as numerical solution techniques for solving 1D and 2D steady state heat equation problems using 2nd and 4th order finite difference.

2 Executive Summary

As of 12/14/18, there are still issues with convergence analysis. Due to this, while most tests can be performed, it is dubious to draw any conclusions because solver correctness has not been verified. Also, because much time was spent trying to fix solver convergence problems, `PETSC` is not functioning.

Overall, I learned a great deal from this project and one of the most important lessons was the value of incremental development. Had I done a better job from the jump of adding and verifying functionality bit by bit, I think I could have avoided some of the traps and time sinks that have prevented me from completing all the deliverables for both Project 1 and Project 2

3 Usage

3.1 Build Procedure

3.2 Autotools

Autotools is used to compile the source code. The files `configure.ac` and `Makefile.am` are both setup to link to `MASA`, `GRVY`, and `HDF5` and optionally `PETSC` though functionality for the later seems broken. The `Makefile.am` in `src` is also modified with lines

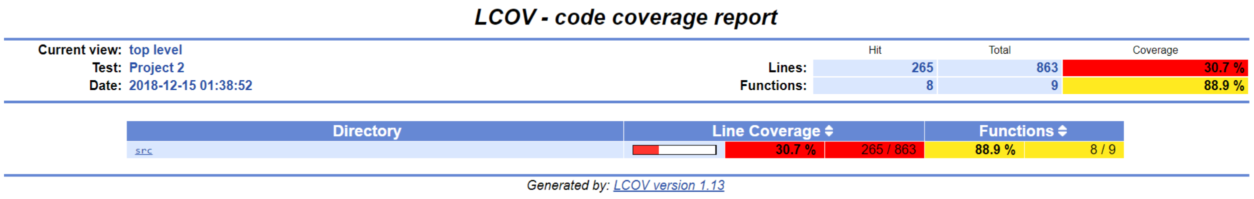
```
AUTOMAKE_OPTIONS = foreign

if PETSC_ENABLED
include $(PETSC_DIR)/lib/petsc/conf/variables
AM_CXXFLAGS += -DINCLUDE_PETSC $(PETSC_CC_INCLUDES)
endif

bin_PROGRAMS = heatFD

heatFD_SOURCES = main.c utilities.c utilities.h

AM_CFLAGS = $(GRVY_CFLAGS)
AM_CFLAGS += $(MASA_CXXFLAGS)
AM_CFLAGS += $(HDF5_CFLAGS)
LIBS = $(GRVY_LIBS)
LIBS += $(MASA_LIBS)
LIBS += $(HDF5_LIBS)
LIBS += -lm

if PETSC_ENABLED
heatFD_LDADD += ${PETSC_LIB}
endif
```

A `test` directory was created to perform regression tests using shell scripts and the `make check` target, but convergence analysis issues (see below) have limited the number of regression tests to just working cases (as of 12/14/18, this is the 1d 2nd order case).

To facilitate troubleshooting, a shell script `bootstrap.sh` can be sourced (very important to `source` the script so environment variables are appropriately set in the parent process) to purge modules, then reload default `TACC` modules, then depending on input either load modules for `PETSC` or load a `gcc` toolchain that has `gcov`. The default behavior is to perform the later, while `PETSC` linking can be accomplished by passing the option `--petsc`. In all cases, the script sets necessary environment variables (`PKGPATH`), then runs `autoreconf -f -i` then `./configure` with appropriate command line options. After that, user can run `make` and `make check` and optionally `make coverage` if enabled.

3.3 Coverage

The `gcov` and `lcov` tools were used to evaluate how well the regression test suite created by the `make check` target covered the use cases of the code. While the requirement is a minimum of 75%, I was only able to achieve approximately 30% coverage (Fig. 3.3) because I did not include regression tests for the problem cases where my code was not achieving correct performance. While I could have written tests and most likely reached the 75% mark, that would have been antithetical to the meaning of regression testing.



LCOV - code coverage report

			Hit	Total	Coverage
Current view:	top level				
Test:	Project 2	Lines:	265	863	30.7 %
Date:	2018-12-15 01:38:52	Functions:	8	9	88.9 %

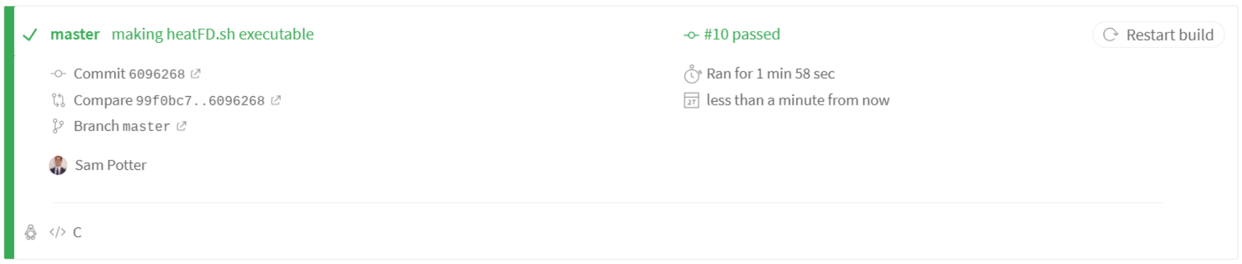
Directory	Line Coverage ⬍			Functions ⬍	
src		30.7 %	265 / 863	88.9 %	8 / 9

Generated by: LCOV version 1.13

Figure 1: Coverage report from lcov

3.4 Continuous Integration

In order to automate my regression testing, I used Travis-CI and a `travis.yml` file to trigger a regression test build every time I pushed code to GitHub. I used the Docker image made available to the class as my base OS. I did have an issue getting Travis to work with my UTHPC repository, but was able to clone my repo into another repository under my own account and get the builds working (Fig. 3.4), so I don't know if this really counts.



✓ master making heatFD.sh executable

Commit 6096268

Compare 99f0bc7..6096268

Branch master

Sam Potter

#10 passed

Ran for 1 min 58 sec

less than a minute from now

C

Figure 2: Passing build from Travis-CI

3.5 Input Options

Input options available to the user are summarized in Table 3.5.

Table 1: Application input options

option	description	acceptable range
method	iterative solver method	(Jacob,Gauss-Seidel)
iter_max	iterative solver max number of iterations	$>= 1$
tol	iterative solver convergence tolerance	positive real double
order	finite difference order	(2,4)
dimension	problem dimension	(1,2)
kappa	material thermal conductivity	positive real double
n	number of nodes along a side	> 2
Txmin	temperature at lower bound of x	real double
Txmax	temperature at upper bound of x	real double
Tymin	temperature at lower bound of y	real double
Tymax	temperature at upper bound of y	real double
Ax	MASA parameter Ax	real double
By	MASA parameter By	real double
verification	Bool switch: runn verification	(0=no, 1=yes)
out_mode	switch for output verbosity	(0=silent, 1=standard, 2=debug)
timer	Bool switch: timing to stdout	(0=no, 1=yes)
out_file	file name to save results to	string

3.6 Verification Procedure

To run the application in verification mode, the user can either set the value in the input file to 1 or pass the argument `verification 1` on the command line. The user must also specify reasonable numbers for MASA parameters `Ax` and `By` in the input file based on domain size (assumed to be the unit interval in either $\mathbb{R}$ or $\mathbb{R}^2$). Output to `stdout` includes problem details and L2 norm error with MASA exact solution.

3.7 Verification Exercise

Outstanding issues with convergence results in all cases except 1D 2nd order. See Fig 3.7. through Fig. 3.7 for current results. Results for the 2D 4th order case are completely nonsensical. Note, using Gauss-Seidal iterative solver because Jacobi diverges for 4th order finite difference. This divergence stems from the fact that the system matrix A is no longer strictly diagonally dominate, thus the Jacobi method won't converge with an arbitrary initial guess.

3.8 Performance Measures

Outstanding convergence issues in all cases except 1d 2nd order. Showing timing from 1 and 2d 2nd order. As mentioned above, Gauss-Seidal method used. One dimensional results in Table

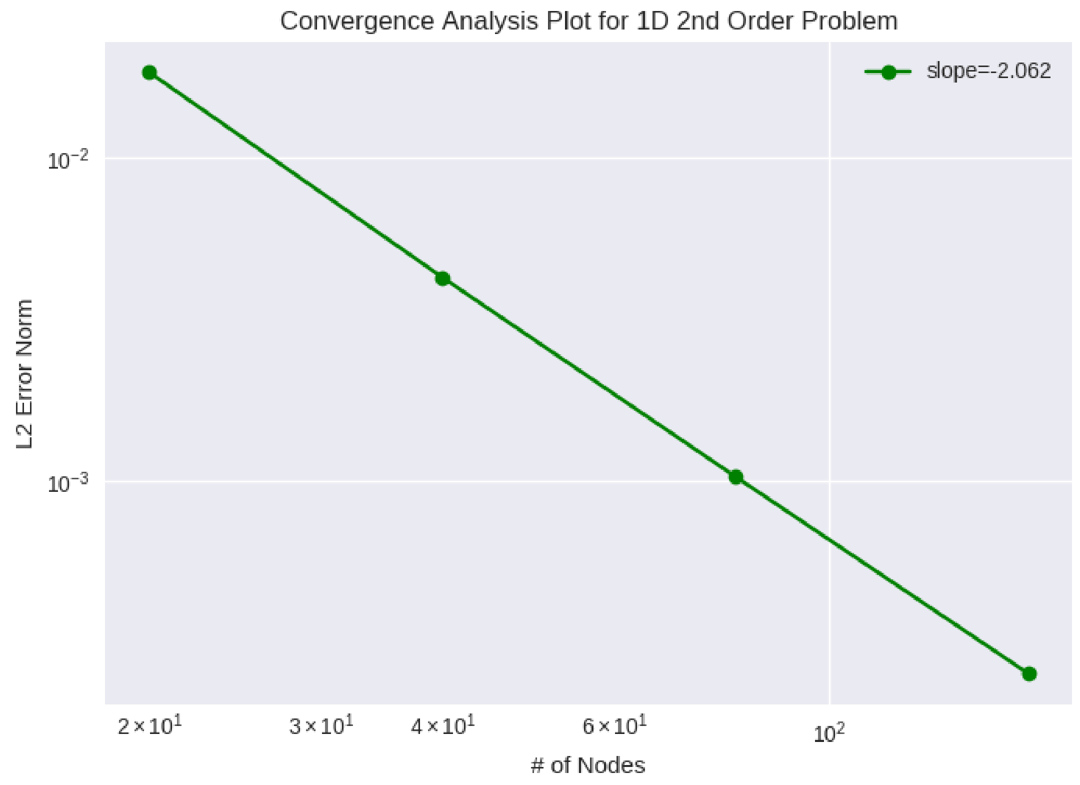


Figure 3: Convergence results for 1D 2nd Order. Working as expected.

3.8. Two dimensional results in Table 3.8. Timings from `PETSC` solves not available due to issues with compilation and linking.

Table 2: Timing results for 1D convergence testing w/ Gauss-Seidel

n	input	assemble	solve	total
20	3.4e-3	4.1e-3	4.7e-4	1.4e-2
40	3.2e-2	1.7e-3	4.9e-3	4.3e-2
80	2.5e-2	1.6e-3	7.5e-2	1.1e-1

4 Results

4.1 2D Plot

I used Paraview to visualize my 2D solution. I wrote a short script in Python that used the `h5py` library to read the HDF5 file and then write that data to an ASCII vtk file using a structured grid format. While I wouldn't say that the result is aesthetically beautiful it is beautiful in the sense

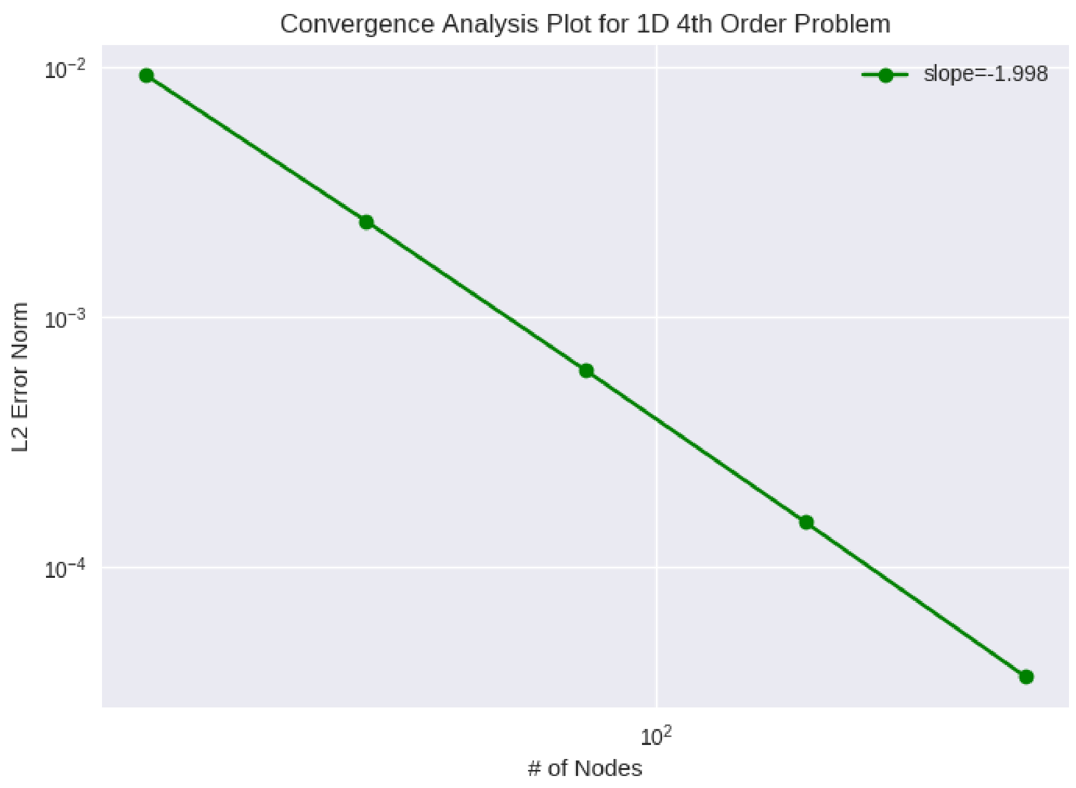


Figure 4: Convergence results for 1D 4th Order. Not working as expected. Convergence rate is half that of theoretical expectation.

that it shows that I clearly have either a boundary value issue somewhere or an issue with how I've ordered my solution vector (Fig. 4.1). This kind of information will be helpful as I continue to debug.

4.2 1D Plot

Finally, while not a required deliverable, I wanted to show a plot of my 1d 4th order solution with 80 nodes (Fig.) because it seems to match the analytical solution well, but I'm still getting slow convergence. This tells me something may be going on in how I'm calculating the L2 error. I am continuing to hunt this issue down.

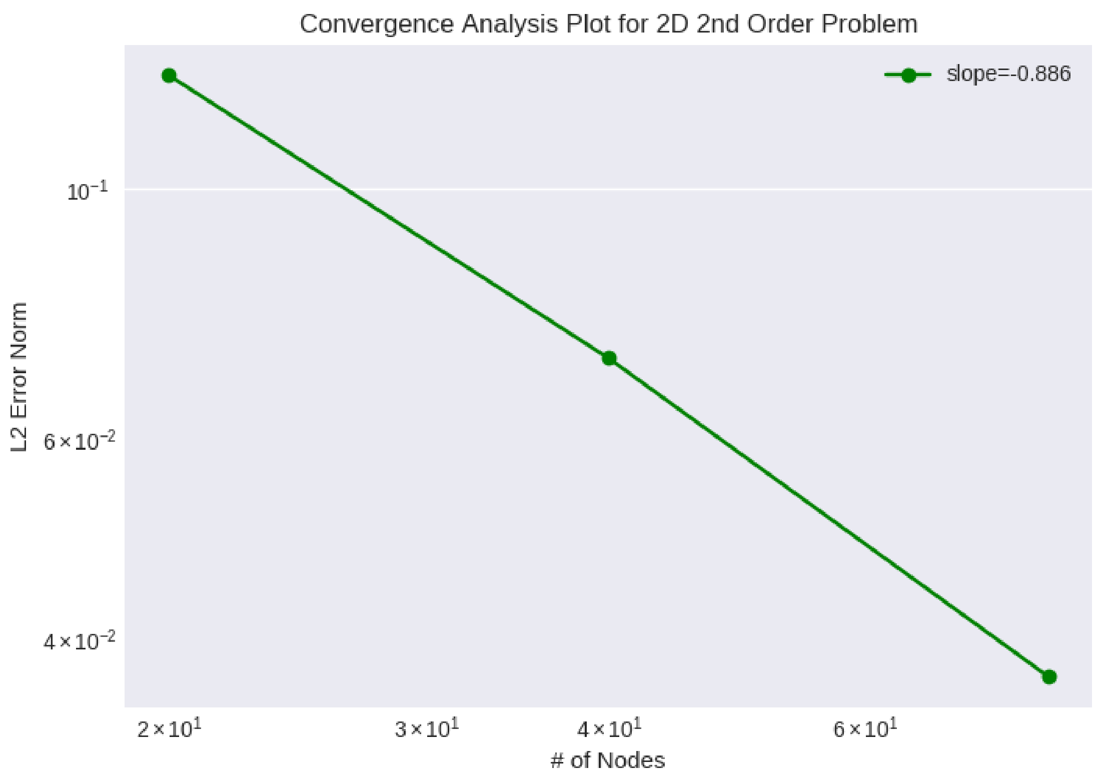


Figure 5: Convergence results for 2D 2nd Order. Not working as expected. Convergence rate is half that of theoretical expectation.

5 Problem Setup

5.1 Governing Equations

5.1.1 One Dimensional Case

In one dimension, the governing equation is

$$-k\frac{\partial^2 T(x)}{\partial x^2} = q(x) \tag{1}$$

5.1.2 Two Dimensional Case

In two dimensions, the governing equation is

$$-k\nabla^2 T(x,y) = q(x,y) \tag{2}$$

Table 3: Timing results for 2D convergence testing w/ Gauss-Seidel

n	input	assemble	solve	total
20	7.1e-3	5.3e-3	9.3e-2	1.1e0
40	3.5e-3	1.4e-2	6.3e0	6.3e0
80	2.9e-3	2.2e-1	4.4e2	4.4e2

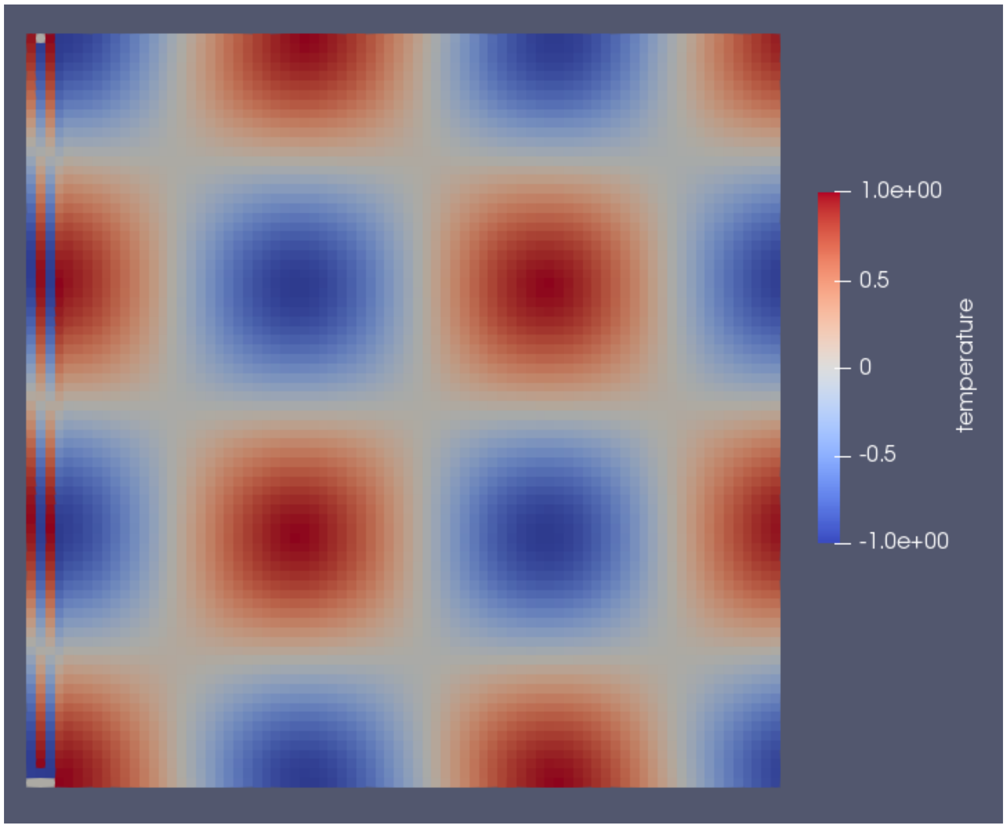


Figure 6: Plot of scalar temperature field for a 2D MASA verification problem. 80 nodes used in the finite difference solution.

5.2 Nomenclature

5.2.1 One Dimensional Case

- $q(x)$: Heat flux at spatial coordinate location x
- x: Spatial coordinate in 1D
- $T(x)$: Temperature of material at spatial coordinate location x
- k: Material thermal conductivity

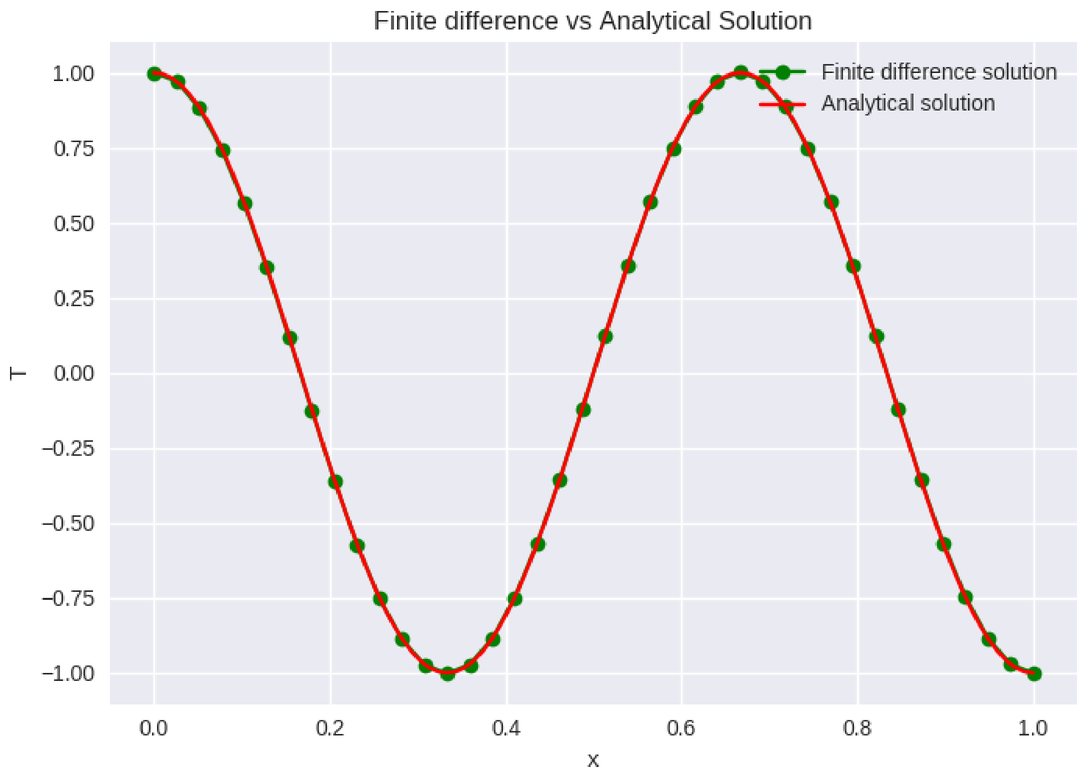


Figure 7: Plot of scalar temperature field for a 1D MASA verification problem. 80 nodes used in the finite difference solution.

5.2.2 Two Dimensional Case

- $q(x, y)$: Heat flux at spatial coordinate location (x, y)
- x: Spatial coordinate in first dimension.
- y: Spatial coordinate in second dimension
- $T(x, y)$: Temperature of material at spatial coordinate location (x, y)
- k: Material thermal conductivity
- ∇: Gradient operator in 2D Cartesian coordinates

5.3 Boundary Conditions

5.3.1 One Dimensional Case

- $T(x = 0)$: **Required:** Temperature at spatial location $x = 0$.

- $T(x = 1)$: **Required:** Temperature at spatial location $x = 1$.
- $q(x)$: **Optional:** Heat flux at spatial coordinate location x

5.3.2 Two Dimensional Case

- $T(x = 0, y)$: **Required:** Temperature at spatial boundary $(x = 0, y)$.
- $T(x = 1, y)$: **Required:** Temperature at spatial boundary $(x = 1, y)$.
- $T(x, y = 0)$: **Required:** Temperature at spatial boundary $(x, y = 0)$.
- $T(x, y = 1)$: **Required:** Temperature at spatial boundary $(x, y = 1)$.
- $q(x, y)$: **Optional:** Heat flux at spatial coordinate location (x, y)

5.4 Constitutive Inputs

5.4.1 One Dimensional Case

- k: **Required:** Material thermal conductivity. Assumed homogeneous across the material domain

5.4.2 Two Dimensional Case

- k **Required:** Material thermal conductivity. Assumed homogeneous across the material domain

6 Assumptions

6.1 One Dimensional Case

- The problem domain is on the interval $\Omega = x \in [0, 1]$.
- The boundary conditions are restricted to Dirichlet types, i.e. only temperature can be specified at the domain boundaries, not heat flux.
- Further, these Dirichlet boundary conditions are given, i.e. temperature at mesh nodes on the boundary are specified
- The material thermal conductivity is constant over the domain
- Mesh step size ($\Delta x = h$) is uniform, i.e. no refinement near boundaries, source terms, etc.

6.2 Two Dimensional Case

- The problem domain is the unit square $\Omega = (x, y) \in [0, 1] \times [0, 1]$
- The boundary conditions are restricted to Dirichlet types, i.e. only temperature can be specified at the domain boundaries, not heat flux.
- Further, these Dirichlet boundary conditions are given, i.e. temperature at mesh nodes on the boundary are specified
- The material thermal conductivity is constant over the domain
- Mesh step size ($\Delta x = \Delta y = h$) is uniform, i.e. no refinement near boundaries, source terms, etc.

7 Numerics

7.1 Finite Difference

7.1.1 One Dimensional Case

2nd Order Finite Difference in One Dimension

$$\frac{\partial^2 T(x)}{\partial x^2} = \frac{T(x_{i+1}) - 2T(x_i) + T(x_{i-1})}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{\partial^4 T(x)}{\partial x^4}|_{x_i} + ... \tag{3}$$

Expansion of 1D Heat Equation with 2nd Order Finite Difference

$$-k\frac{T(x_{i+1}) - 2T(x_i) + T(x_{i-1})}{\Delta x^2} = q(x_i) \tag{4}$$

4th Order Finite Difference in One Dimension

$$\frac{\partial^2 T(x)}{\partial x^2} = \frac{-T(x_{i+2}) + 16T(x_{i+1}) - 30T(x_i) + 16T(x_{i-1}) - T(x_{i-2})}{12\Delta x^2} - \frac{\Delta x^4}{90}\frac{\partial^6 T(x)}{\partial x^6}|_{x_i} + ... \tag{5}$$

Expansion of 1D Heat Equation with 4th Order Finite Difference

$$-k\frac{-T(x_{i+2}) + 16T(x_{i+1}) - 30T(x_i) + 16T(x_{i-1}) - T(x_{i-2})}{12\Delta x^2} = q(x_i) \tag{6}$$

7.1.2 Two Dimensional Case

Finite difference formulas for the second order partial derivatives are the same as in the 1D case. The difference is that there are now two of the terms (one for each spatial direction) in the discrete form of the governing equation

2D Heat Equation with 2nd Order Finite Difference

$$-k\Big(\frac{T(x_{i+1},y_j)-2T(x_i,y_j)+T(x_{i-1},y_j)}{\Delta x^2}+\frac{T(x_i,y_{j+1})-2T(x_i,y_j)+T(x_i,y_{j-1})}{\Delta y^2}\Big)=q(x_i,y_i) \quad (7)$$

2D Heat Equation with 4th Order Finite Difference

$$-k\Big(\frac{-T(x_{i+2},y_j)+16T(x_{i+1},y_j)-30T(x_i,y_j)+16T(x_{i-1},y_j)-T(x_{i-2},y_j)}{12\Delta x^2}+\frac{-T(x_i,y_{j+2})+16T(x_i,y_{j+1})-30T(x_i,y_j)+16T(x_i,y_{j-1})-T(x_i,y_{j-2})}{12\Delta y^2}\Big)=q(x_i,y_j) \quad (8)$$

7.2 Meshing

7.2.1 General Notes

- Mesh is grid based

7.2.2 1D Problem

Mesh and finite difference stencil details can be found in Fig. 8

7.2.3 2D Problem

Mesh details can be found in Fig. 9

Finite difference stencil details can be found in Fig. 10

7.3 Linear System

7.3.1 1D Problem

2nd Order Finite Difference The resulting system of equations has the form

$$2T(x_1)-T(x_2)=\frac{h^2}{k}(q(x_1))+T(x_0) \quad (9)$$

$$-T(x_1)+2T(x_2)-T(x_3)=\frac{h^2}{k}q(x_2) \quad (10)$$

$$\vdots \quad (11)$$

$$2T(x_{n_x-1})-T(x_{n_x-2})=\frac{h^2}{k}(q(x_{n_x-1}))+T(x_{n_x}) \quad (12)$$

$$(13)$$

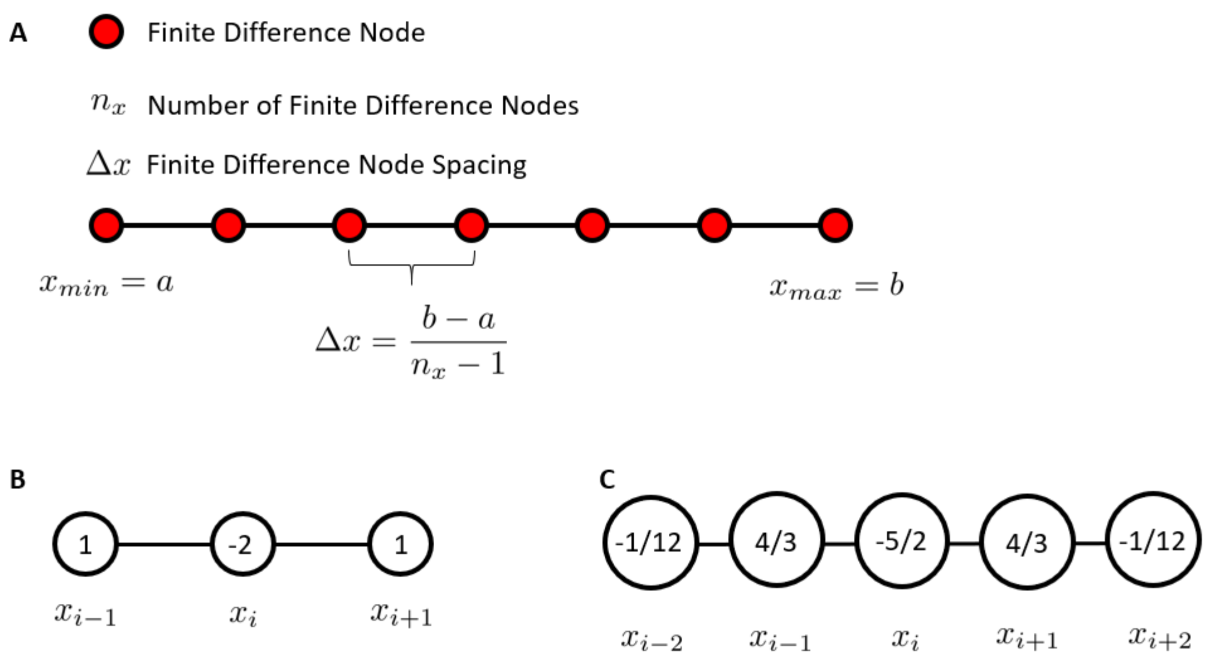


Figure 8: Finite difference mesh and stencil details for the 1D Heat Equation problem. A) Mesh details. B) Stencil for 2nd order finite difference. C) Stencil for 4th order finite difference.

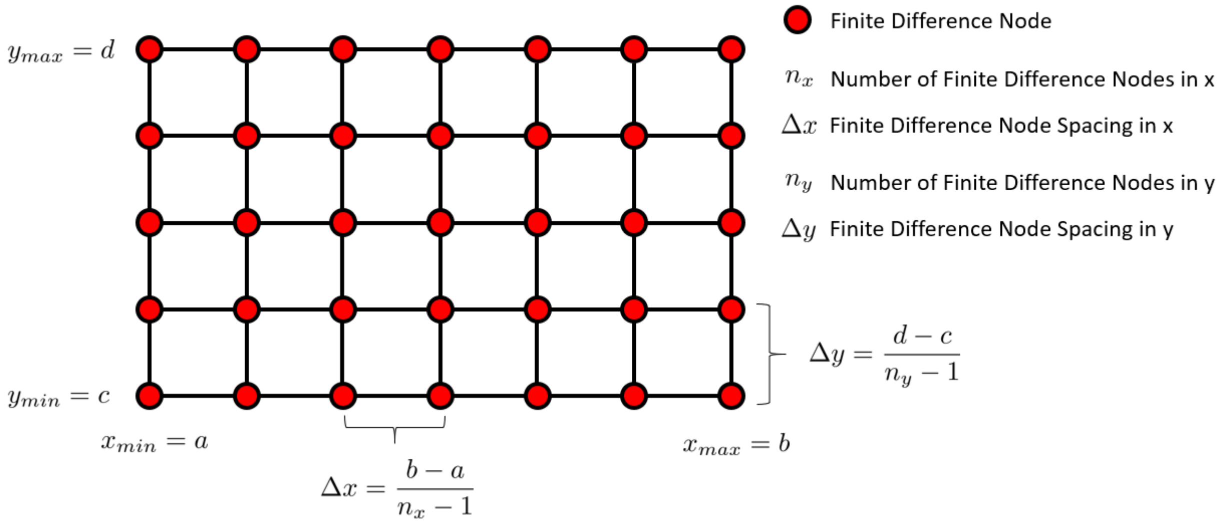
The resulting matrix equation is $AT = Q$ with $A \in \mathbb{R}^{n_x n_y \times n_x n_y}$ given by the matrix

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 & \dots & & 0 \\ -1 & 2 & -1 & 0 & \dots & & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & 0 \\ & & & -1 & 2 & -1 & 0 \\ 0 & \dots & \dots & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & \dots & 0 & -1 & 2 \end{bmatrix}$$

and the RHS vector, $Q \in \mathbb{R}^{n_x}$ by

$$Q = \begin{bmatrix} \frac{h^2}{k} q(x_1) + T(x_0) \\ \frac{h^2}{k} q(x_2) \\ \vdots \\ \frac{h^2}{k} q(x_{n_x - 2}) \\ \frac{h^2}{k} q(x_{n_x - 1}) + T(x_{n_x}) \end{bmatrix}$$

The sparsity of the matrix A is visualized in Fig. 11. There are typically 3 non-zero entries for a interior element row



$y_{max} = d$
$y_{min} = c$
$x_{min} = a$
$x_{max} = b$
$\Delta x = \frac{b-a}{n_x - 1}$
$\Delta y = \frac{d-c}{n_y - 1}$
● Finite Difference Node
n_x Number of Finite Difference Nodes in x
Δx Finite Difference Node Spacing in x
n_y Number of Finite Difference Nodes in y
Δy Finite Difference Node Spacing in y

Figure 9: Finite difference mesh details for the 2D Heat Equation problem.

4th Order Finite Difference The resulting system of equations has the form

$$
\begin{aligned}
2T(x_1) - T(x_2) &= \frac{h^2}{k}(q(x_1)) + T(x_0) \\
-\frac{4}{3}T(x_1) + \frac{5}{2}T(x_2) - \frac{4}{3}T(x_3) + \frac{1}{12}T(x_4) &= \frac{h^2}{k}(q(x_2)) - \frac{1}{12}T(x_0) \\
\frac{1}{12}T(x_1) - \frac{4}{3}T(x_2) + \frac{5}{2}T(x_3) - \frac{4}{3}T(x_4) + \frac{1}{12}T(x_5) &= \frac{h^2}{k}q(x_3) \\
&\vdots \\
\frac{1}{12}T(x_{n_x-5}) - \frac{4}{3}T(x_{n_x-4}) + \frac{5}{2}T(x_{n_x-3}) - \frac{4}{3}T(x_{n_x-2}) + \frac{1}{12}T(x_{n_x-1}) &= \frac{h^2}{k}q(x_{n_x-3}) \\
-\frac{4}{3}T(x_{n_x-3}) + \frac{5}{2}T(x_{n_x-2}) - \frac{4}{3}T(x_{n_x-1}) + \frac{1}{12}T(x_{n_x-4}) &= \frac{h^2}{k}(q(x_{n_x-2})) - \frac{1}{12}T(x_{n_x}) \\
2T(x_{n_x-1}) - T(x_{n_x-2}) &= \frac{h^2}{k}(q(x_{n_x-1})) + T(x_{n_x})
\end{aligned}
\tag{14}
$$

where second order finite difference approximations are used on the first interior boundary nodes to deal with the fact that in those locations the 4th order approximations require information from nodes that do not exist.

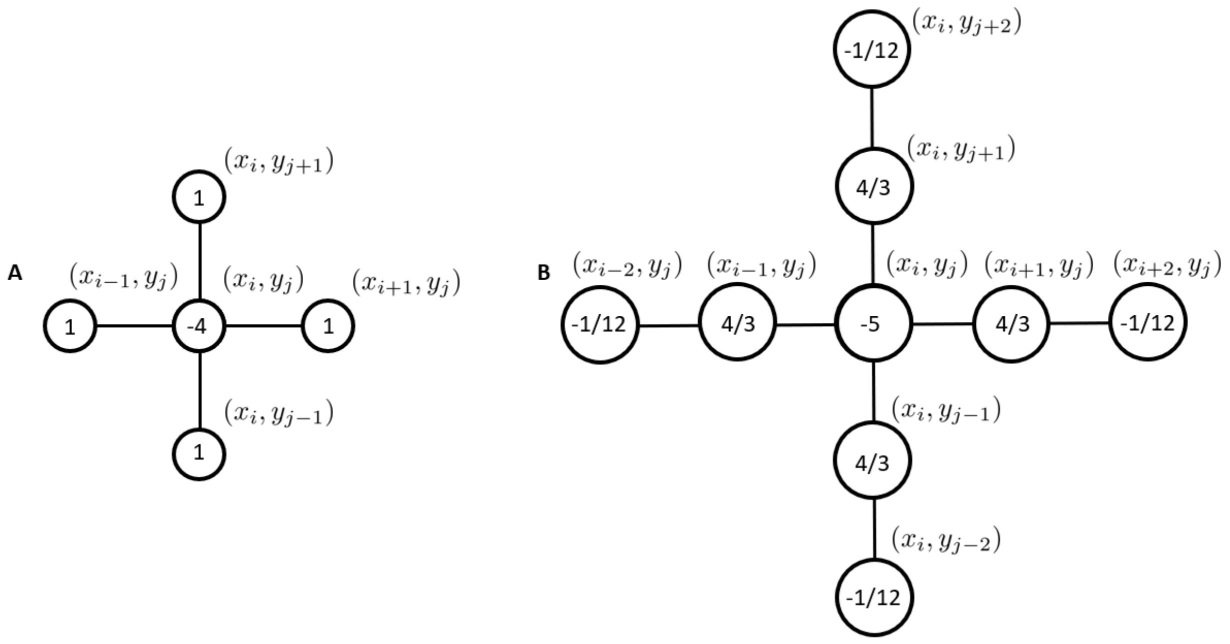


Figure 10: Finite difference mesh details for the 2D Heat Equation problem.

The resulting linear system of equations is $AT = Q$ with $A \in \mathbb{R}^{n_x n_y \times n_x n_y}$ given by the matrix

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 & \dots & & & 0 \\ -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \dots & & 0 \\ \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \dots & 0 \\ 0 & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} \\ 0 & \dots & \dots & 0 & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} \\ 0 & \dots & & & \dots & 0 & -1 & 2 \end{bmatrix}$$

and the RHS vector, $Q \in \mathbb{R}^{n_x}$ by

$$Q = \begin{bmatrix} \frac{h^2}{k} q(x_1) + T(x_0) \\ \frac{h^2}{k} q(x_2) - \frac{1}{12} T(x_0) \\ \frac{h^2}{k} q(x_3) \\ \vdots \\ \frac{h^2}{k} q(x_{n_x-3}) \\ \frac{h^2}{k} q(x_{n_x-2}) - \frac{1}{12} T(x_{n_x}) \\ \frac{h^2}{k} q(x_{n_x-2}) + T(x_{n_x}) \end{bmatrix}$$

The sparsity of the matrix A is visualized in Fig. 12. There are typically 5 non-zero entries for a interior element row

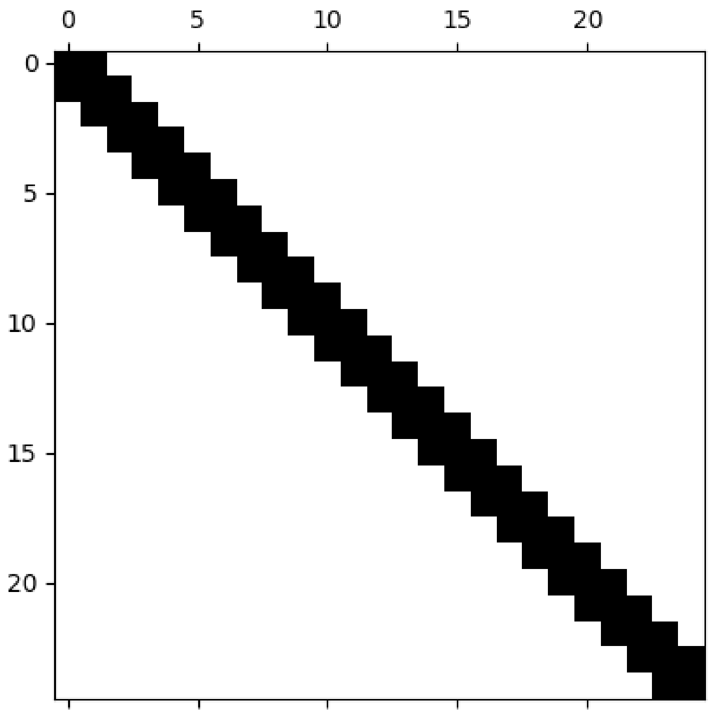


Figure 11: Sparsity of problem system in 1D and 2nd order finite difference for an example 25 degrees of freedom system. Blocks in black indicate non-zero entries

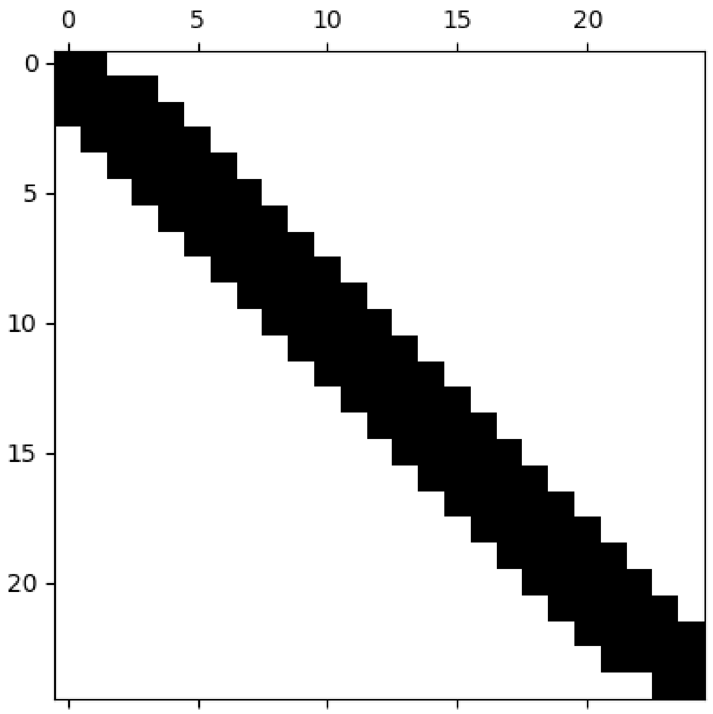


Figure 12: Sparsity of problem system in 1D and 4th order finite difference for an example 25 degrees of freedom system. Blocks in black indicate non-zero entries

7.3.2 2D Problem

2nd Order Finite Difference The resulting system of equations has the form (stepping through x first) and is a simple extension of the 1D problem.

$$\begin{aligned}
4T(x_1, y_1) - T(x_2, y_1) &= \frac{h^2}{k}(q(x_1, y_1)) + T(x_0, y_1) \\
-T(x_1, y_1) + 4T(x_2, y_1) - T(x_3, y_1) &= \frac{h^2}{k}q(x_2, y_1) \\
&\vdots \\
4T(x_{n_x-1}, y_1) - T(x_{n_x-2}, y_1) &= \frac{h^2}{k}(q(x_{n_x-1}, y_1)) + T(x_{n_x}, y_1) \qquad (15) \\
&\vdots \\
4T(x_1, y_2) - T(x_2, y_2) &= \frac{h^2}{k}(q(x_1, y_2)) + T(x_0, y_2) \\
&\vdots \\
4T(x_{n_x-1}, y_2) - T(x_{n_x-2}, y_2) &= \frac{h^2}{k}(q(x_{n_x-1}), y_2) + T(x_{n_x}, y_2)
\end{aligned}$$

The resulting linear system of equations is $AT = Q$ with $A \in \mathbb{R}^{n_x n_y \times n_x n_y}$ given by the block, tridiagonal matrix

$$A = \begin{bmatrix} S & -I & & & & \\ -I & S & -I & & & \\ & -I & S & -I & & \\ & & \ddots & \ddots & \ddots & \\ & & & -I & S & -I \\ & & & & -I & S \end{bmatrix} S \in \mathbb{R}^{n_x \times n_x} = \begin{bmatrix} 4 & -1 & 0 & 0 & \dots & & 0 \\ -1 & 4 & -1 & 0 & \dots & & 0 \\ 0 & -1 & 4 & -1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & 0 \\ & & & -1 & 4 & -1 & 0 \\ 0 & \dots & \dots & 0 & -1 & 4 & -1 \\ 0 & \dots & \dots & \dots & 0 & -1 & 4 \end{bmatrix}$$

and I is the identity matrix in $\mathbb{R}^{n_x \times n_x}$. The RHS vector, $Q \in \mathbb{R}^{n_x n_y}$ is

$$Q = \begin{bmatrix} \frac{h^2}{k} q(x_1, y_1) + T(x_0, y_1) \\ \frac{h^2}{k} q(x_2, y_1) \\ \vdots \\ \frac{h^2}{k} q(x_{n_x-2}, y_1) \\ \frac{h^2}{k} q(x_{n_x-1}, y_1) + T(x_{n_x}, y_1) \\ \vdots \frac{h^2}{k} q(x_1, y_1) + T(x_0, y_2) \\ \frac{h^2}{k} q(x_2, y_2) \\ \vdots \\ \frac{h^2}{k} q(x_{n_x-2}, y_2) \\ \frac{h^2}{k} q(x_{n_x-1}, y_2) + T(x_{n_x}, y_2) \end{bmatrix}$$

The sparsity of the matrix A is visualized in Fig. 13. There are typically 5 non-zero entries for a interior element row

4th Order Finite Difference As in the 2nd order case, the resulting system of equations has form that is a simple extension of the 1D problem. The resulting linear system of equations is $AT = Q$ with $A \in \mathbb{R}^{n_x n_y \times n_x n_y}$ given by the block, tridiagonal matrix

$$A = \begin{bmatrix} S & -I & & & & \\ -I & S & -I & & & \\ & -I & S & -I & & \\ & & \ddots & \ddots & \ddots & \\ & & & -I & S & -I \\ & & & & -I & S \end{bmatrix} S \in \mathbb{R}^{n_x \times n_x} = \begin{bmatrix} 4 & -1 & 0 & 0 & \dots & & & 0 \\ -\frac{4}{3} & 5 & -\frac{4}{3} & \frac{1}{12} & 0 & \dots & & 0 \\ \frac{1}{12} & -\frac{4}{3} & 5 & -\frac{4}{3} & \frac{1}{12} & 0 & \dots & 0 \\ 0 & \frac{1}{12} & -\frac{4}{3} & 5 & -\frac{4}{3} & \frac{1}{12} & 0 & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & \frac{1}{12} & -\frac{4}{3} & 5 & -\frac{4}{3} & \frac{1}{12} \\ 0 & \dots & \dots & 0 & \frac{1}{12} & -\frac{4}{3} & 5 & -\frac{4}{3} \\ 0 & \dots & & & \dots & 0 & -1 & 4 \end{bmatrix}$$

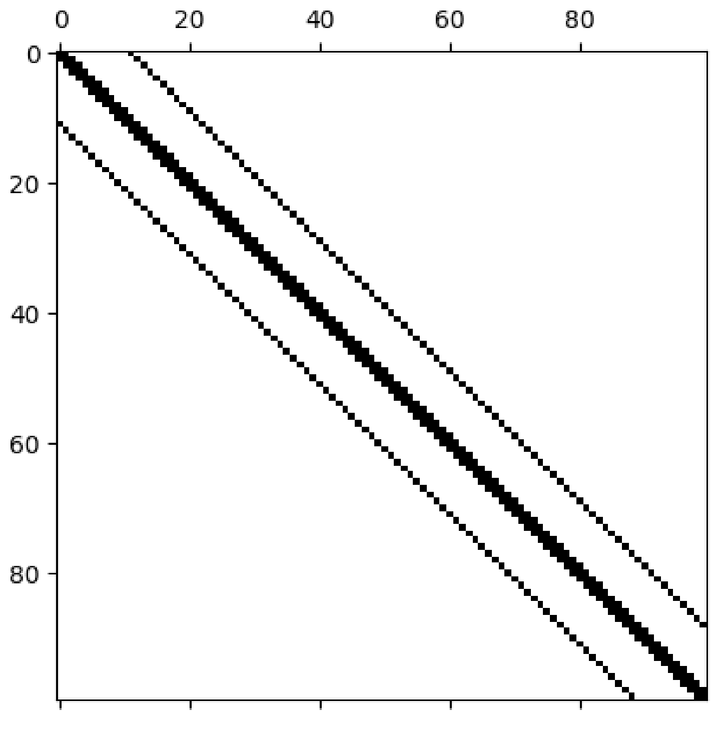


Figure 13: Sparsity of problem system in 2D and 2nd order finite difference for an example 10 x 10 degrees of freedom system. Blocks in black indicate non-zero entries

and I is the identity matrix in $\mathbb{R}^{n_x \times n_x}$. The RHS vector, $Q \in \mathbb{R}^{n_x n_y}$ is

$$Q = \begin{bmatrix} \frac{h^2}{k}q(x_1, y_1) + T(x_0, y_1) \\ \frac{h^2}{k}q(x_2, y_1) - \frac{1}{12}T(x_0, y_1) \\ \frac{h^2}{k}q(x_3, y_1) \\ \vdots \\ \frac{h^2}{k}q(x_{n_x-3}, y_1) \\ \frac{h^2}{k}q(x_{n_x-2}, y_1) - \frac{1}{12}T(x_{n_x}, y_1) \\ \frac{h^2}{k}q(x_{n_x-2}, y_1) + T(x_{n_x}, y_1) \\ \frac{h^2}{k}q(x_1, y_2) + T(x_0, y_2) \\ \frac{h^2}{k}q(x_2, y_2) - \frac{1}{12}T(x_0, y_2) \\ \frac{h^2}{k}q(x_3, y_2) \\ \vdots \\ \frac{h^2}{k}q(x_{n_x-3}, y_2) \\ \frac{h^2}{k}q(x_{n_x-2}, y_2) - \frac{1}{12}T(x_{n_x}, y_2) \\ \frac{h^2}{k}q(x_{n_x-2}, y_2) + T(x_{n_x}, y_2) \end{bmatrix}$$

The sparsity of the matrix A is visualized in Fig. 14. There are typically 7 non-zero entries for a interior element row

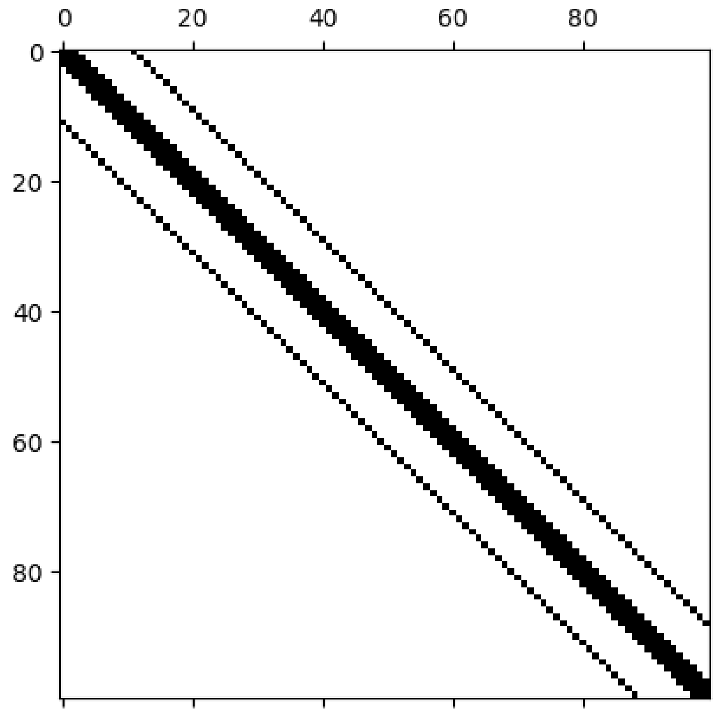


Figure 14: Sparsity of problem system in 2D and 4th order finite difference for an example 10 x 10 degrees of freedom system. Blocks in black indicate non-zero entries

7.4 Solvers

7.4.1 Jacobi

Algorithm Outline Given $Ax = B$, decompose A into $A = D + R$ with D being the diagonal and R the off diagonal terms. Solve for next iterative guess of x via

$$x^{k+1} = D^{-1}(b - Rx^k) \tag{16}$$

and terminate when difference norm term $||x^k - x^{k-1}||$ falls below user specified tolerance ϵ. User must also specify an initial guess x^0.

Psuedo-Code

```
$k = 0$;
error = $||b - Ax^{(k)}||_2$ ;
**while** *error* $>$ *epsilon* **do**
    **for** $i = 1$ **to** $n$ **do**
        $\sigma = 0$;
        **for** $j = 1$ **to** $n$ **do**
            **if** $j \neq i$ **then**
                $\sigma = \sigma + a_{ij}x_j^{(k)}$;
            **end**
        **end**
        $x_i^{(k+1)} = \frac{1}{a_{ii}}(b_i - \sigma)$ ;
    **end**
    $k = k + 1$ ;
    error = $||b - Ax^{(k+1)}||_2$ ;
**end**
```

7.4.2 Gauss-Seidel

Algorithm Outline Given $Ax = B$, decompose A into $A = L + R$ with L being lower triangular and U upper triangular. Solve for next iterative guess of x via

$$x^{k+1} = L^{-1}(b - Ux^k) \tag{17}$$

and terminate when difference norm term $||x^k - x^{k-1}||$falls below user specified tolerance ϵ. Note, this method only requires storage of a single vector sized to the number of variables, whereas the Jacobi requires storage of two such vecotrs. User must also specify an initial guess ϕ.

Psuedo-Code

```
error = $||b - A\phi||_2$ ;
**while** *error* $>$ *epsilon* **do**
    **for** $i = 1$ **to** $n$ **do**
        $\sigma = 0$;
        **for** $j = 1$ **to** $n$ **do**
            **if** $j \neq i$ **then**
                $\sigma = \sigma + a_{ii}\phi_j$;
            **end**
        **end**
        $\phi_i = \frac{1}{a_{ii}}(b_i - \sigma)$ ;
    **end**
    error = $||b - A\phi||_2$ ;
**end**
```

7.5 Memory Considerations

A conservative memory estimate would be to calculate the memory required to store each element of the matrix A and vectors T, Q in double precision floating point as a function of the problem size. Count the T vector twice to accommodate the need to store two of these vectors if using Jacobi solution method. Note, the storage could be vastly improved if matvec storage is used for A.

7.5.1 1D Problem

- A: $n_x \times n_x$ floating point numbers
- Q: n_x floating point numbers
- T: n_x floating point numbers

Total Floating Point Numbers: $n_x^2 + 3n_x$

Memory estimation: 64 bits $* (n_x^2 + 3n_x)$

7.5.2 2D Problem

- A: $n_x n_y \times n_x n_y$ floating point numbers
- Q: $n_x n_y$ floating point numbers
- T: $n_x n_y$ floating point numbers

Total Floating Point Numbers: $(n_x n_y)^2 + 3(n_x n_x)$

Memory estimation: 64 bits $* ((n_x n_y)^2 + 3(n_x n_x))$