FYS3150 Computational Physics - Project 1

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A look at different algorithms for solving a second-order differential equation with a known analytical solution, comparing both their speed and accuracy. Found that a specialized algorithm implemented in an efficient manner can speed up the computation significantly.

INTRODUCTION

THEORY, ALGORITHMS AND METHODS

We have second order inhomogeneous differential equation, Eqn. 1

$$\frac{d^2u(x)}{dx^2} = f(x) \tag{1}$$

With boundary conditions $\ddot{u}(x) = f(x)$, $u(0) = u(1) = 0$ and $x \in (0, 1)$.

If we let $f(x) = 100e^{-10x}$, then it can be shown analytically that the differential equation has a solution Eqn. 2

$$u(x) = 1 - (1 - e^{-10})x - e^{-10x} \tag{2}$$

This problem can also be solved numerically by discretization. By the use of taylor expansions, it can be shown that there is a discrete, iterative solution in the form Eqn. 3 [1]

$$-\frac{v_{i+1} + v_{i-1} + 2v_i}{h^2} = f_i \tag{3}$$

where $h = 1/(n + 1)$ is the step size for $n + 1$ points.

This problem can be written in the form

$$A\vec{v} = \vec{b} \tag{4}$$

Where A $\in R^{n\times n}$ is a tridiagonal matrix with diagonal elements 2 and -1 (Eqn. 5) and $\vec{b} = h^2(f_1, \dots, f_n)$.

$$A = \begin{bmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & -1 \\ \dots & \dots & \dots & \dots & -1 & 2 \end{bmatrix} \tag{5}$$

By matrix multiplication, when we multiply the i-th row of A by $\vec{v}$, we get

$$\begin{aligned} -1v_{i-1} + 2v_i - 1v_{i+1} &= -(v_{i+1} + v_{i-1} - 2v_i) \\ &= h^2 f_i \end{aligned} \tag{6}$$

Which is equivalent to the discretized differential equation Eqn. 3, showing that the differential equation can be solved as a linear algebra problem rather than iteratively.

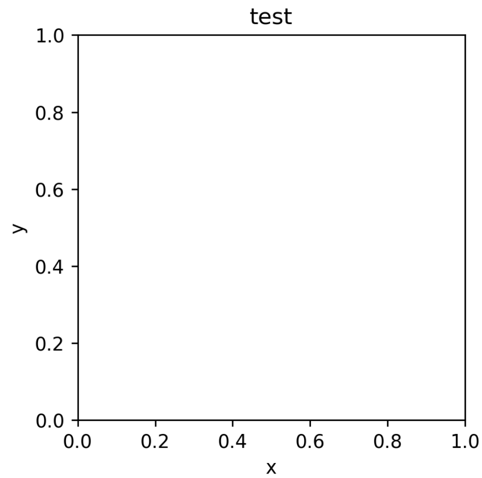

FIG. 1. This is a caption

RESULTS AND DISCUSSIONS

https://github.com/nicholaskarlsen/FYS3150

CONCLUSIONS

[1] M. Hjorth-Jensen, Computational Physics - Lecture Notes 2015, (2015).