ME614 Fall 2018 - Homework 1

Spatial Discretization

(Due September 19, 2018)

Please submit your homework on Blackboard in the form of a (1) report in PDF (keep file size smaller than 5MB) and (2) a working code, zipped in one file. The submitted code needs to run and create all (and possibly only) the plots you are including in your report. The use of LaTeX for your report is strongly recommended (but not required) and you can start with a template from http://www.latextemplates.com/. Discussions and sharing of ideas are encouraged but individually prepared submissions (codes, figures, written reports, etc.) are required. Due to the sensitivity of some numerical results to the specific coding choices, and sometimes even hardware, it is easy for the instructor to flag homeworks as suspicious. A plagiarism detection algorithm will be run against all codes submitted. Do NOT include in your submisison any files that are not required (e.g. the syllabus, zip files with python libraries, other PDFs, sample python sessions etc).

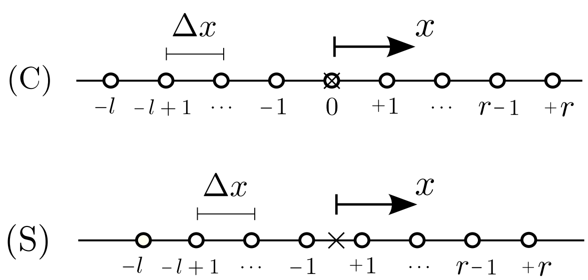
Points will be deducted from late submissions at a rate of 20% of the overall homework value per day late. Homeworks are due at 11:59 PM of the due date.

Problem 1

With the use of explicitly evaluated Lagrangian polynomials, consider the numerical approximation of the first derivative of the function

$$f(x) = \tanh(x)\sin(5x + 1.5) \tag{1}$$

at $x = 0$ (indicated with an '×') with the uniformly spaced computational stencils shown below.



	centered	biased
(C)	$l = r = 1$	$l = 0,\ r = 1$
(C)	$l = r = 2$	$l = 0,\ r = 2$
(C)	$l = r = 3$	$l = 0,\ r = 3$
(S)	$l = r = 1$	$l = 1,\ r = 1$
(S)	$l = r = 2$	$l = 1,\ r = 2$
(S)	$l = r = 3$	$l = 1,\ r = 3$

The polynomial interpolant should exploit the full number of points in the stencil (indicated with circles), that is $N = l+r+1$ for the (C) arrangement, and $N = l+r$ for the (S) arrangement, for every given value of l and r. Please perform the following tasks:

(a) Plot a few sample Lagrangian polynomials as done in class for a large and a small value of N; Are there any patterns you are noticing for large values of N that look potentially troublesome?

[5%]

(b) Plot in log-log scale the absolute value of the truncation error, ϵ_{TR} at $x = 0$, versus the inverse of the grid spacing, Δx^{-1}, as the grid is refined ($\Delta x \to 0$), starting with a unitary spacing ($\Delta x = 1.0$). Compare results among all combinations of collocated (C) and staggered (S) arrangements, and centered and biased reconstructions shown in the table above[1]. Plot with a thin dashed line the reference truncation error $\epsilon_{\text{ref}} \propto \Delta x^n$ for various values of n (order of accuracy). Make sure to label the line on the plot with the corresponding value of n.

[20%]

(c) Does the order of accuracy always correspond to the order of the polynomial interpolant? For a given polynomial order, p, what is the minimum and maximum order of accuracy you can achieve when evaluating numerically the first derivative? Briefly discuss by relying on your numerical results from the previous task.

[5%]

[1] The biased case for $l = r = 1$ is not technically biased but it is convenient to define it for scripting purposes.

(d) Pick one of the cases above (staggered or collocated, centered or biased) for a large value of N (at least 4 or 5) and compare the log-log plot of ϵ_{TR} versus Δx^{-1} obtained with the Lagrangian polynomials, as done above, with the (theoretically identical) numerical approximation of the first derivative obtained by constructing the Vandermonde matrix of a polynomial interpolant of $N-1$-th order for the same stencil, inverting it to find the coefficient and *then* evaluating its derivative. Good luck.

[5%]

Problem 2

Perform the following numerical tasks associated with a uniformly-spaced grid with N points discretizing the one-dimensional interval $[x_0, x_{N-1}]$, with x_0 and x_{N-1} fixed and of your choice:

(a) Generate an $N \times N$ discrete numerical operator in the form of a sparse matrix implementing the first and second derivative on said grid, each with second-order and third-order-*accurate* discretization schemes (derived 'by hand' via Taylor-Series expansion). This results in a total of 4 operators. With the `spy` plot function plot the resulting matricial pattern for $N = 10$, for example, and show the analytical derivations to derive the discretization weights. Careful with the end points – that's the tricky part.

[20%]

(b) Solve the following one-dimensional boundary value problem (BVP) in the domain $[x_0, x_{N-1}]$:

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

with the following boundary conditions,

$$\begin{aligned} \widehat{u}_0 &= f(x)\big|_{x=x_0} \\ \left.\widehat{\frac{du}{dx}}\right|_{N-1} &= \left.f^{(1)}(x)\right|_{x=x_L} \end{aligned} \tag{3}$$

where $f^{(n)}(x)$ is the n-th-derivative of an arbitrary function, $f(x)$, of your choice, and 0 and $N-1$ are the first and last points of the computational domain, corresponding to $[x_0, x_{N-1}]$, which are also arbitrary. Please pick a function $f(x)$ with several sign changes (i.e. very wavy) in the interval $[x_0, x_{N-1}]$. Plot the root-mean-square (RMS) of the error[2], $\epsilon = |\hat{u} - f|$, against the inverse of the grid spacing, Δx^{-1} for the *two discretization orders* mentioned in part (a). In other words, tackle the given boundary value problem with second-order and third-order-accurate schemes separately.

[25%]

Problem 3

Let $\{x_i\}$ $\forall i \in \{0, \ldots, N-1\}$ be a collection of (initially) uniformly spaced points, with spacing Δx, discretizing a given one-dimensional interval $[x_0, x_{N-1}]$ in space, with x_0 and x_{N-1} fixed and of your choice. Let $L = x_{N-1} - x_0$ be the length of the domain. Consider the following perturbation applied to all of the grid points:

$$\tilde{x}_i = x_i + \overline{\Delta x}\mathcal{N}(0, \sigma), \forall i \in \{0, \ldots, N-1\} \tag{4}$$

where $\mathcal{N}(0, \sigma)$ is a normal distribution with average 0 and standard deviation σ. Via this relation you can pseudo-randomly create different classes of perturbed grids for different values of σ.

Plot the root-mean-square (RMS) of the error versus the inverse of the characteristic grid spacing $\overline{\Delta x} = L/(N-1)$ (characteristic, as in, independent of σ) on the evaluation of the second derivative on the internal points only with a polynomial-based discretization designed for a non-uniform grid with a second-order-accurate and fourth-order-accurate schemes (separated) for increasing values of σ (say, 10^{-5}, 10^{-3}, 10^{-1})[3]. Please comment briefly on the results you are obtaining, trying to justify them.

[20%]

[2] The root-mean-square is the square root of the integral average (or arithmetic average in this case) over the spatial domain of the squares of the local value of the error. Therefore, you need to make sure you average the square of the local truncation error *first* and then take the square root.

[3] If points cross over each other, reduce the amplitude of the perturbation.

Bonus Questions

You can only pick one of the bonus problems below. Note that you don't need to solve a bonus problem to get 100% on this homework. Each bonus question is worth extra +5% of the total homework value and may be used to replace any items above that have not been (intentionally or non intentionally) addressed. Bonus questions may also be used simply as extra credit, which will count towards the final grade.

Problem A

Solve Problem 2(b) with a spatial discretization based on a Chebyshev grid and Chebyshev polynomials. Comment on the resulting matrix operator, performance of the resulting numerical discretization, etc. compared to what executed in Problem 2(b).

[2.5%]

Augment the results shown in Problem 1(d) with a Discrete-Fourier-Transform (DFT) based discretization over the same stencil.

[2.5%]

Problem B

Consider the (unphysical) boundary layer velocity profile:

$$u(y) = -(1-y)^4 + 1 \tag{5}$$

where $y = 0$ is the wall and $y = 1$ is the boundary layer edge.

Analytically derive the expression of the truncation error ϵ_{TR} as a function of the grid spacing Δy for a uniformly spaced grid of N points discretizing the interval $[0, 1]$ in y for the first derivative and a second-order numerical scheme.

[2.5%]

Analytically derive the grid transformation law that would be needed to redistribute the same amount of grid points in the y direction (perhaps clustering them at the wall) such that ϵ_{TR} is as close as possible to being a uniform function of y and/or it is overall minimized/optimized.

[2.5%]