Report: Homework 1

ME:614

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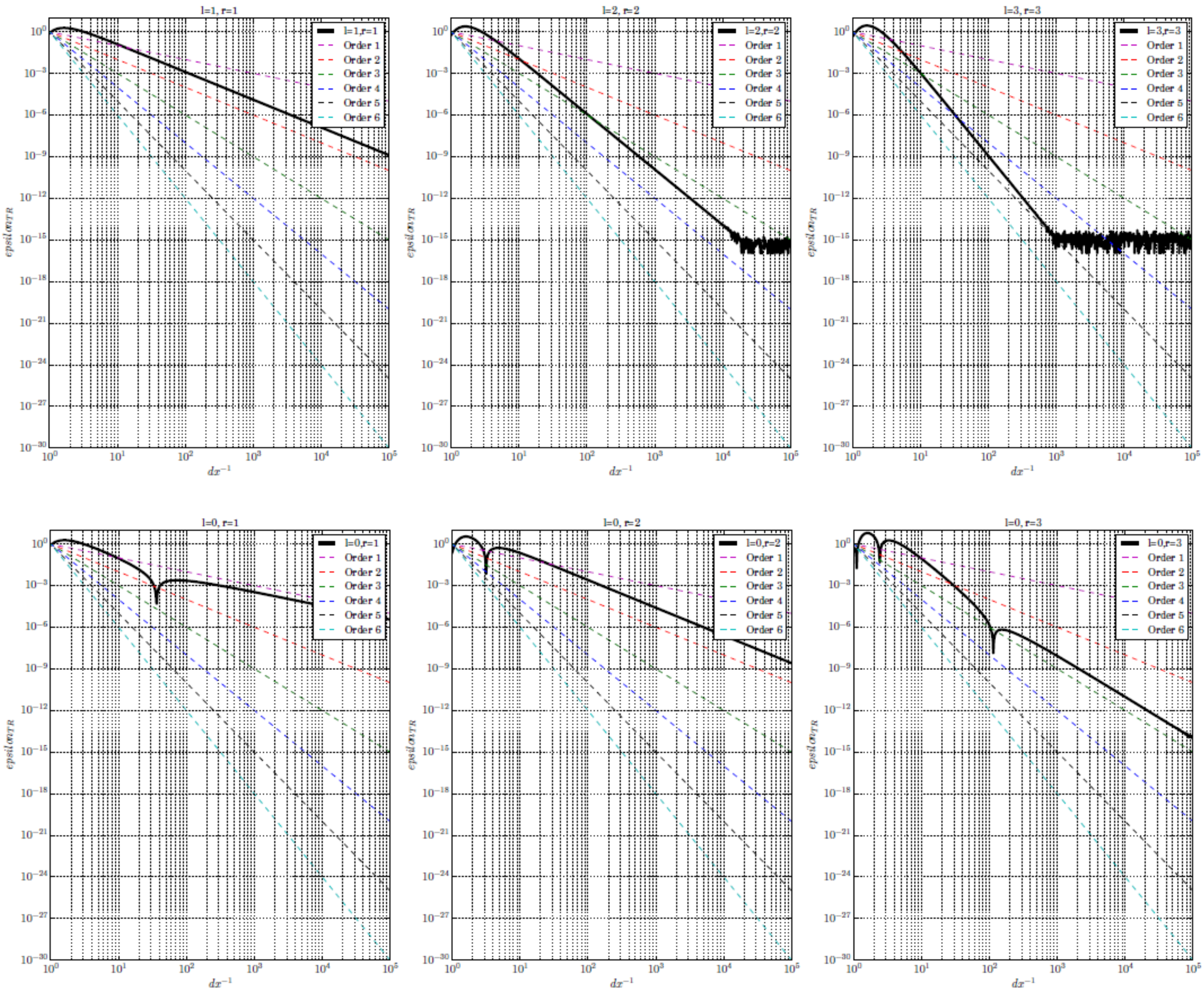
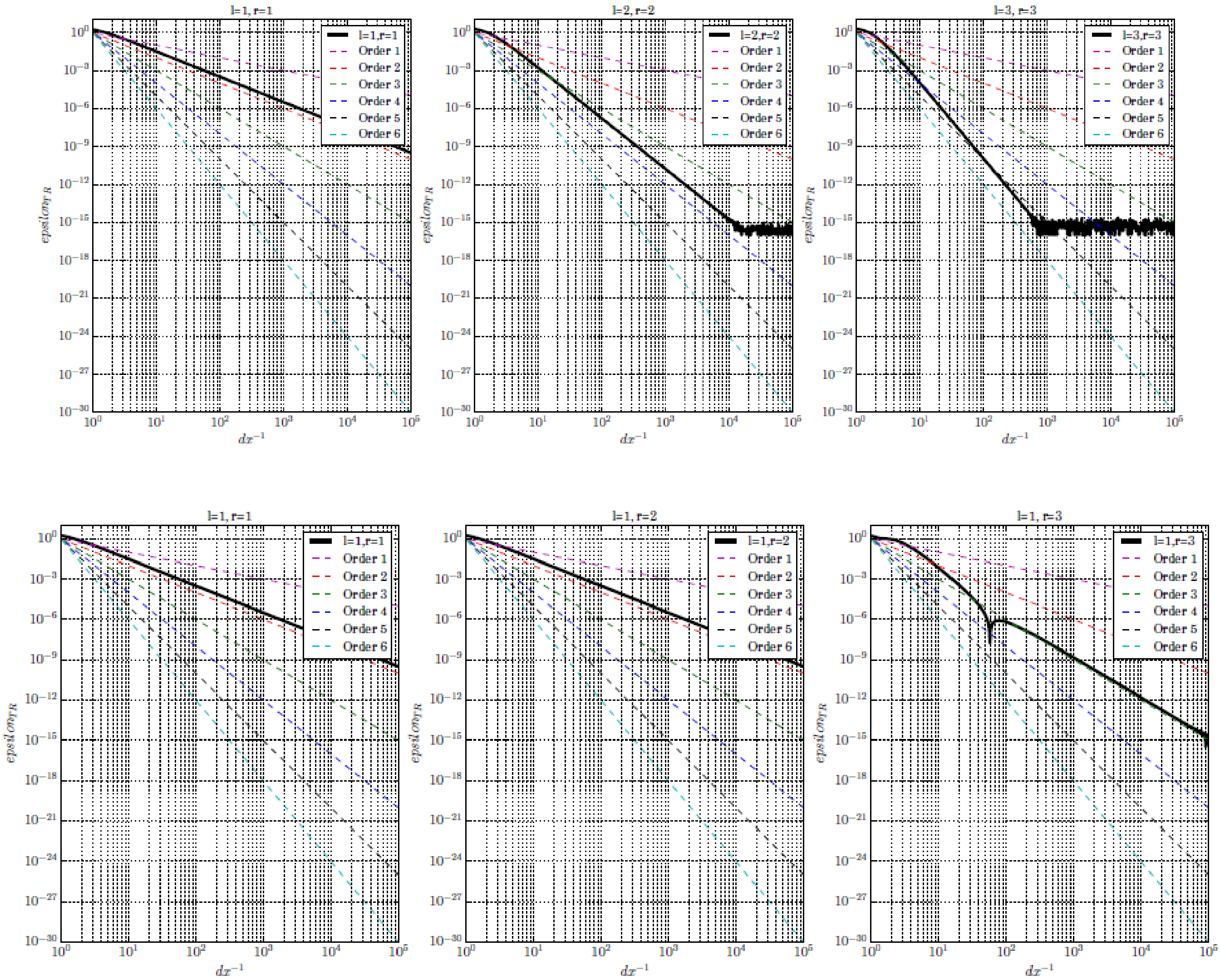
Problem 1

a.) The following plots show the variation of the absolute truncation error with inverse grid spacing for different collocated and staggered schemes:



Absolute truncation error vs inverse grid spacing for collocated schemes



Absolute error vs inverse grid spacing for Staggered schemes

(due to an issue with pasting images from pdfs in word, the pdfs in the report folder give a better view of the plots as compared to the ones in the report)

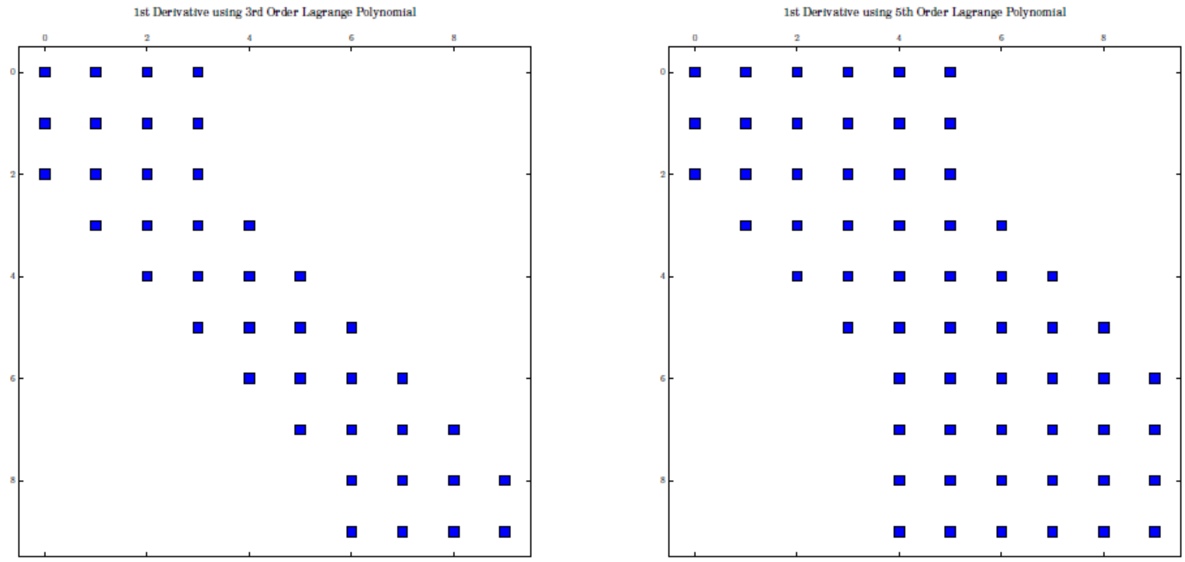
From the plots, we can estimate the following orders of accuracy:

Type of stencil	No. of points	Order of scheme	Degree of polynomial
Collocated scheme	l=1, r=1	2	2
	l=2, r=2	4	4
	l=3, r=3	6	6
	l=0, r=1	1	1
	l=0, r=2	2	2
	l=0, r=3	3	3
Staggered schemes	l=1, r=1	2	1
	l=2, r=2	4	3
	l=3, r=3	6	5
	l=1, r=1	2	1
	l=1, r=2	2	2
	l=1, r=3	3	3

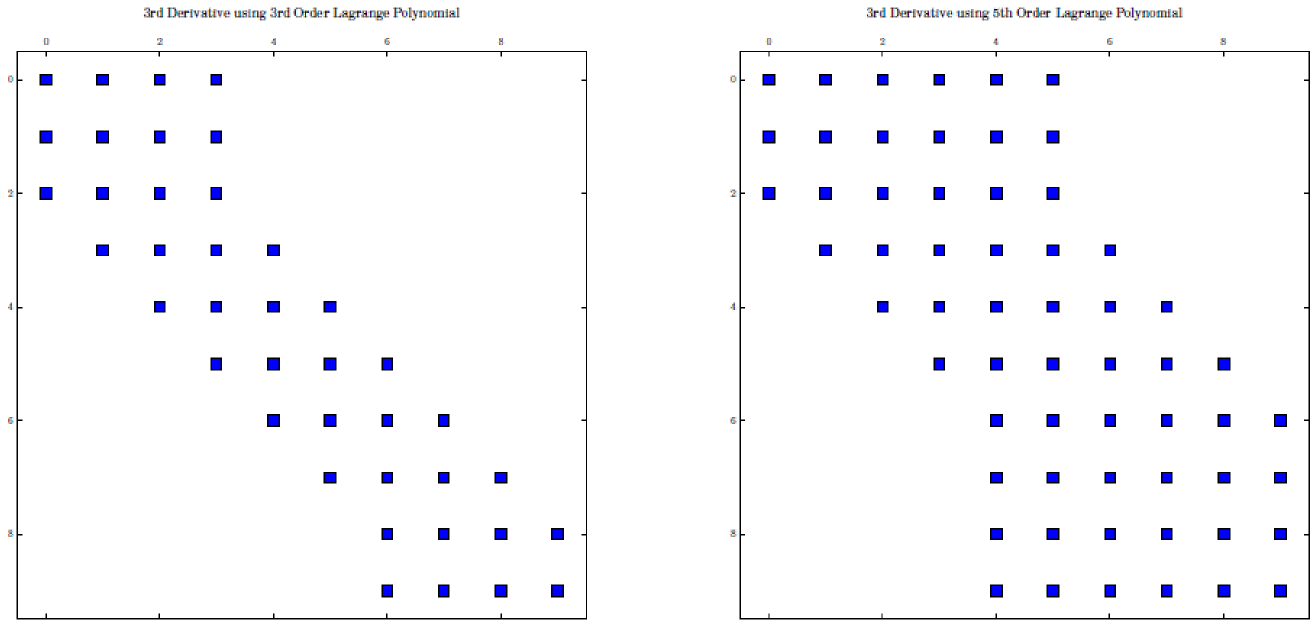
b.) Based on the values above, we can see that the order of the interpolating polynomial is not always equal to the order of accuracy. For staggered unbiased schemes, one can get a higher order of accuracy for a lower order polynomial interpolation.

Problem 2:

a.) The following figure shows the spy plot for the 1^{st} and 3^{rd} derivative operators based on a 3^{rd} and 5^{th} order Lagrange Polynomial reconstruction. A left biased stencil for the 3^{rd} order and a right biased stencil for the 5^{th} order has been used respectively (evident from the spy plot)



Spy plots for 1^{st} derivative



Spy plots for 3^{rd} derivative

b.) The function f(x) chosen is log(x) over (x0, x1) = (15, 1000).

The first and third derivatives are:

$$f^{(3)}(x) = \frac{2}{x^3}$$

$$f^{(1)}(x) = \frac{1}{x}$$

Here, both the 3rd and 5th order operators generated in part a.) have been used. In order to patch the boundary conditions, a 1st order scheme has been used for the derivatives at the edges:

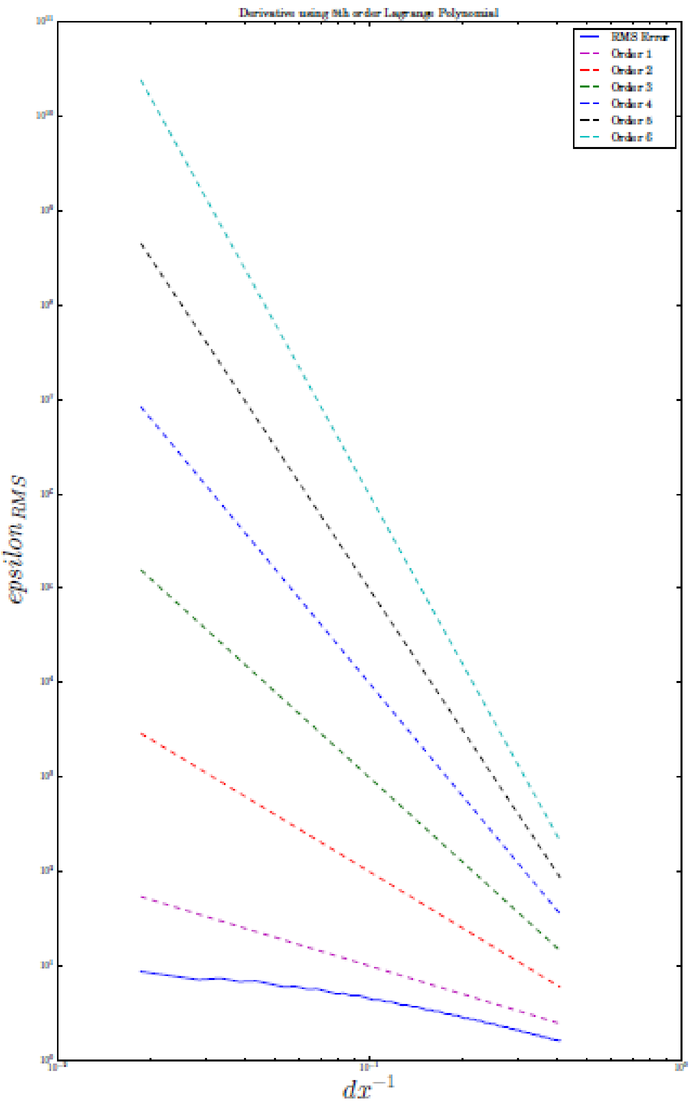
$$f^{(1)}|_{x0} = (f_{x0+\Delta x} - f_{x0})/\Delta$$

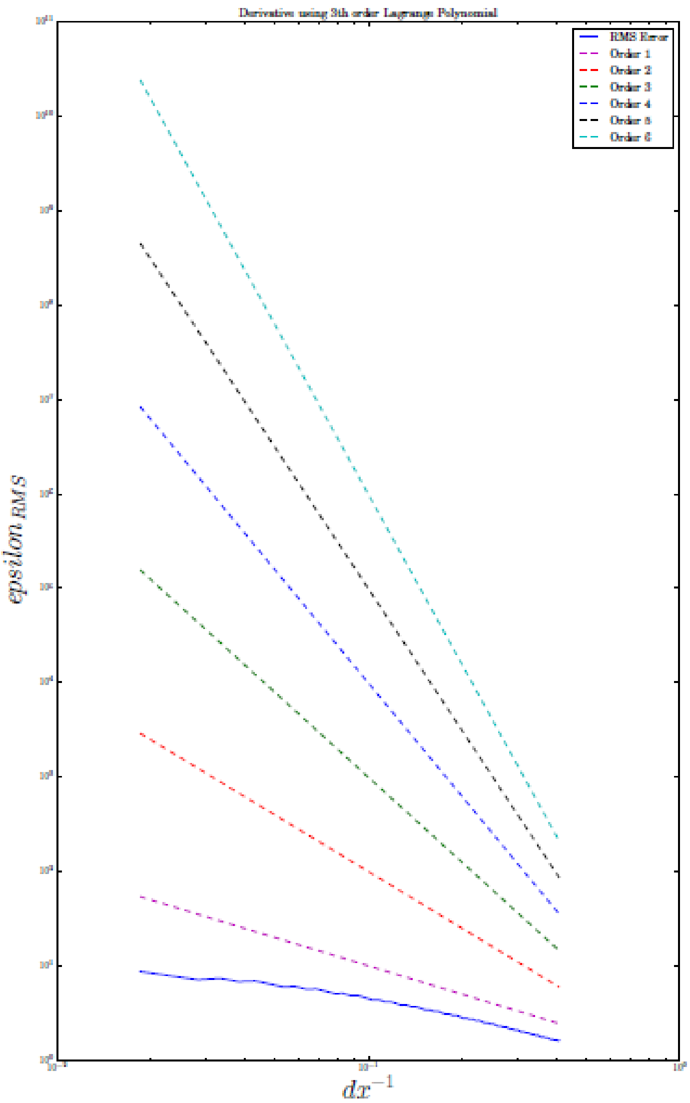
$$f^{(1)}|_{x1} = (f_{x1} - f_{x1-\Delta})/\Delta$$

Where Δ= grid spacing.

(Note: We can also use the 1st and last rows of the 1st order derivative operator generated in 2a, among many other schemes as a means to patch the boundary derivatives, noting the fact that the order of accuracy will be affected accordingly).

The following plot shows the RMS error as a function of the inverse grid spacing:





As seen from the plots, the scheme has effectively been reduced to a 1st order. This implies that the method used to patch the boundary condition does have a significant effect. The effect of patching the derivatives with the operators generated in part 2a might have a significantly different effect (included in the code as a comment but not explicitly studied)

Problem 3:

a.) Derivation of a 4^{th} order Pade' scheme for the 3^{rd} derivative:

From an extension of the expression for 2^{nd} derivative in Lele et. al. (1991), a linear combination of the third derivative of *f* for a 3-point stencil around x_i (i-1, i, i+1 th points) can be expressed as a linear combination of the central difference approximations to the third derivative (d^3f/dx^3) choosing Δ, 2Δ and 3Δ as the grid spacing at x_i

$$\alpha f_{i-1}^{(3)} + f_i^{(3)} + \alpha f_{i+1}^{(3)} = a\left[\frac{-\frac{1}{2}f_{i-2} + f_{i-1} - f_{i+1} + \frac{1}{2}f_{i+2}}{\Delta^3}\right] + b\left[\frac{-\frac{1}{2}f_{i-4} + f_{i-2} - f_{i+2} + \frac{1}{2}f_{i+4}}{8\Delta^3}\right] + c\left[\frac{-\frac{1}{2}f_{i-6} + f_{i-3} - f_{i+3} + \frac{1}{2}f_{i+6}}{27\Delta^3}\right]$$

The Pade' scheme is obtained by choosing b=c=0. Using Taylor expansion to evaluate the derivatives and function values at the surrounding points in terms of the values at x_i , we get:

$$\begin{aligned}
&\alpha\left[\Delta^3\left(f_i^{(3)} - f_i^{(4)}\frac{\Delta}{1!} + f_i^{(5)}\frac{\Delta^2}{2!} - f_i^{(6)}\frac{\Delta^3}{3!} + O(\Delta^4)\right)\right] + f_i^{(3)} \\
&\quad + \alpha\left[\Delta^3\left(f_i^{(3)} + f_i^{(4)}\frac{\Delta}{1!} + f_i^{(5)}\frac{\Delta^2}{2!} + f_i^{(6)}\frac{\Delta^3}{3!} + O(\Delta^4)\ldots\right)\right] \\
&\quad = a\left[\frac{-1}{2}\left[f_i - f_i^{(1)}(2\Delta) + f_i^{(2)}\frac{(2\Delta)^2}{2!} - f_i^{(3)}\frac{(2\Delta)^3}{3!} + f_i^{(4)}\frac{(2\Delta)^4}{4!} - f_i^{(5)}\frac{(2\Delta)^5}{5!} + f_i^{(6)}\frac{(2\Delta)^6}{6!}\right.\right. \\
&\quad \left. + O(\Delta^7)\right] \\
&\quad + \left[f_i - (\Delta)f_i^{(1)} + f_i^{(2)}\frac{(\Delta)^2}{2!} - f_i^{(3)}\frac{(\Delta)^3}{3!} + f_i^{(4)}\frac{(2\Delta)^4}{4!} - f_i^{(5)}\frac{(2\Delta)^5}{5!} + f_i^{(6)}\frac{(2\Delta)^6}{6!} + O(\Delta^7)\right] \\
&\quad - \left[f_i + (\Delta)f_i^{(1)} + f_i^{(2)}\frac{(\Delta)^2}{2!} + f_i^{(3)}\frac{(\Delta)^3}{3!} + f_i^{(4)}\frac{(2\Delta)^4}{4!} + f_i^{(5)}\frac{(2\Delta)^5}{5!} + f_i^{(6)}\frac{(2\Delta)^6}{6!} + O(\Delta^7)\right] \\
&\quad + \frac{1}{2}\left[f_i + 2\Delta f_i^{(1)} + f_i^{(2)}\frac{(2\Delta)^2}{2!} + f_i^{(3)}\frac{(2\Delta)^3}{3!} + f_i^{(4)}\frac{(2\Delta)^4}{4!} + f_i^{(5)}\frac{(2\Delta)^5}{5!} + f_i^{(6)}\frac{(2\Delta)^6}{6!}\right. \\
&\quad \left.\left. + O(\Delta^7)\right]\right]
\end{aligned}$$

Clubbing terms together on either side based on the derivatives of f and equating their coefficients of derivatives of *f* (1^{st} , 2^{nd} , 4^{th} and 6^{th} derivatives don't survive on the RHS), we get following two equations (equating for the 3rd and 5th derivative and dropping terms from the 7th derivative):

$$2\alpha + 1 = a$$

$$a = 4\alpha$$

Solving the system gives:

α=1/2 and a=2

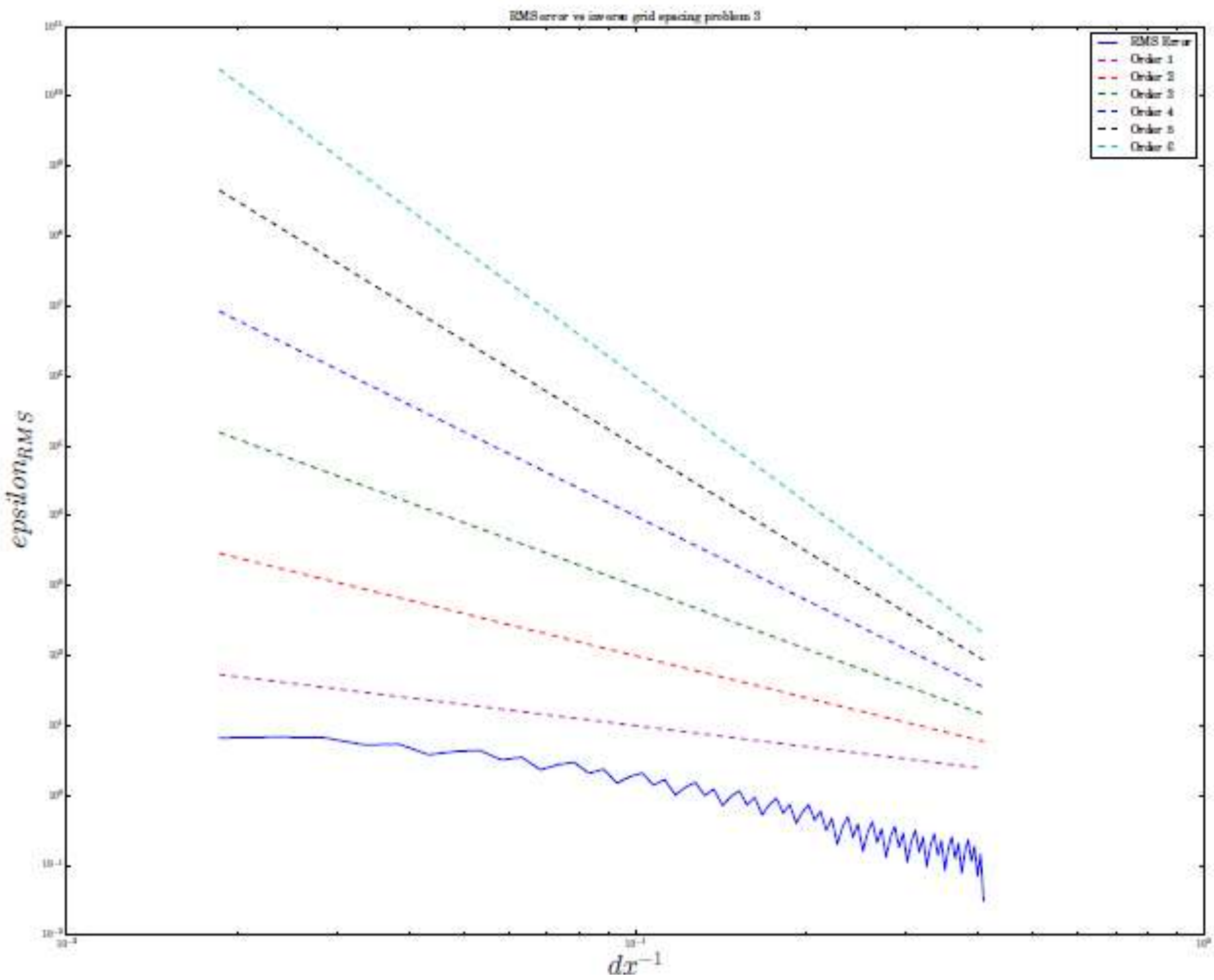
Hence, the final scheme is (after dividing by Δ^3):

$$\frac{1}{2}f^{(3)}{}_{i-1} + f^{(3)}{}_{i} + \frac{1}{2}f^{(3)}{}_{i+1} = \frac{-f_{i-2} + 2f_{i-1} - 2f_{i+1} + f_{i+2}}{\Delta^3} + O(\Delta^4)$$

Here, the scheme has been truncated at the 4th power of Δ, making it a 4th order accurate Pade' scheme.

Problem 3b)

Fig 3b) shows the root-mean-square of the error using the adopted 4th order Pade' scheme, against the inverse of the grid spacing. The function used is the same one as in problem 2b. Here, the 1st order derivative based on a 5th order Lagrange polynomial has been used to patch the derivatives at the boundary.



RMS error vs inverse grid spacing

From the figure, it can be seen that the plot (minus the oscillations) goes parallel to the order 3 line, suggesting a 3rd order accurate scheme overall (the no. of discretization points can be increased to check if the accuracy improves, but the scheme appears to be atleast 3rd order, if not more) . This is one less than the order of the derived Pade' scheme. This suggests that even global schemes are sensitive to the patching of boundary conditions and the overall accuracy of the entire scheme may suffer if the patching were bad. However, on comparison with problem 2b, where the scheme effectively became a 1st order scheme due to bad patching at the boundary, global schemes seem to be more stable and can mitigate effects of bad boundary patching with a relatively low compromise in accuracy.