Verification and Validation in Scientific Computing - Homework 4

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The source code for this assignment is available at `https://github.com/Steven-Roberts/VVSC-Project`.

The Allen–Cahn PDE is a reaction-diffusion PDE governed by equation

$$\begin{aligned} \frac{\partial u(t,x,y)}{\partial t} &= \alpha \nabla^2 u(t,x,y) + \beta \left(u(t,x,y) - u(t,x,y)^3 \right), \\ u(0,x,y) &= \cos(2\pi x) + \cos^2(4\pi y), \\ t,x,y &\in [0,1] \end{aligned} \tag{1}$$

with zero Neumann boundary conditions on all four boundary edges. The parameters α and β are both taken to be 1. This PDE is discretized in space on an using second order finite differences on a uniform grid with cells of size $h \times h$. In time, a second order Rosenbrock method is used with a fixed timestep of h. The system response quantity I consider is the average value of u over the spatial domain $[0,1]^2$ at time $t = 1$.

Table 1 presents the discretization error for the system response quantity approximating using extrapolation.

rh \ h	$\frac{1}{96}$	$\frac{1}{128}$	$\frac{1}{192}$	$\frac{1}{256}$
$\frac{1}{64}$	3.4364e-04	2.0364e-04	9.2936e-05	5.2584e-05
$\frac{1}{96}$		2.3318e-04	1.0464e-04	5.8780e-05
$\frac{1}{128}$			1.0606e-04	5.9283e-05
$\frac{1}{192}$				5.8215e-05

Table 1: All discretization error estimates computed using extrapolation with a finer mesh.

To compute the observed order of accuracy, I used the system response quantities for $h = \frac{1}{64}, \frac{1}{128}, \frac{1}{256}$, which I will denote at f_3, f_2, f_1, respectively:

$$\widehat{p} = \frac{\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{\ln(2)} \approx 1.78.$$

This is slightly less than the theoretical order of 2, indicating the discretization error estimate is somewhat unreliable. I suspect this is because I have not quite reached the asymptotic regime that is required for these extrapolation-based estimated to be accurate. Unfortunately, using finer meshes was prohibitively expensive. Consequently, the safety factor was selected to be the conservative values of $F_s = 3$. Using the definition

$$CGI = \frac{F_s}{r^p - 1}|f_2 - f_1|, \tag{2}$$

the CGI values are provided in table 2.

rh \ h	$\frac{1}{96}$	$\frac{1}{128}$	$\frac{1}{192}$	$\frac{1}{256}$
$\frac{1}{64}$	1.0309e-03	6.1091e-04	2.7881e-04	1.5775e-04
$\frac{1}{96}$		6.9953e-04	3.1393e-04	1.7634e-04
$\frac{1}{128}$			3.1817e-04	1.7785e-04
$\frac{1}{192}$				1.7464e-04

Table 2: CGI values for all pairs of meshes.

As iterative error is not relevant here and I was unable to determine uncertainties due to roundoff error, table 2 also provides the numerical uncertainties. We can see that on the finest mesh, $U_{NUM} \approx 0.000175$, while for a more practical value of $h = \frac{1}{128}$, $U_{NUM} \approx 0.000248$.