Problem Set 3

Problems to Computational Astrophysics, WS 2013/2014

Prof. Dr. Friedrich Röpke, Prof. Dr. Christian Klingenberg, Sebastian Ohlmann
Offices: Campus Hubland Nord, 31.01.017, 30.02.012, 31.01.003

Hand in until Monday, 11.11.2013, 12.00 pm
Tutorial on Tuesday, 12.11.2013, 10.15 am

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1. Step size dilemma (P)

As seen in the first problem of problem set 2, the accuracy of the outcome is not only determined by the truncation error of the finite difference (FD) method, but also by roundoff errors. There are two sources of roundoff errors we will consider here: *cancellation errors* and *condition errors*.
A cancellation error occurs when two nearly equal numbers are subtracted because of their finite representation. The error can be estimated by assuming that the error occurs in the least significant digit,

$$|(a-b)_{\text{true}} - (a-b)| \leq \delta \max(|a|, |b|). \tag{1}$$

δ is the precision of the representation, which is given by $\delta = 2^{-53}$ for usual double precision representations on computers.
A condition error occurs when the given function $f(x)$ is only known to a certain precision. Elementary operations and functions (such as trigonometric functions etc.) are accurate to machine precision, but a function using an integration or iterative computation may only be accurate to a certain error ε. Then, all digits below this threshold are affected and we can estimate the error as

$$|f(x)_{\text{true}} - f(x)| \leq \varepsilon |f(x)|. \tag{2}$$

For elementary functions, $\varepsilon = 2^{-53}$ is the machine precision for usual double precision numbers.
Now consider the forward FD scheme for the first derivative,

$$\text{FD}_1^{(1)}(x,h) = \frac{f(x+h) - f(x)}{h} + O(h), \tag{3}$$

which is based on the Taylor expansion of $f(x+h)$,

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \frac{f''(\xi)}{2}h, \tag{4}$$

where ξ is between x and $x+h$.

a) Compute an upper bound for the total error for this method, which consists of cancellation and condition errors, as well as the truncation error. Sketch this as a function of h.

   Hint: For the roundoff errors, find an upper bound for $|\text{FD}_{\text{true}} - FD|$. The truncation error comes from the last term in the Taylor expansion.

b) A general nth order FD scheme for the dth derivative can be written as

$$\mathrm{FD}_n^{(d)}(x,h) = \frac{\Delta f_n^{(d)}(x,h)}{h^d} + O(h^n), \tag{5}$$

where $\Delta f_n^{(d)}$ is given by a certain combination of function evaluations at different points. Using the true derivative, $f_{\text{true}}^{(d)} = \mathrm{FD}_{\text{true}} + C_{\text{true}} h^n$, the total error can be bounded by

$$\begin{aligned} |f_{\text{true}}^{(d)} - \mathrm{FD}| &= |\mathrm{FD}_{\text{true}} - \mathrm{FD} + C_{\text{true}} h^n| && (6) \\ &\leq |\mathrm{FD}_{\text{true}} - \mathrm{FD}| + |C_{\text{true}}| h^n && (7) \\ &\leq \frac{\varepsilon |F_\varepsilon| + \delta |F_\delta|}{h^d} + |C_n| h^n, && (8) \end{aligned}$$

where the exact form of F_ε, F_δ, and C_n depends on the FD method.

Compute the optimum step size h_{opt} which minimizes this error expression.

Hint: Assume F_ε, F_δ, and C_n to be independent of h for $h \to 0$.

c) Compute F_ε, F_δ, and C_n for the forward and central FD schemes for the first derivative. Use these to get an expression for the optimum step size for both schemes.

d) Compute the optimum step size for problem 1 from problem set 2 ($f(x) = \exp(x)$ at $x = 0$) for the forward, backward and central schemes. Compare this to the plot you made for the error.

2. Von Neumann stability analysis (P)

Consider the centered method

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{2\Delta x}\, a \left(Q_{j+1}^n - Q_{j-1}^n\right)$$

for the linear advection equation $u_t + a\, u_x = 0$. Use von Neumann analysis to show that this method is unstable for fixed $\frac{\Delta t}{\Delta x}$.
Hint: As the equation is linear, you can analyze the behaviour of one Fourier component $\hat{Q}^n(\xi) = \exp(-i\xi j \Delta x) Q_j^n$.

Exercises marked with (P) have to be presented in the exercise, those marked with (H) have to be handed in. Programs can be sent per e-mail to `sohlmann@astro.uni-wuerzburg.de`.