Always check the class bboard on the blackboard site from home.nyu.edu (click on academics, then on Numerical Methods II) before doing any work on the assignment.

Assignment 5, due March 8

Corrections: (none yet)

Consider the first order ODE for $x(t) \in \mathbb{R}^d$

$$\dot{x} \;=\; f(x) \;. \tag{1}$$

This is equivalent to differential equations $\frac{d}{dt}x_i(t) \;=\; f_i(x)$ for $i \;=\; 1,\ldots,d$. *Runge Kutta* methods are derived using Taylor series expansions of f as a function of x, and x as a function of t. For f, we have

$$f(x+\Delta x) \;=\; f(x) \;+\; f'(x)\Delta x \;+\; O\left(\|\Delta x\|^2\right) \tag{2}$$

Here f' is the $d \times d$ *Jacobian* matrix with entries

$$f_{ij}(x) \;=\; \partial_{x_j} f_i(x) \;.$$

And $f'\Delta x$ is the matrix-vector product. If it were to occur, $f'(x)f'(x)$ would be the matrix-matrix product. The next term in the Taylor expansion may be expressed as a *bilinear form*. A general bilinear form is a mapping $(u,v) \rightarrow B(u,v)$ that is linear in u for fixed v, and linear in v for fixed u. Being linear both ways (as a function of u and v)makes it bilinear. A bilinear form from $\mathbb{R}^d$ to $\mathbb{R}^d$ may be expressed using a $d \times d \times d$ array of numbers, $(u,v) \;\rightarrow\; w = B(u,v)$ means (with or without the *summation convention*)

$$B(u,v)_i \;=\; w_i \;=\; B_{ijk}u_jv_k \;=\; \sum_{j=1}^{d}\sum_{k=1}^{d} B_{ijk}u_jv_k \;.$$

In this notation, the next order Taylor series is

$$f(x+\Delta x) \;=\; f(x) \;+\; f'(x)\Delta x \;+\; \frac{1}{2}f''(x)(\Delta x,\Delta x) \;+\; O\left(\|\Delta x\|^3\right) \;. \tag{3}$$

Here, f'' is an array with three indices

$$f''_{ijk} \;=\; \partial_{x_j}\partial_{x_k} f_i(x) \;.$$

The next Taylor series term uses a trilinear form defined in terms of the four index array of third partials, etc.

1. Differentiate the ODE with respect to time to find expressions for $\ddot{x}(t) = \partial_t^2 x(t)$ and $\partial_t^3 x(t)$ in terms of $f = f(x(t))$, $f' = f'(x(t))$, and f''. Use this to write a formula of the form (fill in the dots)

$$x(t + \Delta t) \; = \; x(t) \; + \; \cdots \; + \; O\left(\Delta t^3\right) \; ,$$

in terms of data at time t.

2. Consider an approximation

$$\begin{aligned} y &= x \, + \, \alpha \Delta t f(x) \\ u &= x \, + \, \beta \Delta t f(x) \, + \, \gamma \Delta t f(y) \end{aligned}$$

Here α, β, and γ are constants that do not depend on f or Δt. Find two equations for α, β, and γ so that $u = x(t + \Delta t) + O(\Delta t^3)$.

3. Use this to show that the resulting time stepping method

$$\begin{aligned} y_n &= x_n \, + \, \alpha \Delta t f(x_n) \\ x_{n+1} &= x_n \, + \, \beta \Delta t f(x_n) \, + \, \gamma \Delta t f(y_n) \end{aligned}$$

is stable (in our old sense of stable ODE solvers) and second order accurate. This is a *two stage* (because there are two f evaluations per time step) and second order explicit Runge Kutta method.

4. Consider the predictor-corrector approximation to the implicit *trapezoid rule* $x_{n+1} = x_n + \frac{\Delta t}{2} \left[f(x_n) + f(x_{n+1}) \right]$. Show that this is one of the two stage second order Runge Kutta methods of part 3.

5. Show that all second order two stage explicit Runge Kutta methods give the same results when applied to $\dot{x} = \lambda x$.

6. Show that two stage second order time stepping is unstable at any CFL for linear advection with centered differencing in space.

7. Find the CFL limit for two stage second order time stepping for the heat equation. The PDE is $\partial_t u = D \partial_x^2 u$. The CFL limit is an inequality of the form $\Delta t \leq (\text{CFL}) \cdot \Delta x^2 / D$ as equivalent to stability of the method. Do this in two stages. First figure out the spectrum (range of eigenvalues) of the second difference operator in space using Fourier analysis. Second, figure out what value of Δt puts this whole set inside the stability region of the time stepping method.

8. Consider a three stage method

$$\begin{aligned} y &= x \, + \, \alpha \Delta \alpha t f(x) \\ z &= x \, + \, \Delta t \left(\beta f(x) \, + \, \gamma f(y) \right) \\ u &= x \, + \, \Delta t \left(\delta f(x) \, + \, \epsilon f(y) \, + \, \phi f(z) \right) \end{aligned}$$

Find the four equations involving the six parameters that lead to a three stage third order explicit Runge Kutta method. There is one equation for each of the four Taylor series terms f, f', $f''(f,f)$, and $f'f'f$ (all evaluated at x). Use this to show that this particular three stage method is third order accurate:

$$\begin{aligned} y_n &= x_n + \frac{2\Delta t}{3} f(x_n) \\ z_n &= x_n + \frac{\Delta t}{3} \left(f(x_n) + f(y_n) \right) \\ x_{n+1} &= x_n + \frac{\Delta t}{4} \left(f(x_n) + 3f(z_n) \right) \end{aligned}$$

9. Show that all explicit three stage third order Runge Kutta methods do the same thing for $\dot{x} = \lambda x$. If you are so inclined, you might try instead to prove the general theorem that a p stage explicit Runge Kutta method that is order p accurate must give the order p Taylor series for $e^{\lambda \Delta t}$

$$x_{n+1} = \left(\sum_{k=0}^{p} \frac{(\lambda \Delta t)^k}{k!} \right) x_n \; .$$

(This is less useful than it seems because there are no p stage methods of order p for $p > 4$.) Hint: p applications of $\lambda \Delta t$ gives a polynomial of degree p in $\lambda \Delta t$. What else could this polynomial be?

10. Consider applying this three stage time stepper to linear advection in one dimension: $\partial_t u + a \partial_x u = 0$. Use second order centered differencing in space. Show that the stability limit is $a\Delta t / \Delta x \leq \sqrt{3}$. It probably is easier if you use the hint of part 7, as modified for this case.

11. The overall method of part 10 is only second order accurate despite using a third order accurate time stepper. Try to find a second order three stage time stepper with a larger CFL limit.

12. Apply the time stepper from part 10 or part 11 to linear acoustics in 2D. These equations are

$$\begin{aligned} 0 &= \partial_t \rho + \rho_0 \left(\partial_x v_x + \partial_y v_y \right) \\ 0 &= \rho_0 \partial_t v_x + c_0^2 \partial_x \rho \\ 0 &= \rho_0 \partial_t v_y + c_0^2 \partial_y \rho \end{aligned}$$

Take initial data corresponding to a small localized density disturbance: $v_x(x,y,0) = 0$, $v_y(x,y,0) = 0$, $\rho(x,y,0) = e^{-(x^2+y^2)/2\sigma^2}$ with σ as small as you can while still getting accurate results (this depends on your computer – how fine a mesh can it do in a reasonable amount of time). Use periodic boundary conditions in the x and y directions. Do a convergence study at a fixed reasonable time to show that the result is second order accurate. Organize the program in a modular way. There should be a procedure that computes the semi-discrete operator (does the necessary space differencing, etc.) and a different one that does the time stepping and just calls the space differencing procedure. Use VisIt to visualize the solution at several times. It should look like an outgoing wave. If you have extra time and nothing else to do, try go get VisIt to make a movie. Verify using a convergence study that your method is second order accurate.