Advanced Computational Methods in Condensed Matter Physics

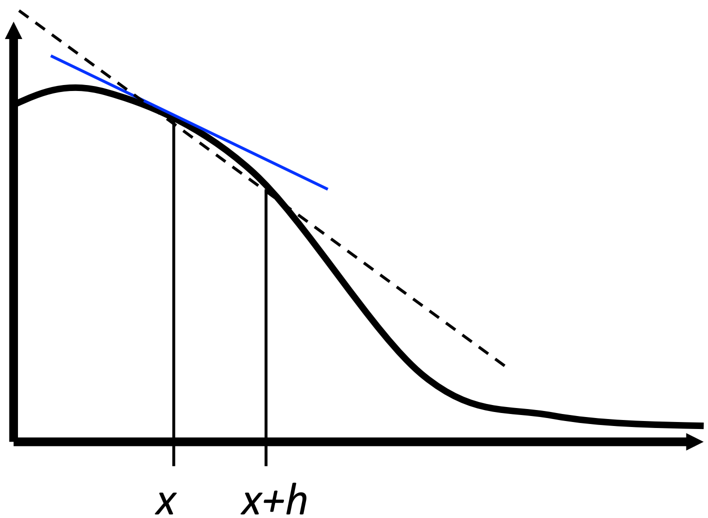
Lecture 4

Explicit and implicit PDE discretization

Numerical Differentiation

- The mathematical definition: $f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$

- Graphically, as the tangential line:



- Numerically, we can not calculate the limit as *h* goes to zero, so we need to approximate it.
- Apply directly for a non-zero *h* leads to the slope of the secant curve.

…

- This is called **Forward Differences** and can be derived using Taylor's Series:

$$f(x+h) = f(x) + f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f(x+h) - f(x) = f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f'(x) = \frac{f(x+h) - f(x)}{h} - f''(\xi)\frac{h}{2!}$$

$$\therefore \frac{f(x+h) - f(x)}{h} \rightarrow f'(x) \;\; as \;\; h \rightarrow 0$$

Reminder: errors

- ***Truncation Error:*** introduced in the solution by the approximation of the derivative
- ***Round-off Error:*** introduced in the computation by the finite number of digits used by the computer

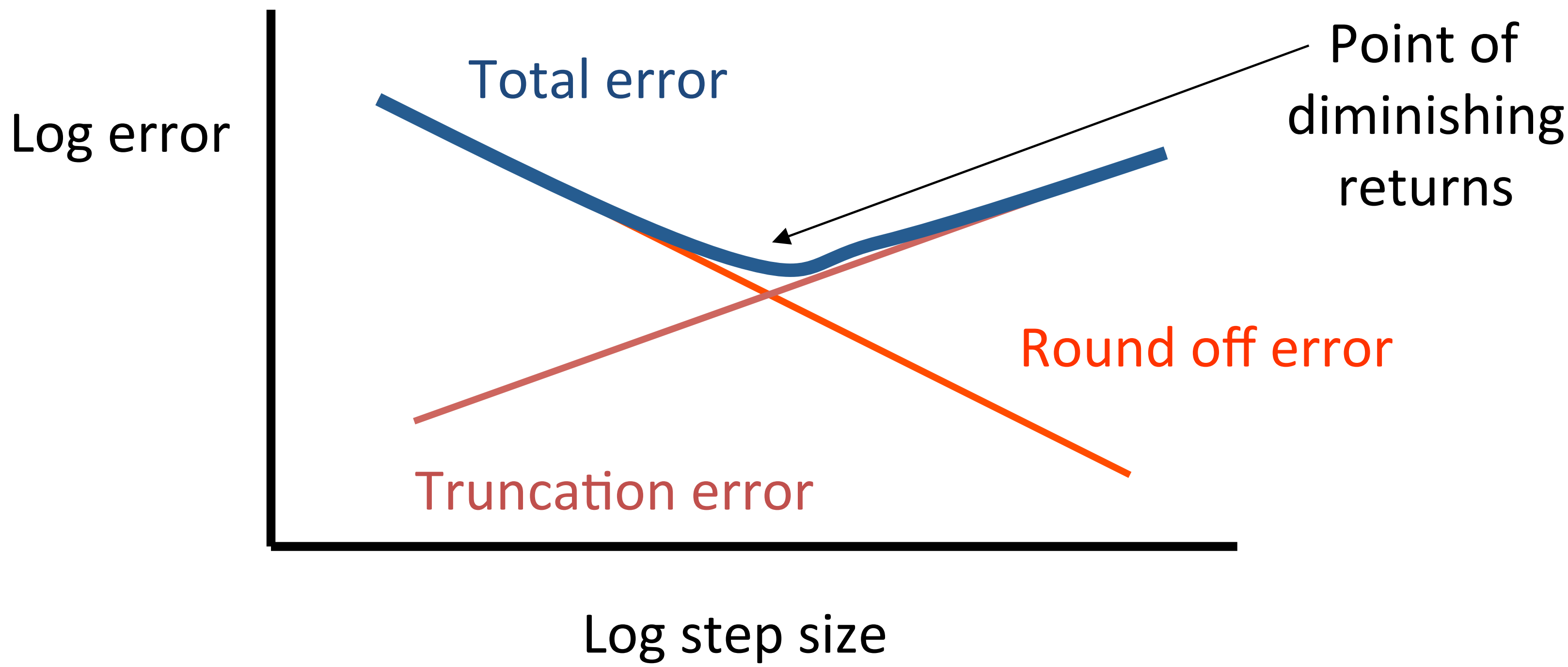
- Solving differential equations is done in multiple steps. Therefore we also have:
  - ***Local Error:*** from each term of the equation
  - ***Global Error:*** from the accumulation of local error

Truncation errors

- Let *f(x)* = a+e, and *f(x+h)* = a+f.
- Then, as *h* approaches zero, e<<a and f<<a.
- With limited precision on our computer, our representation of *f(x)* ≈ a ≈ *f(x+h)*.
- We can easily get a random round-off bit as the most significant digit in the subtraction.
- Dividing by *h*, leads to a very wrong answer for *f'(x).*

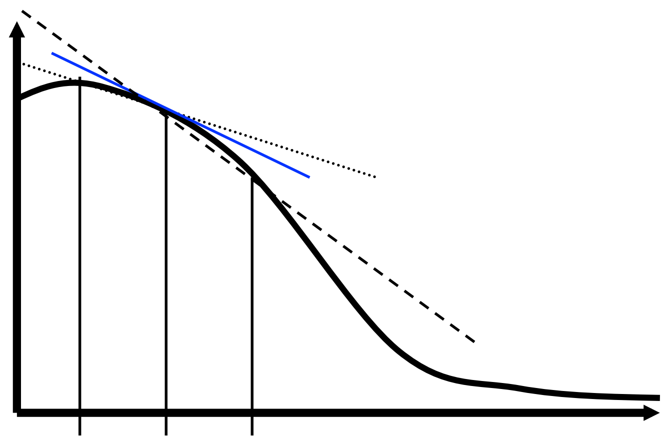
Error trade-off

- Using a smaller step size reduces truncation error.
- However, it increases the round-off error.
- Trade off/diminishing returns occurs: Always think and test!



"Backward" Differentiation

- This forward differentiation formula favors (or biases towards) the right-hand side of the curve.
- Why not use the left?
- This leads to the **Backward Differences** formula:



$$f(x-h) = f(x) - f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f'(x) = \frac{f(x) - f(x-h)}{h} + f''(\xi)\frac{h}{2!}$$

$$\therefore \frac{f(x) - f(x-h)}{h} \to f'(x) \;\; as \;\; h \to 0$$

Central difference

- Can we do better?
- Let's average the two:

$$f'(x) \approx \frac{1}{2}\left(\underbrace{\frac{f(x+h)-f(x)}{h}}_{\textit{Forward difference}} + \underbrace{\frac{f(x)-f(x-h)}{h}}_{\textit{Backward difference}}\right) = \frac{f(x+h)-f(x-h)}{2h}$$

- This is called the **Central Difference** formula.
- This formula does not *seem* very good.
  - It does not follow the calculus formula.
  - It takes the slope of the secant with width 2h.
  - The actual point we are interested in is not even evaluated.

…

- But, is this any better?
- Use the Taylor series to examine the error:

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(\xi)\frac{h^3}{3!}$$

$$f(x-h) = f(x) - f'(x)h + f''(x)\frac{h^2}{2} - f'''(\varsigma)\frac{h^3}{3!}$$

subtracting

$$f(x+h) - f(x-h) = 2f'(x)h + \left(f'''(\xi)\frac{h^3}{3!} + f'''(\varsigma)\frac{h^3}{3!} \right)$$

- The central differences formula has much better convergence.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6} f'''(\zeta)h^2, \zeta \in \left[x-h, x+h\right]$$

- Approaches the derivative as h^2 goes to zero!!

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O\left(h^2\right)$$

But:

- **Still have truncation error problem.**

- Consider the case of:

- Build a table with smaller values of *h*.

- What about large values of *h* for this function?

$$f(x) = \frac{x}{100}$$

$$f'(x) \simeq \frac{\left\lfloor \frac{x+h}{100} \right\rfloor - \left\lfloor \frac{x-h}{100} \right\rfloor}{2h}$$

$$at\ \ x = 1, h = 0.000333, with\, 6\, significant\, digits$$

$$f'(x) \simeq \frac{0.0100033 - 0.0099966}{0.000666666} = 0.010050$$

Relative error:

$$\frac{|0.01\text{-}0.010050|}{0.01} = 0.5\%$$

Richardson Extrapolation

- Can one do better?
- Is my choice of *h* a good one?
- Let's start with the Taylor series of the difference:

$$f(x+h)-f(x-h)=2f'(x)h+2\frac{f'''(x)}{3!}h^3+2\frac{f'''(x)}{3!}h^3+2f^{(5)}(x)\frac{h^5}{5!}+\cdots$$

- Assuming the higher derivatives exist:

$$f'(x)=\varphi(h)+a_2h^2+a_4h^4+a_6h^6+\cdots$$
$$\text{with } \varphi(h)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]$$

- Richardson Extrapolation examines the operator φ(h) as a function of h, which approximates $f'(x)$ to $O(h^2)$.
- For h→0:

$$\varphi(h)=f'(x)-a_2h^2-a_4h^4-a_6h^6-\mathrm{L}$$
$$\varphi(\frac{h}{2})=f'(x)-a_2\left(\frac{h}{2}\right)^2-a_4\left(\frac{h}{2}\right)^4-a_6\left(\frac{h}{2}\right)^6-\mathrm{L}$$

…

- Using these two formula's, we can come up with another estimate for the derivative that cancels out the h^2 terms.

$$\varphi(h) - 4\varphi(\frac{h}{2}) = -3f'(x) - \frac{3}{4}a_4 h^4 - \frac{15}{16}a_6 h^6 - \cdots$$

$$\text{or } f'(x) = \varphi(\frac{h}{2}) + \frac{1}{3}\left[\varphi(\frac{h}{2}) - \varphi(h)\right] + O\left(h^4\right)$$

new estimate

difference between old and new estimates

- If h is small (h<<1), then h^4 goes to zero much faster than h^2.
- Can we cancel out the h^6 term?
  - Yes, by using h/4 to estimate the derivative.

Generalization

- Let us define the central differences operator for different values of *h*:

$$D\left(n,0\right) \equiv \varphi\left(\frac{h}{2^n}\right)$$

$$= L + \sum_{k=1}^{\infty} A\left(k,0\right)\left(\frac{h}{2^n}\right)^{2k}$$

$$L = \lim_{h\to 0} \varphi(h) = f'\left(x\right)$$

- I.e.

$$f'(x) = \varphi(\frac{h}{2}) + \frac{1}{3}\left[\varphi(\frac{h}{2}) - \varphi(h)\right] + O\left(h^4\right)$$

$$= D(1,0) + \frac{1}{4-1}\left[D(1,0) - D(0,0)\right] + O\left(h^4\right)$$

- Or for $h \to h/2$:

$$f'(x) = D(n,0) + \frac{1}{4-1}\left[D(n,0) - D(n-1,0)\right] + O\left(\left(\frac{h}{2^n}\right)^4\right)$$

- Define Richardson's extrapolation operator:

$$D\left(n,m\right) = D(n,m-1) + \frac{1}{4^m - 1}\left[D\left(n,m-1\right) - D\left(n-1,m-1\right)\right], \quad \left(1 \le m \le n\right)$$

Giving: $f'(x) = D(n,1) + O\left(\left(\frac{h}{2^n}\right)^4\right)$

Richardson Extrapolation Theorem

- These terms approach *f'(x)* very quickly.

$$D(n,m) = L + \sum_{k=m+1}^{\infty} A(k,m)\left(\frac{h}{2^n}\right)^{2k}$$

Order starts much higher!!!!

- Since $m \leq n$, this leads to a two-dimensional triangular array of values as follows:

$$\begin{array}{lllll} D(0,0) & & & & \\ D(1,0) & D(1,1) & & & \\ D(2,0) & D(2,1) & D(2,2) & & \\ \vdots & \vdots & \vdots & \ddots & \\ D(N,0) & D(N,1) & D(N,2) & \cdots & D(N,N) \end{array}$$

- We must pick an initial value of *h* and a max iteration value *N.*

Example

$$f(x) = \frac{\left(\cos(100x^2)\right)^5}{x^3}$$

$$x = 1.3,\ h = \frac{1}{128},\ N = 5$$

16.696386					
40.583393	48.583393				
109.322528	132.235574	137.814897			
135.031747	143.601487	144.359214	144.463092		
142.068615	144.414238	144.468421	144.470154	144.470182	
143.866937	144.466377	144.469853	144.469876	144.469875	$D(5,5) = 144.469875$

Which converges up to eight decimal places, exact result:

f'(13/10)=-((30000 $\cos^5$(169))/28561) - 100000/169 $\cos^4$(169) sin(169)

≈144.46987425310895128951775669783203991279122284388…

Second Derivative

- For the second derivative we can start with

$$f(x+h)=f(x)+f'(x)h+f''(x)\frac{h^2}{2}+f'''(x)\frac{h^3}{3!}+f^{(4)}(x)\frac{h^4}{4!}+f^{(5)}(x)\frac{h^5}{5!}+\cdots$$
$$f(x-h)=f(x)-f'(x)h+f''(x)\frac{h^2}{2}-f'''(\varsigma)\frac{h^3}{3!}+f^{(4)}(x)\frac{h^4}{4!}-f^{(5)}(x)\frac{h^5}{5!}+\cdots$$

- And add them (cancelling odd derivatives):

$$f(x+h)+f(x-h)=2f(x)+2f''(x)\frac{h^2}{2}+2f^{(4)}(x)\frac{h^4}{4!}+\cdots$$

- And therefore:

$$f''(x)\approx\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

- With error term: $-\frac{1}{12}h^2 f^{(4)}(\xi)$

Partial derivatives

- Nothing special about them:

$$\frac{\partial f}{\partial x}(x,y) \approx \frac{f(x+h,y)-f(x-h,y)}{2h}$$

$$\frac{\partial f}{\partial y}(x,y) \approx \frac{f(x,y+h)-f(x,y-h)}{2h}$$

differential equations

Ordinary differential equations (ODE)

- Define:

$$x^{(k)}(t) = \frac{d^k x}{dt^k}\ , \quad k = 1, 2, \cdots, n$$

- the ODE is an equation involving t and $x^{(k)}(t)$: $F(t,x,x',x'',\ldots,x^{(n)})=0$.
- A restricted family of ODEs can be written as $x^{(n)}(t)=F(t,x,x',x'',\ldots,x^{(n-1)})$,
- and can be reduced to a system of the first order ODEs

$$\frac{dy_i}{dt} = f_i(t, y_1, y_2, \ldots, y_n)\ , \ \ y_k := \frac{d^{k-1}x}{dt^{k-1}}.$$

- Therefore, we consider ODEs with one variable, since most of results for this single ODE can be applicable for the above n-coupled ODEs.

$$\frac{dy}{dt} = f(t, y)$$

Existence, uniqueness, and stability of solution for ODEs

$$\frac{dy}{dt} = f(t, y)$$
$$y(a) = \alpha.$$

Definition:(Lipschits condition)

$D \subset \mathbf{R}^2$, $f : D \to \mathbf{R}$: a function, $f : (t, y) \mapsto \mathbf{R}$

A function $f(t, y)$ satisfies a Lipschits condition, if

$\exists L > 0$: a constant such that, $|f(t, y_1) - f(t, y_2)| < L|y_1 - y_2|$

for $\forall (t, y_1)$, $(t, y_2) \in D$. L: Lipschitz constant for f

Theorem:(Existence and uniqueness)

$D := \{(r, y) \,|\, a \leq t \leq T, |y - \alpha| \leq \beta\}$ for some $\beta > 0$.

If $f(t, y)$ is continuous on D (or $\exists M > |f(t, y)|$),

and $f(t, y)$ satisfies Lipschitz codition in y on D,

then $\exists [a, b] \subset [a, T]$ on which a unique solution to the ODE

$y = \phi(t)$ exists with an initial value $\phi(a) = \alpha$.

Definition:(Stability)

Consider a *perturbed* equation $\frac{dz}{dt} = f(t, z) + \delta(t)$.

The initial value problem is called stable, if $\exists \epsilon > 0$, and $K > 0$,

such that, whenever $|\epsilon_0| < \epsilon$ and $|\delta(t)| < \epsilon$ for $\forall t \in [a, b]$,

the perturbed equation has a unique solution that satisfies

$|z(t) - y(t)| < K\epsilon$ for $\forall t \in [a, b]$.

Euler's method

Consider the initial value problem $\frac{dy}{dt} = f(t,y) \quad y(a) = \alpha\,,\ t \in [a,b]$

- Let w_i be the numerical approximation to the exact value $y_i := y(t_i)$,
- It is determined at the set of discrete points, $a = t_0 < t_1 < \cdots < t_n = b$
- We choose equally spaced points $t_i := a + ih$, with $h := (b-a)/N$, $i = 0, \cdots N$.

From Taylor expansion of $y(t)$ in $t \in [t_i, t_{i+1}]$, $\exists \xi \in [t_i, t_{i+1}]$

$$y(t) = y_i + y_i'(t - t_i) + \frac{1}{2!} y''(\xi)(t - t_i)^2,$$

we have at $t = t_{i+1}$,

$$y_i' = \frac{y_{i+1} - y_i}{h} - \frac{1}{2!} y''(\xi) h = f(t_i, y_i).$$

Euler's method approximate this equation by

$$w_0 = \alpha,$$

$$\frac{w_{i+1} - w_i}{h} = f(t_i, w_i), \text{ where } \ i = 0, \cdots, N-1$$

…

Error of the Euler method:

- Assuming f is twice differentiable on [a,b], the error at time step i is given by

$$\tau_i = \frac{y_{i+1} - y_i}{h} - f(t_i, y_i) = \frac{h}{2!} y''(\xi_i),$$

- And

$$|\tau_i| = \frac{h}{2!} \max_{t \in [a,b]} |y''|, \quad \text{(local error)}.$$

Note that $|y_i - w_i| = O(h)$, and, clearly, $|y_i - w_i| \to 0$ as $h \to 0$

Theorem: (Global error for Euler's method)

Let $y(t)$ be the unique solution to $\frac{dy}{dt} = f(t, y)$, $y(a) = \alpha$, $t \in [a, b]$.

Let $w_0, w_1, \cdots, w_N$ be generated by Euler's method.
If f satisfies Lipschitz condition in y on $D = \{(t, y) \,|\, t \in [a, b], y \in \mathbb{R}\}$
with Lipschits constant L, and $\exists M$ a constant such that

$$\max_{t \in [a.b]} |y''(t)| \le M$$

then

$$|\, y_i - w_i \,| \le \frac{hM}{2L} \left[e^{L(t_i - a)} - 1 \right].$$

If $\frac{\partial f}{\partial y}$ and $\frac{\partial f}{\partial y}$ exists, $y'' = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} y' = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f$ may be used to estimate the bound M

Stability of Euler's method

Theorem:

$y(t)$: the unique solution to $\dfrac{dy}{dt} = f(t,y), \quad y(a) = \alpha, \quad t \in [a,b]$.

u_i: generated by Euler's method with finite precision arithmetic,

$$\begin{aligned} u_0 &= \alpha + \delta_0, \\ u_{i+1} &= u_i + hf(t_i, u_i) + \delta_i, \\ \text{where} |\delta_i| &< \delta \quad \text{for} \quad i = 0, \cdots, N. \end{aligned} \tag{1}$$

If f satisfies Lipschitz condition in y on $D = \{(t,y) \,|\, t \in [a,b], y \in \mathbf{R}\}$ with Lipschits constant L, and $\exists M$ a constant such that

$$\max_{t \in [a.b]} |y''(t)| \le M$$

then

$$|\, y_i - u_i \,| \le \left(\frac{hM}{2L} + \frac{\delta}{hL}\right)\left[e^{L(t_i - a)} - 1\right] + \delta e^{L(t_i - a)}.$$

Remarks: $\dfrac{hM}{2} \gg \dfrac{\delta}{h}$, we will observe $O(h)$ convergence, while global error would grow for sufficintly small h.
Difference in the initail data α results in $|\tilde{w}_i - w_i| \le e^{L(t_i - a)} |\tilde{\alpha} - \alpha|$.
Therefore the Euler's method is stable.

Taylor's method

If the higher order continuous derivatives of $y(t)$, and those for $f(t,y)$ exist, Taylor expansion of $y(t)$, $t \in [t_i, t_{i+1}]$, is written; namely, $\exists \xi \in [t_i, t_{i+1}]$,

$$\begin{aligned} y(t) &= y_i + y_i'(t-t_i) + \frac{1}{2!}y_i''(t-t_i)^2 + \cdots + \frac{1}{n!}y_i^{(n)}(t-t_i)^n \\ &\quad + \frac{1}{(n+1)!}y^{(n+1)}(\xi)(t-t_i)^{(n+1)}. \end{aligned}$$

We may substitute the followings to the higher derivatives terms

$$y_i'' = \frac{d}{dt}f(t,y)|_{t=t_i} = \left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}f\right)_{t=t_i},$$

$$y_i''' = \frac{d^2}{dt^2}f(t,y)|_{t=t_i} = \left(\frac{\partial^2 f}{\partial t^2} + 2f\frac{\partial^2 f}{\partial t \partial y} + \frac{\partial^2 f}{\partial y^2}f^2 + \frac{\partial f}{\partial y}\frac{\partial f}{\partial t} + \left(\frac{\partial f}{\partial y}\right)^2 f\right)_{t=t_i},$$

and so on.

The second order Taylor method: $w_{i+1} = w_i + hf(t_i, w_i) + \frac{h^2}{2}\frac{df}{dt}(t_i, w_i)$.

The fourth order Taylor method:

$$w_{i+1} = w_i + hf(t_i, w_i) + \frac{h^2}{2}\frac{df}{dt}(t_i, w_i) + \frac{h^3}{3!}\frac{d^2 f}{dt^2}(t_i, w_i) + \frac{h^4}{4!}\frac{d^3 f}{dt^3}(t_i, w_i).$$

Definitions

(Consistency, Convergence and Stability)

If $\tau_i \to 0$ as $h \to 0$, the method is called consistent.
If $\tau_i = O(h^p)$, the method is of order p.

If $\lim\limits_{h\to 0} \max\limits_{1\le i\le N} |y_i - w_i| = 0$, the method is called convergent.

If $\exists k(t)$ s.t. $|\tilde{w}_i - w_i| \le k(t_i)|\tilde{\alpha} - \alpha|$ for $\forall i$, the method is called stable.

One-step methods

$$\frac{w_{i+1} - w_i}{h} = \phi(f, t_i, w_i, h)$$

$$\lim_{h \to 0} \tau_i = \frac{dy}{dt}(t_i) - \phi(f, t_i, y_i, 0) = f(t_i, y_i) - \phi(f, t_i, y_i, 0)$$

One-step method is consistent if $f(t_i, y_i) = \phi(f, t_i, y_i, 0)$.

Remark: If the one-step method is consistent $\Rightarrow$ convergent.
It can be shown that under certain conditions: one-step method is convergent $\Leftrightarrow$ consistent.

2nd order Runge-Kutta method.

$$\frac{w_{i+1} - w_i}{h} = \phi(f, t_i, w_i, h)$$
$$\phi(f, t, y, h) = a_1 f(t, y) + a_2 f(t + \delta_2, y + \Delta_2 f(t, y))$$

Determine constants a_1, a_2, δ_2, Δ_2, so that ϕ becomes $O(h^2)$ approximation of the $O(h^2)$ Taylor method.

$$a_1 + a_2 = 1, \quad \text{and } \delta_2 = \Delta_2 = \frac{h}{2a_2}.$$

- **Modified Euler method.** (Half step Euler + Midpoint integration.)

$$\tilde{w} = w_i + \frac{h}{2} f(t_i, w_i),$$
$$w_{i+1} = w_i + hf\left(t_i + \frac{h}{2}, \tilde{w}\right).$$

$\Longrightarrow$

$$k_1 = f(t_i, w_i),$$
$$k_2 = f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} k_1\right),$$
$$w_{i+1} = w_i + h\, k_2.$$

- **Heun method.** (One step Euler + Trapezoidal integration.)

$$\tilde{w} = w_i + h\, f(t_i, w_i),$$
$$w_{i+1} = w_i + \frac{h}{2} [f(t_i, w_i) + f(t_i + h, \tilde{w})]$$

$\Longrightarrow$

$$k_1 = f(t_i, w_i),$$
$$k_2 = f(t_i + h, w_i + h\, k_1),$$
$$w_{i+1} = w_i + \frac{h}{2}(k_1 + k_2).$$

- Optimal RK2 method.

$$\tilde{w} = w_i + \frac{2h}{3} f(t_i, w_i),$$
$$w_{i+1} = w_i + \frac{h}{4} f(t_i, w_i) + \frac{3h}{4} f\left(t_i + \frac{2h}{3}, \tilde{w}\right)$$

$\Longrightarrow$

$$k_1 = f(t_i, w_i),$$
$$k_2 = f\left(t_i + \frac{2h}{3}, w_i + \frac{2h}{3} k_1\right),$$
$$w_{i+1} = w_i + \frac{h}{4}(k_1 + 3k_2).$$

- Classical 4th order Runge-Kutta method.

$$k_1 = f(t_i, w_i),$$
$$k_2 = f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} k_1\right),$$
$$k_3 = f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} k_2\right),$$
$$k_4 = f(t_i + h, w_i + h k_3),$$
$$w_{i+1} = w_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

The local truncation error of the classical 4th-order Runge-Kutta method is $O(h^4)$.

Linear (m-step) Multistep method

$$\frac{w_{i+1} - \sum_{j=1}^{m} a_j w_{i+1-j}}{h_i} = \sum_{j=0}^{m} b_j f(t_{i+1-j}, w_{i+1-j})$$

$b_0 = 0$: Explicit

$b_0 \neq 0$: Implicit

Adams method: $a_j = 0$, for j = 2, .. , m

Derivation: Integrating the both side of the ODE,

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))dt. \quad \Leftrightarrow \quad \frac{dy}{dt} = f(t, y)$$

- The Implicit linear multistep method is derived from interpolating f(t,y(t)) to polynomial of order m.
- The Explicit linear multistep method from interpolating polynomial of order m-1

Substitute the form f(t,y(t)) = p(t) + R(t) in the integral form of ODE, and integrate it to calculate b_j .

Remarks

- The explicit scheme is also called Adams-Bashforth, implicit Adams-Moulton.
- Explicit scheme may be efficient since the $f(t_i,w_i)$ of earlier steps are used.
- The starting values for w_0 (initial value), w_1, …, w_{m-1} are required for the m-step method.
- These are calculated from one-step method of the same order.
- For the implicit method, value at t_{i+1}, w_{i+1}, is calculated from an algebraic equation. It is iteratively solved using w_{i+1} of an explicit multistep method of the same order as an initial guess.
- Usually this iteration is done by direct substitution, and only one or two iterations are made. This procedure is called predictor – corrector schemes.
- For this scheme, the 4th-order formula is the most popular.

Predictor step (explicit formula)

$$\frac{\tilde{w}_{i+1} - w_i}{h} = \sum_{j=1}^{4} b_j f(t_{i+1-j}, w_{i+1-j})$$

Corrector step (implicit formula)

$$\frac{w_{i+1} - w_i}{h} = b_0 f(t_{i+1}, \tilde{w}_{i+1}) + \sum_{j=1}^{3} b_j f(t_{i+1-j}, w_{i+1-j})$$

PDEs

- In contrast to ODEs, PDEs are differential equation that contains unknown *multivariable* (ODE: single variable) functions and their partial derivatives:

$$F\left(x_1,\ldots,x_n,u,\frac{\partial u}{\partial x_1},\ldots,\frac{\partial u}{\partial x_n},\frac{\partial^2 u}{\partial x_1 \partial x_1},\ldots,\frac{\partial^2 u}{\partial x_1 \partial x_n},\ldots\right)=0.$$

- They describe a wide variety of phenomena such as:
  sound, heat, electrostatics, electrodynamics, fluid flow, elasticity, or quantum mechanics.
- If F is a linear function of u and its derivatives, then the PDE is called linear. Common examples of linear PDEs include the heat equation, the wave equation, Laplace's equation, Helmholtz equation, Klein–Gordon equation, and Poisson's equation.
- ODEs often model one-dimensional dynamical systems, PDEs often model multidimensional systems. [for the ODEs before: n=1, u=y, x_1=t]

…

- Common notation:

$$u_x = \frac{\partial u}{\partial x}$$

$$u_{xy} = \frac{\partial^2 u}{\partial y\, \partial x} = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)$$

$$\ddot{u} = c^2 \nabla^2 u$$

$$\ddot{u} = c^2 \Delta u$$

- subscripts for spatial derivatives
- dots for time derivatives
- ∇ for gradients
- And Δ for the Laplacian

- Many methods for ODEs are simply adapted to PDEs

Example: 1D heat equation

- Consider $u_t = u_{xx}$ and initial condition $u(x,0) = g(x)$
- We will use the finite difference method to approximate the solution
- Forward difference for u_t
- Centered difference for u_{xx} (we discretize function u with respect to x with grid size h_x and denote the value at $x=jh_x$ as u_j)
- Re-write equation in terms of the finite difference approximations:

$$(u_j^{n+1} - u_j^n)/h_t = (u^n_{j+1} - 2u_j^n + u^n_{j-1})/h^2_x$$

- ***Error:*** The local truncation error is $O(h_t)$ from the left hand side and is $O(h^2_x)$ from the right hand side. The parameter $s=h_t/h^2_x$ determines the stability
- *Remarks:* Now all function values u_j need to be stored and calculated separately. All initial value of u_j at t=0 need to be given by $g_{j.}$ The finite difference method above is explicit.

Boundary condition types

- The normal derivative of the problem is given: ***Neumann boundary condition.***
  For example, if there is a heater at one end of an iron rod, then energy would be added at a constant rate but the actual temperature would not be known.
  For an ODE on an interval [a,b]: $y'(a) = \alpha \text{ and } y'(b) = \beta$
  For a PDE $$\frac{\partial y}{\partial \mathbf{n}}(\mathbf{x}) = \nabla y(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = f(\mathbf{x}) \quad \forall \mathbf{x} \in \partial\Omega.$$
- The boundary values to the problem are given: ***Dirichlet boundary condition.***
  For example, if one end of an iron rod is held at absolute zero, then the value of the problem would be known at that point in space.
  $$y(x) = f(x) \quad \forall x \in \partial\Omega$$
- Boundary has the form of a curve or surface that gives a value to the normal derivative and the variable: ***Cauchy boundary condition.***
  These are natural for, e.g., second order ODE, where y(a) and y'(a) are given

Crank-Nicolson scheme

- Let us consider again the heat equation and define $(\delta u^2)^n_j=(u^n_{j+1} - 2u_j^n + u^n_{j-1})/h^2_x$
- Define the θ-scheme for $0<\theta<1$:

$$\frac{u_j^{n+1} - u_j^{n}}{\Delta t} = (1-\theta)(\delta u^2)_j^n + \theta(\delta u^2)_j^{n+1}$$

- For θ=1/2: Crank-Nicolson
- Can avoid any restrictions on stability conditions
- Unconditionally stable no matter what the value of s is if $½\leq\theta\leq 1$.
- Is implicit: to get the "next" value of u in time and that a system of algebraic equations must be solved. In many problems, especially linear diffusion, the algebraic problem is tridiagonal and may be efficiently solved with the tridiagonal matrix algorithm
- For θ<1/2 we need the condition $s<1/(2-4\theta)$ for stability

Summary

- Forward Euler method (explicit):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^n\left(u,\, x,\, t,\, \frac{\partial u}{\partial x},\, \frac{\partial^2 u}{\partial x^2}\right)$$

- Backward Euler method (implicit):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^{n+1}\left(u,\, x,\, t,\, \frac{\partial u}{\partial x},\, \frac{\partial^2 u}{\partial x^2}\right)$$

- Crank-Nicolson (implicit):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left[F_i^{n+1}\left(u,\, x,\, t,\, \frac{\partial u}{\partial x},\, \frac{\partial^2 u}{\partial x^2}\right) + F_i^n\left(u,\, x,\, t,\, \frac{\partial u}{\partial x},\, \frac{\partial^2 u}{\partial x^2}\right)\right]$$

Iterative Solvers for PDE's

Many PDE's can be rewritten as linear equation systems after discretization (in particular for implicit schemes). For the following equation:

$$F\left(x_1, \ldots, x_n, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_n}, \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_1 \partial x_n}, \ldots\right) = \frac{\partial u}{\partial t},$$

where x_i are spatial coordinates and t time

- If *F* is linear in *u* this is clear: spatial derivative discretizations lead to off-diagonal elements in the matrix for the linear equation
- In the presence of non-linear terms in *u*, those can be approximated by, e.g., explicit solvers and then used as constants for the iterative scheme
- Then iterative solver for the linear(ized) equation system can be used
- If the time discretization is sufficiently small, changes in *u* are typically small and the convergence of the iterative solvers can be fast

Spectral methods

- Finite difference method – approximate a function locally using lower order interpolating polynomials.
- Spectral method – approximate a function using global higher order interpolating polynomials.
- Using spectral method, a higher order approximation can be made with moderate computational resources.

Next lecture:

- (Pseudo) random number generators
- Data analysis