Contents

Important concepts, definitions, etc.

Convergence: Numerical solution tends to exact solution as stepsizes tend to zero.

Well-posedness (Hadamard):
If the solution of a mathematical problem

- exists
- is unique, and
- depends continuously on data,

the problem is called well-posed.
Unique: We accept the existence of several but isolated solutions, like the roots of a polynomial, but **not** several infinitely close solutions, like solutions to a singular linear system with a compatible right hand side.
Continuous: We have to define

- a metric, i.e. for PDE's, norms of the functions appearing,
- which perturbations are "allowed".

For initial value problems we shall consider only perturbations to the initial data.

d'Alembert solution: to wave equation $u_{tt}= c^2 u_{xx}$: $u(x,t) = f(x - ct) + g(x + ct)$

Traveling wave: solution of the form $u(x,t) = v(x - st)$ with s a constant.

Jacobian matrix
of a function **f** U –> V, U,V finite dimensional normed linear spaces, dim(U) = n, dim(V) = m, is the matrix of partial derivatives:

$\mathbf{J}(\mathbf{x}) = \{df_i/dx_j\}$, $1 \le i \le m$, $1 \le j \le n$.

Note - be careful ...
If in a given problem there are several mappings, there are also several different "Jacobians". As an example, take the boundary value problem for the first order system,

$\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{G}(\mathbf{y}(0),\mathbf{y}(1)) = 0$, $\mathbf{y}$ in $\mathbf{R}^n$.

The initial value problem for the ODE defines a mapping from $\mathbf{R}^n$ to $\mathbf{R}^n$ which we may call **F**: $\mathbf{y}(1) = \mathbf{F}(\mathbf{y}(0))$. Linearizing this equation gives an nxn Jacobian $d\mathbf{F}/d\mathbf{y}(0)$ which is of course related to but quite distinct from $d\mathbf{f}/d\mathbf{y}$!

Courant number
$c\, \Delta t/\Delta x$ (wave speed c, time step Δt, space step Δx)

Iteration

- Let **P** be a matrix with spectral radius $\rho(\mathbf{P})$. Then, **iff** $\rho(\mathbf{P}) < 1$, the sequence defined by $\mathbf{x}^{(n+1)} = \mathbf{P}\mathbf{x}^{(n)} + \mathbf{c}$ converges to $\mathbf{x}^{(*)} = (\mathbf{I} - \mathbf{P})^{-1}\mathbf{c}$ for all initial values $\mathbf{x}^{(0)}$. Equivalently, the series $\mathbf{I} + \mathbf{P} + \mathbf{P}^2 + \mathbf{P}^3 + \ldots$ converges to $(\mathbf{I} - \mathbf{P})^{-1}$
- For all operator norms $\|\,.\,\|$, $\|\mathbf{P}\| \ge \rho(\mathbf{P})$.
- If $\|\mathbf{P}\| \le R < 1$, $\|\mathbf{x}^{(n)} - \mathbf{x}^{(*)}\| \le R/(1-R)\, \|\mathbf{x}^{(n)} - \mathbf{x}^{(n-1)}\|$

Exact solutions of some differential equations

Linear, constant coefficients

$d\mathbf{y}/dt = \mathbf{A}\mathbf{y} + \mathbf{f}(t)$

$\mathbf{f} = 0$: $\mathbf{y}(t) = \exp(\mathbf{A}t)\,\mathbf{y}(0)$

Duhamel's formula $\mathbf{y}(t) = e^{\mathbf{A}t}\left(\mathbf{y}(0) + \int_0^t e^{-\mathbf{A}\tau}\mathbf{f}(\tau)d\tau\right)$

Computation of $e^{\mathbf{A}}$, or other matrix function $f(\mathbf{A})$

1) If $\mathbf{A}$ is diagonalizable, $\mathbf{AS} = \mathbf{SD}$, $\mathbf{D} = \mathrm{diag}(\lambda_i)$, $f(\mathbf{A}) = \mathbf{S}\,f(\mathbf{D})\,\mathbf{S}^{-1}$ where $f(\mathbf{D}) = \mathrm{diag}(\,f(\lambda_i)\,)$.

2) $e^{\mathbf{A}} = \sum_{k=0}^{\infty}\frac{\mathbf{A}^k}{k!}$ which converges for any $\mathbf{A}$. Can use "argument reduction" to require fewer terms in the sum: $\exp(\mathbf{A}) = [\exp(\mathbf{A}/2)]^2$ etc.

Rule: $\exp(\mathbf{A}+\mathbf{B}) = \exp(\mathbf{A})\exp(\mathbf{B})$ **iff** $\mathbf{AB} = \mathbf{BA}$.

Example

Non-diagonalizable $\mathbf{A}$, a Jordan block:

$$\mathbf{A} = \begin{pmatrix} \lambda & 1 & 0 & \ldots 0 \\ 0 & \lambda & 1 & \ldots 0 \\ 0 & 0 & \ldots & 1 \\ 0 & 0 & \ldots & \lambda \end{pmatrix} = \lambda\mathbf{I} + \mathbf{S}; \mathbf{S}^p = 0 \text{ when } p > n,\; e^{\mathbf{A}} = e^{\lambda\mathbf{I}+\mathbf{S}} = e^{\lambda}e^{\mathbf{S}} = e^{\lambda}\sum_{j=0}^{n}\frac{1}{j!}\mathbf{S}^j$$

Estimates of solutions to differential and difference equations

- **Cauchy-Schwarz inequality.** Let $\mathbf{x}$, $\mathbf{y}$ be elements in an innerproduct space. Then $|(\mathbf{x},\mathbf{y})| \le \|\mathbf{x}\|\,\|\mathbf{y}\|$

where $\|\mathbf{x}\|^2 = (\mathbf{x},\mathbf{x})$

- **Triangle inequality**: $\|\mathbf{x} + \mathbf{y}\| \le \|\mathbf{x}\| + \|\mathbf{y}\|$
- **Completing the square**: If $a > 0$, then $a\|\mathbf{x}\|^2 + 1/a\,\|\mathbf{y}\|^2 \ge 2|(\mathbf{x},\mathbf{y})|$
- $1 + x \le e^x$ for all real x, and $e^x \le 1/(1 - x)$ for $x < 1$. Equality only for $x = 0$.
- $\|\exp(\mathbf{A})\| \le \exp(\|\mathbf{A}\|)$

Positivity Theorem (folklore ?)

Let $\mathbf{y}_t = \mathbf{f}(\mathbf{y})$ and $\mathbf{f}$ be Lipschitz in the open domain D, and $\mathbf{y}(0)$ in D. The outward normal $\mathbf{n}(\mathbf{x})$ to the boundary ∂D exists, except for a finite number of isolated points. Then $\mathbf{y}(t)$ never leaves the closure of D, if $\mathbf{f}(\mathbf{x}) \bullet \mathbf{n}(\mathbf{x}) \le 0$ on ∂D.

- **Corollary**

Let y satisfy the differential inequality $y' \le f(y)$, f Lipschitz-L, and z be a solution to $z' = f(z)$ with $z(0) \ge y(0)$. Then $y(t) \le z(t)$ for $t > 0$.

• **Logarithmic norm** of a matrix

$$\mu[\mathbf{A}] = \lim_{\varepsilon \to 0+} \frac{\| \mathbf{I} + \varepsilon \mathbf{A} \| - 1}{\varepsilon}$$

• **Perturbation estimate**

$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \mathbf{y}(0) = \mathbf{y}0;$

$\mathbf{z}' = \mathbf{f}(\mathbf{z}) + \mathbf{g}(\mathbf{z},t), \mathbf{z}(0) = \mathbf{z}0,$

Assume a priori the existence of a domain D with $\mathbf{y}(t)$, $0 \le t \le T$, and $\mathbf{z}0$ in D, such that $\mathbf{f}$ is Lipschitz-L in D.

The difference $\mathbf{e} = \mathbf{y} - \mathbf{z}$ satisfies the differential inequality

$\|\mathbf{e}\|' \le \mu(t)\|\mathbf{e}\| + \|\mathbf{g}(\mathbf{z}(t),t)\|, \|\mathbf{e}(0)\| = \|\mathbf{y}0 - \mathbf{z}0\|$

where $\mu = \max_{\mathbf{x} \in D}\left(\mu\left[\mathbf{J}(\mathbf{x})\right]\right)$, and $\mathbf{J}$ is the Jacobian $\partial \mathbf{f}/\partial \mathbf{x}$.

The inequality holds for $t \le T^*$ where $T^* = \min(T,T^+)$ and T^+ is the largest t for which the inequality guarantees that $\mathbf{z}(t)$ is in D.

Models

The following models are all discussed in class. Note that the RHS (all zeros here) may well be some source terms $Q(x,t,u)$. These do not in general influence the most important features of the equations.

Conservation laws, 1D (+ time)

$u_t + q_x = Q$, $q = q(x,t,u,u_x)$ = flux function, Q = source term

Convective flux

$q = a(x,t,u)u$, a = advection velocity

Diffusive flux

$q = -C(x,t,u)u_x$

Fourier's law of heat conduction (u = temperature)

$q = -k\, u_x$, k = heat conductivity

Fick's law of diffusion (u = concentration)

$q = -Du_x$, D = diffusion coefficient

Hyperbolic	**Parabolic**	**Elliptic**
Wave operators with wave speed c: One-way / convection $u_t + cu_x = 0$ Standard $u_{tt} - c^2 u_{xx} = 0$ As first order system $u_t - c^2 p_x = 0$ $p_t - u_x = 0$ Maxwell $\varepsilon E_t - H_x = 0$, $\mu H_t - E_x = 0$ with $c = 1/\sqrt{\varepsilon\mu}$ Inviscid Burgers $u_t + u\, u_x = 0$ Schrödinger $i\, u_t - u_{xx} - V(x)u = 0$ Shallow water $h_t + (hu)_I = 0$ $(hu)_t + (hu^2 + 1/2h^2 g)_x = 0$	Convection-Diffusion $u_t + au_x - (Du_x)_x = 0$ Heat, Diffusion $u_t - \alpha\, u_{xx} = 0$ Burgers $u_t + u\, u_x - \varepsilon u_{xx} = 0$	Laplace operator Δ $\Delta u = u_{xx} + u_{yy}$ Poisson equation $\Delta u = f(x,y)$

Convergence of Euler's method

Assume

The initial value problem $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{c}$, $t \geq 0$.

1) $\mathbf{f}$ is Lipschitz-L. The existence of smooth solution $\mathbf{y}(t)$ on [0,T] follows. Let

$R = \max \|\mathbf{y}''(t)\|$ for $t \leq T$.

2) Initial values $\mathbf{y}_0(h)$ are chosen such that $\|\mathbf{E}_0\| = \| \mathbf{y}_0(h) - \mathbf{c} \| \to 0$ as $h \to 0$

The Euler scheme is

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n), \qquad (1)$$

and the exact solution satisfies

$$\mathbf{y}(t_{n+1}) = \mathbf{y}(t_n) + h\mathbf{f}(\mathbf{y}(t_n)) + 1/2\, h^2\, \mathbf{r}(t_n) \text{ with } \|\mathbf{r}\| \leq \mathrm{R} \qquad (2)$$

Note The mean value theorem in the form $\int_0^h f(t+s)ds = hf(t + \theta h)$

or a remainder term of the type in the Taylor series

$$f(t+h) = \sum_{j=0}^{n} \frac{h^j}{j!} f^{(j)}(t) + \frac{h^{n+1}}{(n+1)!} f^{(n+1)}(t + \theta h)$$

has no simple generalization to **vector** valued functions. An integral form is required,

$$\mathbf{y}(t+h) - \mathbf{y}(t) = \int_0^h \mathbf{y}'(t+s)ds = \int_0^h \left(\mathbf{y}'(t) + \int_0^s \mathbf{y}''(t+p)dp \right) ds \Rightarrow$$

$$\Rightarrow \| \mathbf{y}(t+h) - \mathbf{y}(t) - h\mathbf{y}'(t) \| \leq \frac{h^2}{2} \max_{t \leq \xi \leq t+h} \left\| \mathbf{y}''(\xi) \right\|$$

Introducing the **global error** $\mathbf{E}_n = \mathbf{y}_n - \mathbf{y}(t_n)$ the subtraction of (2) from (1) gives

$$\mathbf{E}_{n+1} = \mathbf{E}_n + h(\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{y}(t_n)) - 1/2\, h^2\, \mathbf{r}(t_n)$$

and for the norm $e_n = \|\mathbf{E}_n\|$, using the Lipschitz continuity,

$$e_{n+1} \leq e_n + hLe_n + 1/2\, h^2 R = (1 + hL)e_n + 1/2\, h^2 R$$

Lemma (Exercise: Prove!)

If $u_{n+1} = Au_n + B$, $u_0 = b$, $u_n = bA^n + B/(1-A)\,(A^n - 1)$

It follows that

$$e_n \leq \| \mathbf{E}_0 \| (1 + hL)^n + hR \frac{(1+hL)^n - 1}{L} \leq \| \mathbf{E}_0 \| e^{nhL} + hR \frac{e^{nhL} - 1}{L} =$$

$$= \| \mathbf{E}_0 \| e^{Lt_n} + hR \frac{e^{Lt_n} - 1}{L}$$

and if $\mathbf{E}_0 = 0$ (easy!) the error is $O(h)$.

How to test your PDE solver - some hints

We assume that the code works and produces results that seem stable on the first test case you have devised. So you are very happy ... but much remains before the solver can be considered tested. In a KTH course we will focus just on the *numerics* for the given simple equations whereas industrial validation of a code also must address the *models* - more or less heuristic - for the physical phenomena such as turbulence, combustion, conditions at "infinite" boundaries, etc.

There will always be physical parameters in the model, like gravitational acceleration, viscosity coefficients, etc., and of course the parameters of the discretization and method - stepsizes, tolerances, number of multi-grid levels, …
The basic idea of testing is to change parameters and verify that the numerical results are consistent with what you know about the model and method.
Here are a few suggestions.

1. Choose parameters that allow an analytical solution. Ex: constant material properties, no gravity, no viscous forces, periodic conditions, …
2. Check that the solutions converge as Δx, Δy , Δt –> 0. If you know what the order of consistency should be, say p, check that by looking at $\|u_h - u_{2h}\| / \|u_{2h} - u_{4h}\|$ which should be approximately $(1/2)^p$.
3. Check that tolerances, artificial diffusion, etc., do influence the solution; **Caveat:** It may be hard to guess what the natural range for these parameters is ("Is 10^{-6} small ?? Is Re = 1000 a *large* Reynolds number ? … ")
4. The order of consistency may be hard to check, especially if it is more than two. Always include coding for non-zero source functions for all the equations, PDE and boundary conditions alike. Then it is always possible to compute the source functions for any prescribed exact solution. This is sometimes called the MMS -

Method of Manufactured Solutions

Recipe:
Let the equations be

$$P(\partial t, \partial x, \partial y, u, x, y, t) = f(x,y,t)$$

with boundary conditions

$$B(\partial x,\partial y, u, x, y, t) = g(x,y,t)$$

and initial conditions

$$u = U$$

This problem has the solution w(x,y,t) if f and g are computed from w as

$$f(x,y,t) = P(\partial t,\partial x,\partial y,w(x,y,t),x,y,t)$$
$$g(x,y,t) = B(\partial x,\partial y, w(x,y,t), x, y, t)$$
$$U(x,y,0) = w(x,y,0)$$

Of course, it is a chore to compute $P(\ldots)$ etc. Choosing w as a linear combination of sines, cosines and exponential functions has several advantages:

- Derivatives are easy
- It is easy to change the spatial and temporal rates of change to see how the grid resolution influences the solution.

Example

As an example of the source function method, consider the incompressible Navier-Stokes equations driven by body forces (F,G) on a square $[0,1]^2$. At y = 0 and 1, u = v = 0, at x = 0, u(y) = U(y), v = 0; at x = 1: v = 0, ∂u/∂x = 0.

$$\begin{cases} u_x + v_y = 0 \\ u_t + uu_x + vu_y + p_x = \mathrm{Re}^{-1}\left(u_{xx} + u_{yy}\right) + F \\ v_t + uv_x + vv_y + p_y = \mathrm{Re}^{-1}\left(v_{xx} + v_{yy}\right) + G \end{cases}$$

Write the code for

$$\begin{cases} u_x + v_y = D(x,y,t) \\ u_t + uu_x + vu_y + p_x = \mathrm{Re}^{-1}\left(u_{xx} + u_{yy}\right) + F(x,y,t) \\ v_t + uv_x + vv_y + p_y = \mathrm{Re}^{-1}\left(v_{xx} + v_{yy}\right) + G(x,y,t) \end{cases}$$

$$u(x,0,t) = U(x,0,t); v(x,0,t) = V(x,y,t)$$
$$u(x,1,t) = U(x,1,t); v(x,1,t) = V(x,1,t)$$
$$u(0,y,t) = U(0,y,t); v(0,y,t) = V(0,y,t);$$
$$\partial u/\partial x(1,y,t) = \partial U/\partial x(1,y,t); \partial v/\partial x(1,y,t) = \partial V/\partial x(1,y,t);$$

so, as an example, for

U(x,y,t) = A sin at sin bx sin cy
V(x,y,t) = B sin dt sin ex sin fy
P(x,y,t) = C sin gt sin hx sin iy

we need only choose

D = Ab sin at cos bx sin cy + Bf sin dt sin ex cos fy
$F = U_t + UU_x + VU_y + P_x - \mathrm{Re}^{-1} (U_{xx} + U_{yy})$
$G = V_t + UV_x + VV_y + P_y - \mathrm{Re}^{-1} (V_{xx} + V_{yy})$

for the exact solution to be u = U, v = V.
Caveat - For the NS equations solved by the projection method we use ∂p/∂n = 0 as boundary condition *but that must also be changed to include a source* if we are to specify an arbitrary *P* !