Splitting methods, part 1

1. Introduction to splitting methods

initial value problem

$$y' = f(y) + g(y), \qquad y(0) = y_0$$

split vector field

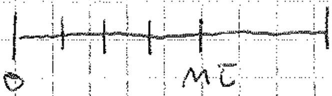
$$v' = f(v), \quad v(0) = v_0 \;\rightarrow\; \varphi_t^{[f]}(v_0) = v(t)$$

$$w' = g(w), \quad w(0) = w_0 \;\rightarrow\; \varphi_t^{[g]}(w_0) = w(t)$$

exact flow

choose step size τ

let $t_n = n\tau$



$$y(\tau) \approx y_1 = \varphi_\tau^{[g]} \circ \varphi_\tau^{[f]}(y_0) = L_\tau(y_0)$$

Lie-Trotter splitting (1959)

is a one-step method

$$y_{n+1} = L_\tau(y_n)$$

Why can this be a good idea?

Example. linear vector field $f(y) = Ay$, $g(y) = By$

$$y(t) = e^{\tau(A+B)} y_0$$

$$\varphi_\tau = e^{\tau(A+B)}, \qquad L_\tau = e^{\tau B} e^{\tau A}$$

splitting error

$$e^{\tau A} = I + \tau A + \frac{\tau^2}{2} A^2 + O(\tau^3)$$

depends on what?

$$e^{\tau B} e^{\tau A} = I + \tau A + \frac{\tau^2}{2} A^2 + \tau B + \tau^2 BA + \frac{\tau^2}{2} B^2 + O(\tau^3)$$

$$= I + \tau(A+B) + \frac{\tau^2}{2}(A+B)^2 + \frac{\tau^2}{2}\underbrace{(BA - AB)}_{[B,A]} + O(\tau^3)$$

$$= e^{\tau(A+B)} + \frac{\tau^2}{2}[B,A] + O(\tau^3)$$

splitting error

(no error if A and B commute)

general approach:
Baker - Campbell - Hausdorff (BCH) formula

$$e^{tB} e^{tA} = e^{tC(t)} \quad \text{with}$$

$$C(t) = C_1 + tC_2 + t^2 C_3 + \cdots$$

$$C_1 = A + B, \qquad C_2 = \frac{1}{2}[B,A]$$

$$C_3 = \frac{1}{12}[B,[B,A]] + \frac{1}{12}[A,[A,B]]$$

etc.

The nonlinear case.

$$\varphi_\tau^{[f]}(v_0) = v_0 + \tau f(v_0) + \frac{\tau^2}{2} f'(v_0) f(v_0) + O(\tau^3)$$

$$\varphi_\tau^{[g]}(w_0) = \ldots$$

$$L_\tau(y_0) = y_1 = y_0 + \tau f(y_0) + \frac{\tau^2}{2} f'(y_0) f(y_0)$$
$$+ \tau g(y_0 + \tau f(y_0) + O(\tau^2))$$
$$+ \frac{\tau^2}{2} g'(y_0 + O(\tau))\, g(y_0 + O(\tau)) + O(\tau^3)$$

$$= y_0 + \tau\big(f(y_0) + g(y_0)\big)$$
$$+ \frac{\tau^2}{2} f'(y_0) f(y_0) + \tau^2 g'(y_0) f(y_0)$$
$$+ \frac{\tau^2}{2} g'(y_0) g(y_0) + O(\tau^3)$$

$$= y(\tau) + \frac{\tau^2}{2} \underbrace{(g'f - f'g)}_{[g,f]}(y_0) + O(\tau^3)$$

$[g,f]$ Lie commutator

annoyingly similar to the linear case

(→ explanation: Lie calculus, later)

The splitting is first-order convergent.

Convergence of one step methods

$$y' = F(y) = f(y) + g(y), \quad y(0) = y_0$$

$y_n \approx y(n\tau)$ step size τ

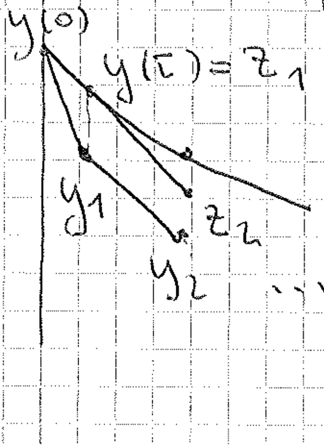
numer. scheme $\quad y_{n+1} = \Phi_\tau(y_n)$

Assumptions:

- local error
$$\| y(t+\tau) - \Phi_\tau(y(t)) \| \le C \tau^{p+1}$$
uniformly on $[0, T-\tau]$
- locally Lipschitz continuous
$$\| \Phi_\tau(v) - \Phi_\tau(w) \| \le \big(\overbrace{1+\tau L}^{\le e^{\tau L}}\big) \| v - w \| \quad \leftarrow \text{clear for splitting}$$
$$v, w \in B_R(y(t)), \quad 0 \le t \le T$$

Then: convergence of order p
$$\| y(n\tau) - \Phi_\tau^n(y_0) \| \le C \tau^p$$
uniformly on $0 \le n\tau \le T$

Proof: Lady Windermere's Fan



stability:
$$\| \Phi_\tau^{n-1}(z_1) - \Phi_\tau^{n-1}(y_1) \| \le \underbrace{(1+\tau L)^{n-1}}_{\le e^{(n-1)\tau L}} \| z_1 - y_1 \|$$

The adjoint scheme

Let $y' = F(y)$ with exact solution

$$y(t) = \varphi_t(y_0)$$

numerical one-step approximation

$$y_{n+1} = \Phi_\tau(y_n)$$

Definition: The map

$$\Phi_\tau^* := (\Phi_{-\tau})^{-1}$$

is called adjoint of Φ_h.

A method is called symmetric if

$$\Phi_\tau^* = \Phi_\tau$$

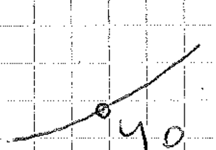
(Q. Why is the adjoint well-defined? Flow maps are perturbations of the identity)

Examples.

(i) The exact flow is symmetric

$$(\varphi_{-\tau})^{-1} = \varphi_\tau$$

(local uniqueness of solution)



(ii) forward Euler method

$$y_1 = y_0 + \tau F(y_0) = \Phi_\tau(y_0)$$

inverse : $y_1 \leftrightarrow y_0$
step size : $\tau \leftrightarrow -\tau$

$$y_0 = y_1 - \tau F(y_1)$$

or $$y_1 = y_0 + \tau F(y_1) = \Phi^*_\tau(y_0)$$

backward Euler

(iii) midpoint rule (Gauß, $s=1$)

$$y_1 = y_0 + \tau F\left(\frac{y_1+y_0}{2}\right)$$

is symmetric.

The adjoint of the splitting is the splitting in <u>reversed</u> order

$$L_\tau = \varphi_\tau^{[g]} \circ \varphi_\tau^{[f]} , \quad L_\tau^* = \varphi_\tau^{[f]} \circ \varphi_\tau^{[g]}$$

Composition with its adjoint gives a symmetric method :

$$\left(\Phi_\tau^* \circ \Phi_\tau\right)^* = \Phi_\tau^* \circ \Phi_\tau$$

Strang splitting

Strang, Marchuk 1968

$$S_\tau = L^*_{\tau/2} \circ L_{\tau/2}$$
$$= \varphi^{[f]}_{\tau/2} \circ \varphi^{[g]}_{\tau} \circ \varphi^{[f]}_{\tau/2}$$

symmetric
second order (metatheorem in numerical analysis)
↳ see, however, later.

Higher order schemes

several possibilities, just two important approaches

(a) Exponential splitting methods

Let $\alpha_1, \dots, \alpha_s$, $\beta_1, \dots, \beta_s$ be given numbers
The scheme

$$\Phi_\tau = \varphi^{[g]}_{\beta_s\tau} \circ \varphi^{[f]}_{\alpha_s\tau} \circ \dots \circ \varphi^{[f]}_{\alpha_2\tau} \circ \varphi^{[g]}_{\beta_1\tau} \circ \varphi^{[f]}_{\alpha_1\tau}$$

is called exponential splitting method (with s stages)
Example.

(i) $s = 1$, $\beta_1 = \alpha_1 = 1$ Lie

(ii) $s = 2$, $\beta_1 = 1$, $\beta_2 = 0$, $\alpha_1 = \alpha_2 = \frac{1}{2}$ Strang

Order conditions with the help of the BCH formula (justification for the nonlinear case later!)

Example.

$$e^{\alpha_2\tau A}\, e^{\beta_1\tau B}\, e^{\alpha_1\tau A} =$$

$$= e^{\alpha_2\tau A}\, e^{\alpha_1\tau A + \beta_1\tau B + \alpha_1\beta_1\frac{\tau^2}{2}[B,A] + O(\tau^3)}$$

$$= e^{(\alpha_1+\alpha_2)\tau A + \beta_1\tau B + \alpha_2\beta_1\frac{\tau^2}{2}[A,B] + \alpha_1\beta_1\frac{\tau^2}{2}[B,A] + O(\tau^3)}$$

$$= e^{\tau(A+B)} + O(\tau^3) \quad \text{falls}$$

$$\left.\begin{aligned} \alpha_1+\alpha_2 &= 1 \\ \beta_1 &= 1 \\ \alpha_2\beta_1 &= \alpha_1\beta_1 \end{aligned}\right\} \quad \begin{aligned} \beta_1 &= 1 \\ \alpha_1 = \alpha_2 &= \tfrac{1}{2} \end{aligned} \quad \text{Strang}$$

(b) Composition methods

Let ψ_τ be a basic method, choose numbers $\gamma_1, \dots, \gamma_s$

The method

$$\Phi_\tau = \psi_{\gamma_s\tau} \circ \dots \circ \psi_{\gamma_1\tau}$$

is called composition of ψ with stepsizes $\gamma_1\tau, \dots, \gamma_s\tau$.

<u>Theorem</u>. Let Ψ_τ be of order p and

$$\gamma_1 + \dots + \gamma_s = 1$$

$$\gamma_1^{p+1} + \dots + \gamma_s^{p+1} = 0 \qquad (*)$$

Then Φ_τ is of order $p+1$ at least.

(real coefficients γ and $(*)$ require p even)

Proof. Taylor expansion. (see <u>Moch</u>!)

<u>application</u>:

choose Ψ_τ symmetric (e.g. Strang)
(hence p even)

and $\gamma_i = \gamma_{s+1-i}$, $i = 1, \dots, s$

Then Φ_τ is symmetric, hence of even order and construction can be done recursively (with Φ in place of Ψ, etc.)

$s = 3$ and Strang $\rightarrow$ "triple jump"

$s = 5$ and $\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5$

$\rightarrow$ "Suzuki's fractal"

<u>triple jump</u>: $2\gamma_1 + \gamma_2 = 1$ (negative!)
for order 4 $\quad 2\gamma_1^3 + \gamma_2^3 = 0$, $\gamma_2 = -\sqrt[3]{2}\,\gamma_1$

$$\gamma_1 = \frac{1}{2 - \sqrt[3]{2}} \approx 1'35120719\ldots$$

(Strang 1989)

<u>Theorem.</u> If an exponential splitting scheme is of order $p \geq 3$, then at least one α_i and one β_j must be negative.

(HLW, III.3.4)

<u>Example</u>

symmetric order 4 composition of Strang splitting : $\gamma_2 < 0$

$$\cdots \varphi^{[f]}_{\tau\gamma_2/2} \circ \varphi^{[g]}_{\tau\gamma_2} \circ \varphi^{[f]}_{\tau\gamma_2/2} \circ \varphi^{[f]}_{\tau\gamma_1/2} \cdots$$

$$\left| \begin{array}{l} \tau\gamma_2 < 0 \\ \frac{1}{2}\tau(\gamma_1+\gamma_2) < 0 \end{array} \right.$$

↳ Problems with semiflows (e.g. parabolic problems)

<u>Solution</u>: complex time steps

$$2\gamma_1 + \gamma_2 = 1, \quad \gamma_1 = \sigma, \quad \gamma_2 = 1-2\sigma$$

$$2\sigma^3 + (1-2\sigma)^3 = 0$$

$$\left(\frac{\sigma}{1-2\sigma}\right)^3 = -\frac{1}{2} \qquad \sqrt[3]{-1} = \begin{cases} -1 \\ \pm e^{i\frac{\pi}{3}} \end{cases}$$

$$\frac{\sigma}{1-2\sigma} = \frac{1}{\sqrt[3]{2}} e^{i\frac{\pi}{3}}$$

$$\left(1 + \frac{2}{\sqrt[3]{2}} e^{i\frac{\pi}{3}}\right)\sigma = \frac{1}{\sqrt[3]{2}} e^{i\pi/3}$$

$$\sigma = \frac{e^{i\pi/3}}{2^{1/3} + 2e^{i\pi/3}} \approx 0.071847 + 0.124427i$$

A prototypical PDE:

(cubic) nonlinear Schrödinger eq.

$$i u_t = (-\Delta + |u|^2) u$$

with periodic boundary conditions

In previous notation

(a) $f(u) = Au = i\Delta u$

$$\varphi_t^{[1]} = e^{it\Delta}$$ (actually computed with FFT techniques)

(b) $g(u) = -i|u|^2 u$

Flow can be computed exactly.

$$w_t = g(w)$$

$$i w_t \bar{w} = |w|^4 \in \mathbb{R}$$

Thus $w_t \bar{w} \in i\mathbb{R}$ and

$$\underbrace{|w|^2_t}_{\in \mathbb{R}} = w_t \bar{w} + \bar{w}_t w \quad \in i\mathbb{R}$$

Hence $|w|^2_t = 0$, $\quad w(t) = e^{-it|w_0|^2} w_0$

Strang and its composition give efficient splitting methods of high order

Error analysis for a linear problem
(see Jahnke, Lubich 2000)

Consider $u_t = Au + Bu$
(in the situation before: $A = i\Delta$
and $B = -iV(x)$ bounded)

Exact solution:

$$u(\tau) = e^{\tau(A+B)} u_0$$

Lie splitting:

$$u_1 = e^{\tau B} e^{\tau A} u_0$$

Error analysis by Taylor series is
not appropriate (why?)

However, $e^{\tau B}$ can be expanded

$$e^{\tau B} = I + \tau B + \underbrace{O(\tau^2)}_{\|B\|^2}$$

Lie splitting

$$u_1 = e^{\tau A} u_0 + \tau B e^{\tau A} u_0 + O(\tau^2)$$

exact solution: variation of constants

$$u(\tau) = e^{\tau A} u_0 + \int_0^\tau e^{(\tau - s)A} B u(s)\, ds$$

$$= e^{\tau A} u_0 + \int_0^\tau e^{(\tau-s)A} B e^{sA} u_0 \, ds + \underbrace{\int_0^\tau \int_0^s e^{(\tau-s)A} B e^{(s-\xi)A} B u(\xi) \, d\xi \, ds}_{= O(\tau^2)}$$

$\|B\|^2$

$$F(s) = e^{(\tau-s)A} B e^{sA} u_0$$

$$\int_0^\tau F(s) \, ds = \int_0^\tau \left(F(\tau) - \int_s^\tau F'(\xi) \, d\xi \right) d\tau$$

$$= \tau F(\tau) - \int_0^\tau \int_s^\tau F'(\xi) \, d\xi \, ds$$

$$F'(s) = e^{(\tau-s)A} \underbrace{[B, A]}_{} e^{sA} u_0$$

boundedness requires spatial smoothness

For the Schrödinger equation:

$$[B, A] w = V \Delta w - \Delta (V w) =$$

$$= V \Delta w - \nabla \cdot (V \nabla w + w \nabla V) =$$

$$= -2 \nabla V \cdot \nabla w - w \Delta V$$

If F' is (uniformly) bounded, we have

$$u_1 - u(\tau) = O(\tau^2)$$

first-order for ~~[illegible]~~ Lie splitting.

Convergence:

a) telescopic identity

$$a^3 - b^3 = a^3 - a^2 b + a^2 b - a b^2 + a b^2 - b^3$$

$$= a^2(a-b) + a(a-b)b + (a-b)b^2$$

$$a^n - b^n = \sum_{k=0}^{n-1} a^{n-k-1} (a-b) b^k$$

b) $L_\tau^n(u_0) - u(n\tau) =$

$$= \left(\left(e^{\tau B} e^{\tau A}\right)^n - e^{n\tau(A+B)} \right) u_0$$

$$= \sum_{k=0}^{n-1} \left(e^{\tau B} e^{\tau A}\right)^{n-k-1} \left(\underbrace{L_\tau(u(k\tau)) - u((k+1)\tau)}_{= O(\tau^2)} \right)$$

spatial smoothness of exact solution

$$\left.\begin{array}{l} \|e^{\tau B}\| \leq e^{\tau \|B\|} \\ \|e^{\tau A}\| = 1 \end{array}\right\} \to \text{stability}$$

c) $$\|L_\tau^n(u_0) - u(n\tau)\| \leq \underbrace{n\tau}_{\leq T} e^{n\tau\|B\|} \cdot C \cdot \tau$$

local error

$$\leq C\tau \qquad \square$$

Gröbner – Alekseev formula

Semilinear case

$$f' = Gf + R(f)$$

$$g' = Gg \qquad E_G(t, g_0) = e^{tG} g_0$$

$$\partial_2 E_G(t, g_0) = e^{tG} \quad \text{and}$$

$$f(t) = e^{tG} f_0 + \int_0^t e^{(t-s)G} R(f(s))\, ds$$

variation-of-constants formula

Proof of GA formula.

Let u be a solution of

$$u'(t) = G(u(t))$$

Then

$$u(t) = E_G(t-s, u(s))$$

Differentiate with respect to s

$$0 = -\partial_1 E_G(t-s, u(s)) + \partial_2 E_G(t-s, u(s))\, G(u(s))$$

(Choose initial value $u(s) := f(s)$

This shows

$$0 = -\partial_1 E_G(t-s, f(s)) + \partial_2 E_G(t-s, f(s))\, G(f(s))$$

Let $\psi(s) = E_G(t-s, y(s))$

$$\psi(t) - \psi(0) = \int_0^t \psi'(s)\,ds$$

$$y(t) - E_G(t, y_0)$$

$$= \int_0^t \left(-\partial_1 E_G(t-s, y(s)) + \partial_2 E_G(t-s, y(s))\,y'(s)\right) ds$$

$$= \int_0^t \partial_2 E_G(t-s, y(s))\, R(y(s))\,ds \qquad \square$$

Appearance of φ functions

$$\varphi_k(z) = \frac{1}{z^k}\left(e^z - \left(1 + z + \dots + \frac{z^{k-1}}{(k-1)!}\right)\right)$$

$$= \sum_{\ell=0}^{\infty} \frac{z^\ell}{(\ell+k)!} \qquad \text{(entire function)}$$

and $\varphi_0(z) = e^z$

Thus

$$e^{\tau E} = \sum_{j=0}^{k-1} \frac{\tau^j}{j!} E^j + \tau^k E^k \varphi_k(\tau E)$$

Expansion of numerical solution

anticommutator $\{E_1, E_2\} =$

$$= E_1 E_2 + E_2 E_1$$

$$e^{\tau A} = I + \tau A \varphi_1(\tau A)$$
$$= I + \tau A + \tau^2 A^2 \varphi_2(\tau A)$$
$$= I + \tau A + \frac{\tau^2}{2} A^2 + \tau^3 A^3 \varphi_3(\tau A)$$

$$e^{\tau/2 A} e^{\tau B} e^{\tau/2 A} =$$

$$= e^{\tau B} + \frac{\tau}{2} e^{\tau B} A + \frac{\tau^2}{8} e^{\tau B} A^2$$
$$+ \frac{\tau}{2} A e^{\tau B} + \frac{\tau^2}{4} A e^{\tau B} A$$
$$+ \frac{\tau^2}{8} A^2 e^{\tau B} + R_3$$

$$= e^{\tau B} + \{A, e^{\tau B}\} + \{A, \{A, e^{\tau B}\}\} + R_3$$

Lie Calculus

Consider differential equation

$$y' = f(y), \quad y \in \mathbb{R}^d$$

derivative along vector field f
(Lie derivative)

$$D = \sum_{j=1}^{d} f_j \partial_j$$

Let $F : \mathbb{R}^d \to \mathbb{R}^m$ be smooth

$$DF = \sum_{j=1}^{d} f_j \underbrace{\partial_j F}_{j\text{th column of Jacobian}}$$

$$= F' f$$

Denote again $\varphi_t(y_0) = y(t)$, then

$$\frac{d}{dt} F(\varphi_t(y_0)) = F'(\varphi_t(y_0)) \cdot f(\varphi_t(y_0))$$

$$= (\underbrace{DF}_{G})(\varphi_t(y_0))$$

$$\frac{d^2}{dt^2} F(\varphi_t(y_0)) = (DG)(\varphi_t(y_0)) =$$

$$= (D^2 F)(\varphi_t(y_0))$$

etc.

hence

$$\frac{d^k}{dt^k} F(\varphi_t(y_0))\Big|_{t=0} = (D^k F)(y_0)$$

and (Taylor)

$$F(\varphi_t(y_0)) = \sum_{k=0}^{\infty} \frac{t^k}{k!} (D^k F)(y_0) =$$

$$(*) \qquad = (e^{tD} F)(y_0)$$

In particular, for $F = id$

$$\varphi_t(y_0) = \sum_{k=0}^{\infty} \frac{t^k}{k!} (D^k id)(y_0) = (e^{tD} id)(y_0)$$

representation of exact flow.

Consider again

$$y' = f(y) + g(y)$$

and splitting

$$v' = f(v), \quad v(t) = \varphi_t^{[f]}(v_0)$$

$$w' = g(w), \quad w(t) = \varphi_t^{[g]}(w_0)$$

<u>Permutation lemma</u> (Gröbner, 1960).

$$\varphi_t^{[g]} \circ \varphi_s^{[f]}(y_0) = (e^{sD_f} e^{tD_g} id)(y_0)$$

Proof. Formula (*) shows

$$F(\varphi_s^{[f]}(y_0)) = (e^{sD_f} F)(y_0)$$

choose $F = \varphi_t^{[g]} = e^{tD_g}\,\mathrm{id}$ $\square$

Lemma suggests to apply BCH formula.
However, D_f and D_g are (unbounded) differential operators; series will not converge.
Truncated series, applied to smooth functions, however is sensible
(→ justifies formal manipulation with series)

$$e^{tD_f} e^{tD_g} = e^{tD(t)}$$

$$D(t) = D_1 + tD_2 + t^2 D_3 + \dots$$

$$D_1 = D_f + D_g$$

$$D_2 = \tfrac{1}{2}[D_f, D_g]$$

$$D_3 = \tfrac{1}{12}[D_f,[D_f,D_g]] + \tfrac{1}{12}[D_g,[D_g,D_f]]$$

etc.

Note 1101

$$[D_f, D_g] = D_f D_g - D_g D_f =$$

$$= \sum_{j,l} f_l \partial_l (g_j \partial_j) - \sum_{j,l} g_l \partial_l (f_j \partial_j)$$

$$= \sum (\partial_l g_j \, f_l - \partial_l f_j \, g_l) \partial_j$$

$$= D_{[g,f]}$$

where the Lie bracket $[g,f]$ is defined as

$$[g,f] = g'f - f'g$$

(Jacobian times vector)

$\Rightarrow$ this finally permits to work

(see also 1-3).

<u>Consequence</u>. Same order conditions for linear and non-linear vector fields.

Relation between Lie series and elementary differentials

$$y' = f(y)$$

$$y'' = f'(y)\,y' = f'(y)\,f(y)$$

$$y''' = f''(y)\big(f(y), f(y)\big) + f'(y)\,f'(y)\,f(y)$$

$$y(t) = y_0 + t\,f(y_0) + \frac{t^2}{2} f'(y_0)\,f(y_0)$$

$$+ \frac{t^3}{6}\Big(f''(y_0)\big(f(y_0), f(y_0)\big) + f'(y_0)\,f'(y_0)\,f(y_0)\Big) + O(t^4)$$

$$y(t) = \varphi_t(y_0) = \left(e^{tD}\,\mathrm{id}\right)(y_0) =$$

$$= y_0 + t\,(D\,\mathrm{id})(y_0) + \frac{t^2}{2}(D^2\,\mathrm{id})(y_0)$$

$$+ \frac{t^3}{6}(D^3\,\mathrm{id})(y_0) + O(t^4)$$

$$D\,\mathrm{id} = \mathrm{id}'\,f = f$$

$$D^2\,\mathrm{id} = D f = f' f$$

$$D^3\,\mathrm{id} = D f' f = f''(f,f) + f' f' f$$

Method of characteristics for quasilinear hyperbolic problems

$$u_t + Q(t,x,u)\,u_x = 0$$

Find $x = x(t)$ such that

$$u(t, x(t)) = \text{const} = u(0, x_0)$$

$$0 = \frac{d}{dt} u(t, x(t)) = u_t + u_x x'$$
$$\stackrel{!}{=} u_t + Q(t,x,u)\,u_x$$

$$x' = Q(t, x, u(0, x_0))$$

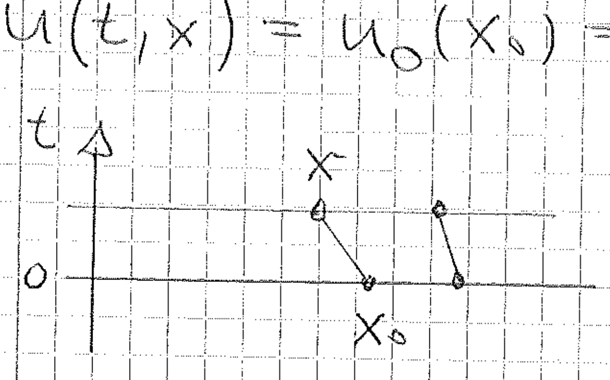
Burgers' equation: $Q(t,x,u) = 6u$

$$x(t) = x_0 + 6t\,u_0(x_0)$$

$$x_0 = x - 6t\,u(t,x)$$

hence

$$u(t,x) = u_0(x_0) = u_0(x - 6t\,u(t,x))$$



slope depends on u

solve with fixed-point iteration
(and interpolation)

Convergence of modified Lie splitting

original problem

$$\begin{cases} u_t = Du + f(u) \\ u|\partial\Omega = b \\ u(0) = u_0 \end{cases}$$

reduction to homog. boundary conditions: solve

$$\begin{cases} Dz = 0 \\ z|\partial\Omega = b \end{cases}$$

and call difference $u - z$ again u

$$u_t + z_t = \underbrace{Du}_{A} + \underbrace{Dz}_{=0} + f(u+z)$$

A generator of analytic semigroup (as u now satisfies homog. b.c.)

Thus

$$u_t = Au + f(u+z) - \underbrace{z_t}_{\text{zero if } b \text{ does not depend on } t}$$

Study splitting of

$$u_t = Au + g(t,u) + k(t)$$

into the sub problems

$$v_t = Av + k(t)$$

$$w_t = g(t,w)$$

classic version: $k(t) = -z_t$

$$g(t,w) = f(w+z)$$

the step from t_n to t_{n+1}:

solve $w_t = g(t,w)$ with $w(t_n) = \eta$

$$w(t_n+\tau) = w(t_n) + \tau\, w'(t_n) + \int_0^\tau (\tau-s)\, w''(t_n+s)\,ds$$

$$\varphi_\tau^{[g]}(\eta) = \eta + \tau\, g(t_n,\eta) + \int_0^\tau (\tau-s)\, w''(t_n+s)\,ds$$

next solve

$v_t = Av + k(t)$ with $v(t_n) = \zeta$

$$v(t_n+\tau) = e^{\tau A}\zeta + \int_0^\tau e^{(\tau-s)A} k(t_n+s)\,ds$$

$$\parallel$$

$$\varphi_\tau^{[A,k]}(\zeta)$$

Lie step

$$L_\tau \eta = \varphi_\tau^{[A,k]} \circ \varphi_\tau^{(g)}(\eta) =$$

$$= e^{\tau A}\eta + \tau e^{\tau A} g(t_n,\eta) + \int_0^\tau e^{(\tau-s)A} k(t_n+s)\,ds$$

$$+ \int_0^\tau e^{\tau A}(\tau-s)\,w''(t_n+s)\,ds$$

exact solution with initial value η.

$$u(t_n+\tau) = e^{\tau A}\underbrace{u(t_n)}_{=\eta} + \int_0^\tau e^{(\tau-s)A} k(t_n+s)\,ds$$

$$+ \int_0^\tau e^{(\tau-s)A} g(t_n+s, u(t_n+s))\,ds$$

local error

$$L_\tau u(t_n) - u(t_n+\tau) =$$

$$= \int_0^\tau e^{\tau A}(\tau-s)\,w''(t_n+s)\,ds - \int_0^\tau\int_0^s l_n'(\sigma)\,d\sigma$$

where

$$l_n(\sigma) = e^{(\tau-\sigma)A} g(t_n+\sigma, u(t_n+\sigma)).$$

local error is $O(\tau^2)$ if $l_n'(\sigma)$ is bounded

However:

$$l_n'(\sigma) = -e^{(\tau-\sigma)A} A\, g(\ldots) + e^{(\tau-\sigma)A}\frac{d}{d\sigma} g(\ldots)$$

The problem comes from

$$A\,\underbrace{g(t_n+\tau,\,u(t_n+\tau))}$$

smooth, but does not satisfy boundary conditions of A

u satisfies homog. Dirichlet b.c.

but $g(t,0) = f(z)$ has boundary values $f(b) \neq 0$, in general.

Remedy: modified splitting

$$u_t = Au + g(t,u) + k(t)$$

$$g(t,u) = f(u+z) - f(z)$$

$$k(t) = f(z) - z_t$$

in this setting

$$g(t,0) = 0 .$$