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Dynamical Low–Rank Approximation for wave phenomena

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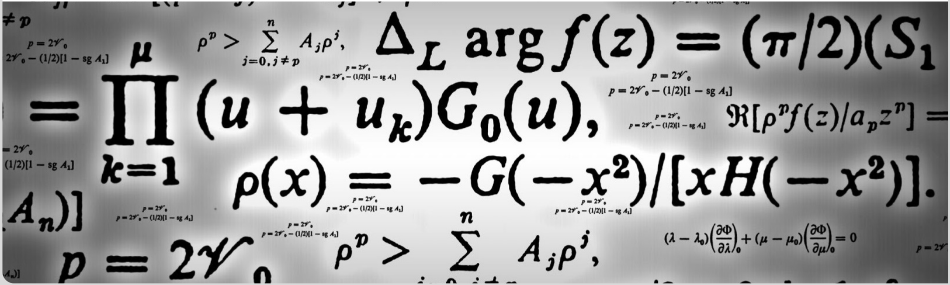

Motivation

Given: Matrix–ODE

$$A'(t) = F(A(t)), \quad A(t_0) = A_0, \tag{A}$$

solution bounded in space $\forall t \in [t_0, T]$.

For all $t \in [t_0, T]$ only some of the a_{ij} are nonzero.

Idea: Use approximation $Y_0 \approx A_0$ with $\operatorname{rank} Y_0 \ll \operatorname{rank} A_0$, solve

$$Y'(t) = G(Y(t)), \quad Y(t_0) = Y_0, \tag{Y}$$

instead of (A), with $A(t) \approx Y(t)$ for all $t \in [t_0, T]$.

Best–approximation

- exact solution of (A) not known $\rightsquigarrow$ use numerical solution
- possible approach: best–approximation by matrix with lower rank

Definition

Let $m, n \in \mathbb{N}$, $r \leq \min\{m, n\}$.

$$\mathcal{M}_r := \{X \in \mathbb{C}^{m \times n} : \mathrm{rank}(X) = r\}$$

denotes the manifold of rank–r–matrices.

For all $t \in [t_0, T]$ use best–approximation in Frobenius norm to $A(t)$ with rank r, i.e. $X(t) \in \mathcal{M}_r$ with

$$\|X(t) - A(t)\|_F = \min! \,. \tag{1}$$

Dynamical low–rank approximation

Ansatz for solving (1): $Y(t) \in \mathcal{M}_r$ fulfills

$$Y'(t) \in \mathcal{T}_{Y(t)}\mathcal{M}_r \quad \text{with} \quad \|Y'(t) - A'(t)\|_F = \text{min!} \quad \forall t \in [t_0, T].$$

- $\mathcal{T}_{Y(t)}\mathcal{M}_r$ denotes solution–dependend tangent space
- $Y'(t)$ as linear projection on $\mathcal{T}_{Y(t)}\mathcal{M}_r$ for given $Y(t)$
- advantage: extend model on situation (A):

$$Y'(t) \in \mathcal{T}_{Y(t)}\mathcal{M}_r \quad \text{with} \quad \|Y'(t) - F(Y(t))\|_F = \text{min!}$$

Decomposition of rank–r matrices

- decompose $Y \in \mathcal{M}_r$ in
$$Y = USV^H,$$
$U \in \mathbb{C}^{m\times r}$, $V \in \mathbb{C}^{n\times r}$ with
$$U^H U = I_r = V^H V, \quad S \text{ nonsigular}$$
- resemblance with economical variant of SVD, here S not assumed to be diagonal
- decomposition is not unique
- substitute for nonuniqueness: uniqueness in tangent space

Projector–splitting

- $Y = USV^H$,

  $Y' = P(Y)A' = A'VV^H - UU^HA'VV^H + UU^HA'$

  orthogonal projection on tangent space $\mathcal{T}_Y\mathcal{M}_r$

- Lie–Trotter splitting:

$$
\begin{aligned}
&\text{(i)} \quad \text{solve } Y_I' &&= A'V_IV_I^H, && Y_I(t_0) &&= Y_0 \\
&\text{(ii)} \quad \text{solve } Y_{II}' &&= -U_{II}U_{II}^HA'V_{II}V_{II}^H, && Y_{II}(t_0) &&= Y_I(t_1) \\
&\text{(iii)} \quad \text{solve } Y_{III}' &&= U_{III}U_{III}^HA', && Y_{III}(t_0) &&= Y_{II}(t_1)
\end{aligned}
$$

- IVPs exactly solvable!

Transfer to matrix-ODE $A'' = F(A)$

Transformation into system of first order ODEs

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- straightforward approach: transform

$$A'' = F(A)$$

into

$$A' = B,$$
$$B' = F(A)$$

and apply integrator from Lubich and Oseledets to

$$C' = G(C), \quad C := \begin{pmatrix} A \\ B \end{pmatrix} \in \mathbb{C}^{2m \times n}, \quad G(C) := \begin{pmatrix} B \\ F(A) \end{pmatrix}$$

- Rieger (2014): convergence degraded, robustness of integrator lost

Störmer–Verlet before Lie–Trotter

- Idea: Use two rank–r–approximations

$$A \approx Y = USV^H, \quad A' \approx Z = TRW^H,$$

solve $Y'' = F(Y)$ with Störmer–Verlet:

$$Z' = F(Y) \ \text{ in } \left[t_0, t_0 + \frac{h}{2}\right] \text{ with expl. Euler,}$$

$$\text{for } k = 1, \dots, n-1:$$

$$\begin{cases} Y' = Z \ \text{ in } [t_{k-1}, t_k] \text{ with midpoint scheme,} \\ Z' = F(Y) \ \text{ in } \left[t_{k-\frac{1}{2}}, t_{k+\frac{1}{2}}\right] \text{ with midpoint scheme,} \end{cases}$$

$$Y' = Z \ \text{ in } \left[t_{n-\frac{1}{2}}, t_n\right] \text{ with impl. Euler.}$$

- each IVP $Z' = F(Y)$, $Y' = Z$ solvable with Lie–Trotter splitting
- good long–term integration in (few) numerical examples

Lie–Trotter before Störmer–Verlet

- Idea: Search for $Y''(t)$ in tangent space $\mathcal{T}_{\delta Y}\mathcal{T}_Y\mathcal{M}_r$ of $\mathcal{T}_Y\mathcal{M}_r$ in δY with $\|Y''(t) - A''(t)\|_F = \min! \quad \forall t \in [t_0, T]$

$$\Rightarrow Y = USV^H,$$

$$Y'' = \widetilde{P}(Y)A'' = A''VV^H - UU^HA''VV^H + UU^HA'' + 2U'S(V')^H$$

$$= P(A) + 2U'S(V')^H$$

- application of Lie–Trotter splitting requires first order ODE

Lie–Trotter splitting for second order ODEs

- second order ODE

$$y'' = f(y), \quad y(t_0) = y_0, \quad y'(t_0) = z_0$$

- application of theory on new situation requires reformulation as system of first order ODEs:

$$\begin{bmatrix} y \\ z \end{bmatrix}' = \begin{bmatrix} z \\ f(y) \end{bmatrix}$$

- decomposition into integrable pieces

$$f(y) = f^{[1]}(y) + f^{[2]}(y) + f^{[3]}(y)$$

leads to

$$\begin{bmatrix} y \\ z \end{bmatrix}' = \begin{bmatrix} \alpha_1 z \\ f^{[1]}(y) \end{bmatrix} + \begin{bmatrix} \alpha_2 z \\ f^{[2]}(y) \end{bmatrix} + \begin{bmatrix} \alpha_3 z \\ f^{[3]}(y) \end{bmatrix}$$

with

$$\alpha_1 + \alpha_2 + \alpha_3 = 1$$

Lie–Trotter splitting for second order ODEs

- backtransformation of i-th system

$$\begin{bmatrix} y \\ z \end{bmatrix}' = \begin{bmatrix} \alpha_i z \\ f^{[i]}(y) \end{bmatrix}$$

gives

$$y'' = \alpha_i f^{[i]}(y), \quad i = 1, \ldots, 3$$

- with $A'' = F(A)$, $A' = \alpha B$, $B' = F(A)$, given initial values, stepsize τ, one step of Störmer–Verlet reads

$$B = B + \frac{\tau}{2} F(A)$$
$$A = A + \alpha \tau B$$
$$B = B + \frac{\tau}{2} F(A)$$

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Lie–Trotter before Störmer-Verlet

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- $Y'' = \widetilde{P}(Y)A'' = A''VV^H - UU^HA''VV^H + UU^HA'' + 2U'S(V')^H$
- new ODEs

$$
\begin{aligned}
&\text{(i)}\ \ Y_I'' = \alpha_1 A'' V_I V_I^H + 2U_I' S_I (V_I')^H, && Y_I(t_0) = Y_0, && Y'(t_0) = Y_0' \\
&\text{(ii)}\ \ Y_{II}'' = -\alpha_2 U_{II} U_{II}^H A'' V_{II} V_{II}^H, && Y_{II}(t_0) = Y_I(t_1), && Y_{II}'(t_0) = Y_I'(t_1) \\
&\text{(iii)}\ \ Y_{III}'' = \alpha_3 U_{III} U_{III}^H A'', && Y_{III}(t_0) = Y_{II}(t_1), && Y_{III}'(t_0) = Y_{II}'(t_1)
\end{aligned}
$$

- IVPs (i) - (iii) solvable for

$$
V_I''(t) = V_I'(t) = V_{II}''(t) = V_{II}'(t) = 0,
$$

$$
U_{II}''(t) = U_{II}'(t) = U_{III}''(t) = U_{III}'(t) = 0,
$$

$$
\begin{cases}
\big(U_I(t)S_I(t)\big)'' = \alpha_1 A''(t) V_I, \\
S_{II}''(t) = -\alpha_2 U_{II}^H A''(t) V_{II}, \\
\big(V_{III}(t)S_{III}^H(t)\big)'' = \alpha_3 \big(A''(t)\big)^H U_{III}
\end{cases}
$$

Lie–Trotter before Störmer–Verlet

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- replacing A'' by $F\big(Y(t)\big)$ and reformulation leads to

$$
\begin{aligned}
\text{(j)} \quad & \big(U_I(t)S_I(t)\big)'' = \alpha_1 F\big(Y(t)\big)V_I, \\
\text{(jj)} \quad & S_{II}''(t) = -\alpha_2 U_{II}^H F\big(Y(t)\big)V_{II}, \\
\text{(jjj)} \quad & \big(V_{III}(t)S_{III}^H(t)\big)'' = \alpha_3 F\big(Y(t)\big)^H U_{III}
\end{aligned}
$$

- choice of weights

$$\alpha_1 = 1 = \alpha_3, \quad \alpha_2 = -1$$

or

$$\alpha_1 = \alpha_2 = \alpha_3 = \frac{1}{3}$$

or ...?

- Does choice of weights affect error?

Splitting for harmonic oszillator

- setting:

$$y'' = -(\omega_1^2 + \omega_2^2 + \omega_3^2)y =: f(y), \quad \omega_i^2 > 0 \; \forall i = 1, \dots, 3$$

- with $\omega^2 := \omega_1^2 + \omega_2^2 + \omega_3^2$, given initial values $y(0) = y_0$ and $y'(0) = z_0$, exact solution given by

$$y(t) = y_0 \cos(\omega t) + \frac{z_0}{\omega} \sin(\omega t)$$

- i-th system

$$\begin{bmatrix} y \\ z \end{bmatrix}' = \begin{bmatrix} \alpha_i z \\ -\omega_i^2 y \end{bmatrix}$$

with solution

$$y(t) = y_0 \cos(k_i t) + \frac{\alpha_i z_0}{k_i} \sin(k_i t)$$

where

$$k_i := \sqrt{\alpha_i \omega_i^2}$$

Splitting for harmonic oszillator

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- numerical experiments showed: for configuration $\alpha_1 = \alpha_3 = 1,\ \alpha_2 = -1$ one additional order in h was obtained for arbitrary frequencies ω_i^2

- for configuration

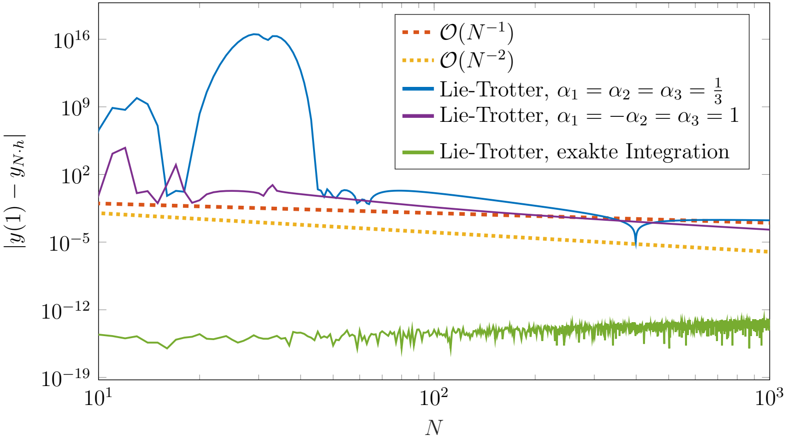
$$\alpha_i = \frac{\omega_i^2}{\omega^2}, \quad \omega^2 = \sum_{i=1}^{3} \omega_i^2 \tag{ex}$$

  splitting is exact for arbitrary frequencies ω_i^2

- verification by Taylor expansion

Splitting for harmonic oszillator

Harmonic oscillator, $\omega_1 = 5, \omega_2 = 10, \omega_3 = 100$, interval of integration $[0, 1]$, absolute error at $T = 1$, stepsize $h = N^{-1}$



Splitting for harmonic oszillator

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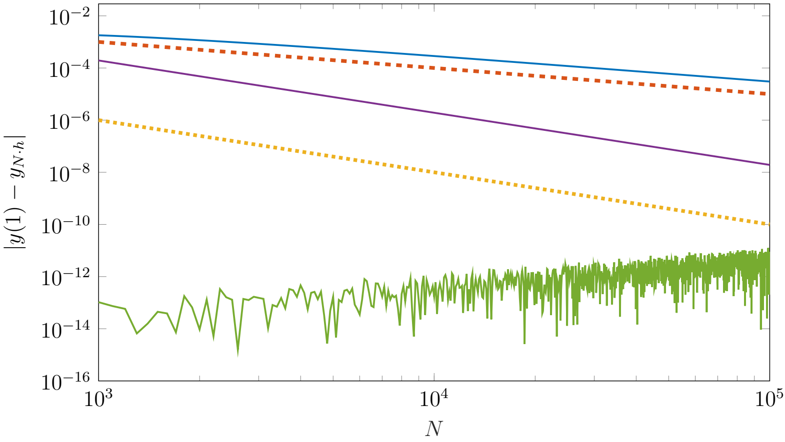

Lie–Trotter splitting: matrix case

- $$Y' = \left(\sum_{i=1}^{n} A_i\right) Y, \quad Y(0) = Y_0 \in \mathbb{R}^{2d}, \quad A_i \in \mathbb{R}^{2d\times 2d}, \quad \forall i = 1, \dots, n$$
- solve $\quad Y_i' = A_i Y_i \quad$ for given initial values $Y_i(0) = Y_0^{[i]}$
- exact solution of i-th subproblem

$$Y_i(t) = \exp(A_i t)\, Y_0^{[i]}$$

- approximation

$$Y(h) \approx \exp(A_n h)\exp(A_{n-1} h)\cdots\exp(A_1 h)\, Y_0$$

- splitting is of order 1

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Lie–Trotter splitting: matrix case

- assume A_i of form

$$A_i = \begin{bmatrix} 0 & c_i I \\ -\Omega_i^2 & 0 \end{bmatrix} \in \mathbb{R}^{2d\times 2d}, \quad c_i \in \mathbb{R}, \quad I \in \mathbb{R}^{d\times d}$$

  with $\sum_i c_i = 1$

- one additional order for $Y_{0,1:d}^{[i]} = 0 \in \mathbb{R}^d$
- exact , if
  - $Y_0^{[i]} = 0 \in \mathbb{R}^{2d}$, solution is constant zero
  - two subproblems: $\Omega_1^2 = a\Omega_2^2$, $a \in \mathbb{R}\backslash\{-1\}$ and

$$c_1 = \frac{a}{1+a}, \quad c_2 = \frac{1}{1+a}$$

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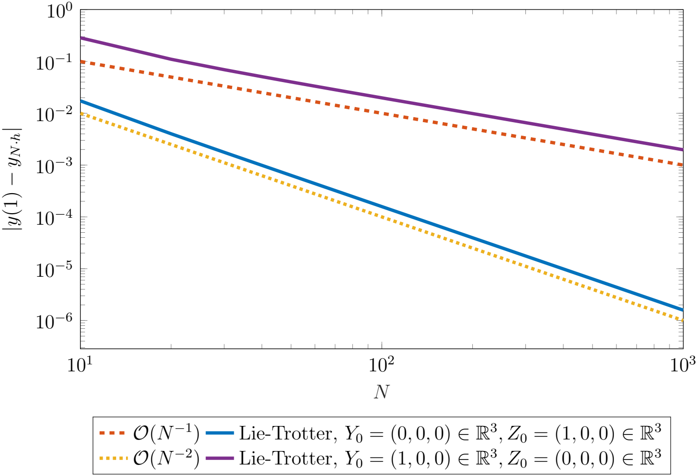
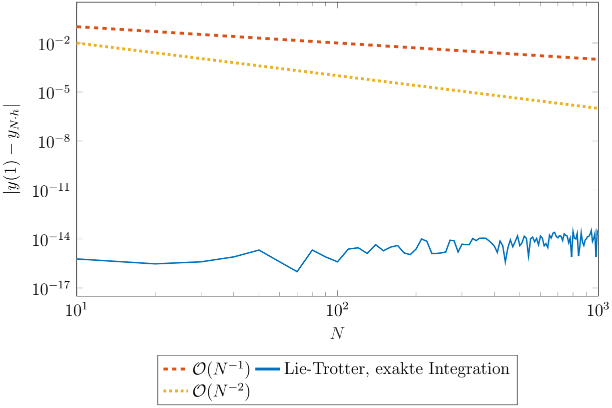
Lie–Trotter splitting: matrix case

$n = 5$, $\Omega_i^2 = Q_i D_i^2 Q_i^T$, with D_i positive definite, diagonal, Q_i orthogonal



Lie–Trotter splitting: matrix case

$$\Omega_1^2 = 0.35 \begin{pmatrix} \sqrt{3} & 1 \\ -1 & \sqrt{3} \end{pmatrix}, \quad \Omega_2^2 = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}, \quad a = 0.7$$



Standing wave

- wave equation

$$\frac{\partial^2}{\partial t^2} a(t,x,y) - \Delta a(t,x,y) = 0, \quad (x,y) \in \Omega = [-\pi,\pi]^2, \quad t \in [t_0, T]$$

- solution

$$\psi(t,x,y) = \frac{1}{2}\cos(2\sqrt{2}t)\sin\big(2(x+y)\big)$$

- discretization:

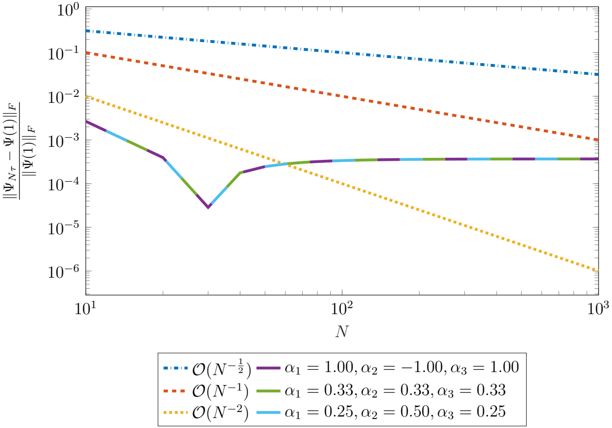
$$\overline{\Omega} = (-\pi + ih, -\pi + jh), \quad i,j = 1,\dots,m = 2^k, \quad k = 2,3,\dots$$

  with $h = \frac{2\pi}{m}$, finite differences, periodic boundary conditions

- discretized problem has rank 2 $\rightsquigarrow$ use rank–2–approximation

Standing wave: results

- LT–SV Algorithm: different weight configurations lead to the same approximations



Standing wave: results

- define $\widehat{\Psi}^{(k)} = \big(\sin(2(x_i + y_j))\big)_{i,j}, \quad i,j = 1,\dots,2^k, \quad k \in \mathbb{N}$
- $t_0 = 0$, $k = 3$, $r = 2$, time stepsize τ, approximation via LT–SV after one time step:

$$\Psi(\tau) \approx \Psi_\tau = \frac{\pi^2 - 32\tau^2(\alpha_1 + \alpha_2 + \alpha_3)}{2\pi^2}\widehat{\Psi}^{(3)},$$

independent of certain choice of weights as

$$\alpha_1 + \alpha_2 + \alpha_3 = 1$$

- approximation via SV–LT after one time step:

$$\Psi(\tau) \approx \Psi_\tau = \frac{\pi^2 - 32\tau^2}{2\pi^2}\widehat{\Psi}^{(3)}$$

Standing wave: results

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Theorem

LT–SV leads to the same approximations independent of the certain choice of the weights α_i, for arbitrary $t_0 \in \mathbb{R}$ and $k \in \mathbb{N}$.

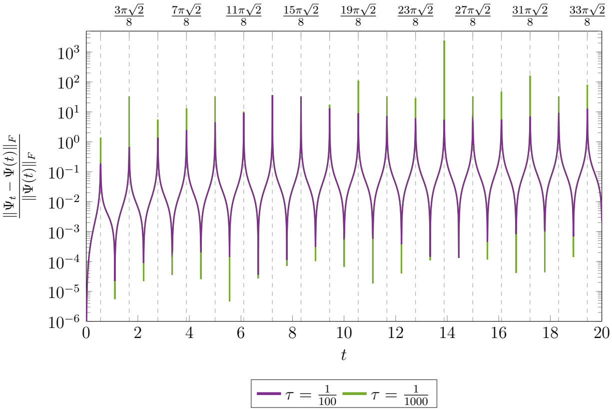
Theorem

SV–LT and LT–SV lead to the same approximations, for arbitrary $t_0 \in \mathbb{R}$ and $k \in \mathbb{N}$.

Proofs: work in progress

Standing wave: results

Relative error in Frobenius norm between LT–SV and exact solution for different time step sizes



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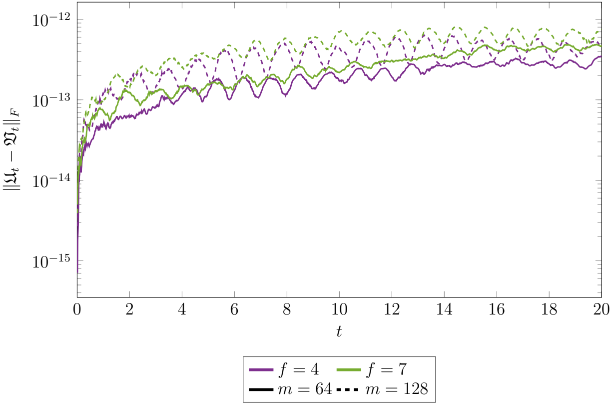
Standing wave: results

Absolute error in Frobenius norm between LT–SV and SV–LT solution for different grid widths (purple: standing wave, green: moving wave)



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Laser–plasma–interaction

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- 2D wave equation with cubic non-linearity

$$\frac{\partial^2}{\partial t^2} a(t,x,y) - \Delta a(t,x,y) = -\hat{c}\vartheta(y)\left(1 - \frac{1}{2}|a(t,x,y)|^2\right)a(t,x,y),$$

  with $\hat{c} = 0.3$ plasma density, $\vartheta(y)$ position of plasma
- no exact solution known, use leapfrog reference solution
- initial value:

$$a(t,x,y) = a_0 e^{-\frac{(y-y_0-k_0 t)^2}{l_0^2}} e^{-\frac{x^2}{\omega_0^2}} e^{i(k_0 y - y_0 - t)}$$

  with $\lambda_0 = \pi$ (wavelength of pulse), $y_0 = 0$, $l_0 = 10\lambda_0$ (length), $w_0 = 100\lambda_0$ (width), $a_0 = 0.12$
- k_0 group velocity: $k_0 = 1$ (starting in vacuum), $k_0 = \sqrt{1-\hat{c}}$ (starting in plasma)

Laser–plasma–interaction: (expected) results

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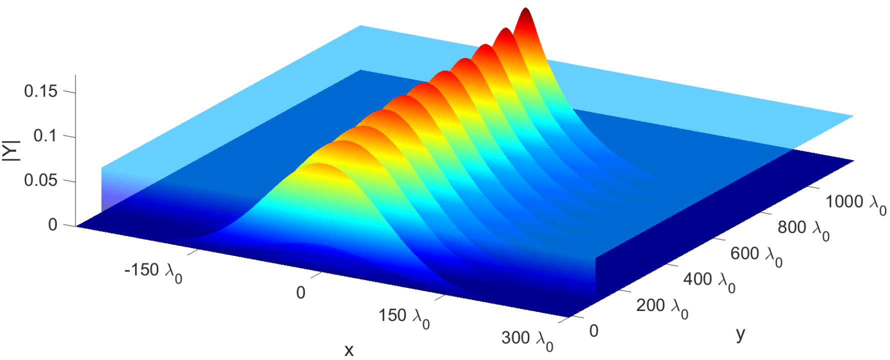
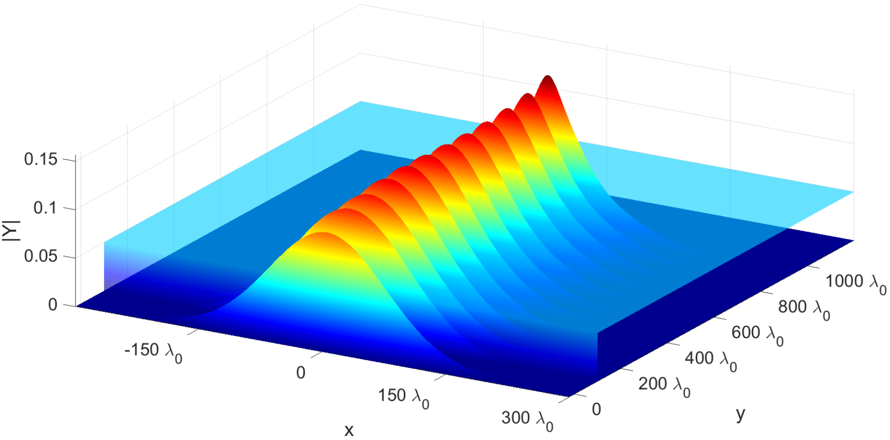
- propagation through vacuum: no change in velocity/shape
- propagation through plasma: focus in transversal direction, group velocity shrinks
- propagation after plasma: still focused in transversal direction
- observation: discretization of Laplacian by Fourier transform needed

Laser–plasma–interaction: leapfrog

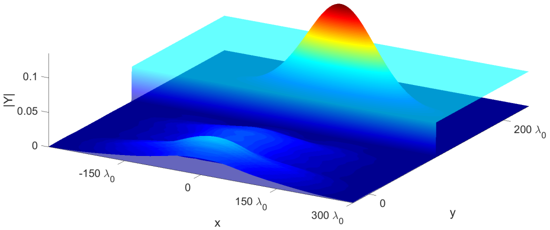


Laser–plasma–interaction: SV–LT



Laser–plasma–interaction: LT–SV

- issue: non-stable for change of medium
- possible approach: increase rank in critical region



- achievement so far: doubled stable time domain

Future work

- solve problems with tangent spaces
- proofs for conjectures
- moving box simulation for laser–plasma–interaction
- useful method for increasing rank in mid–simulation
- expanding theory to other examples
- error and stability estimates