Karlsruher Institut für Technologie

Dynamical Low-Rank Approximation to the Solution of Wave Equations

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joint work with Marlis Hochbruck

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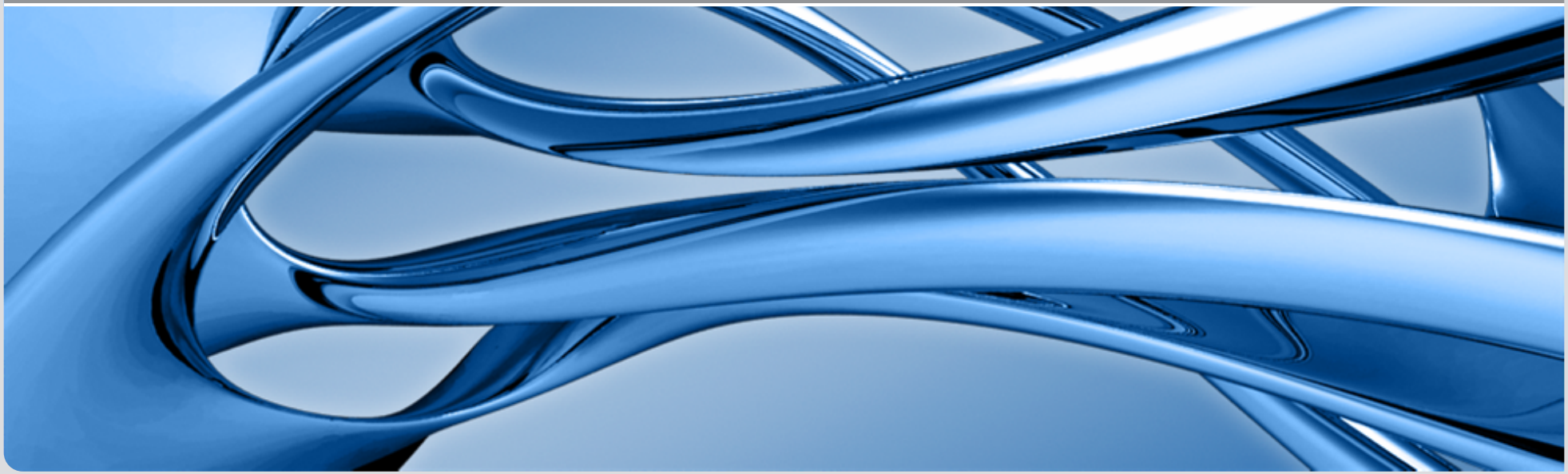
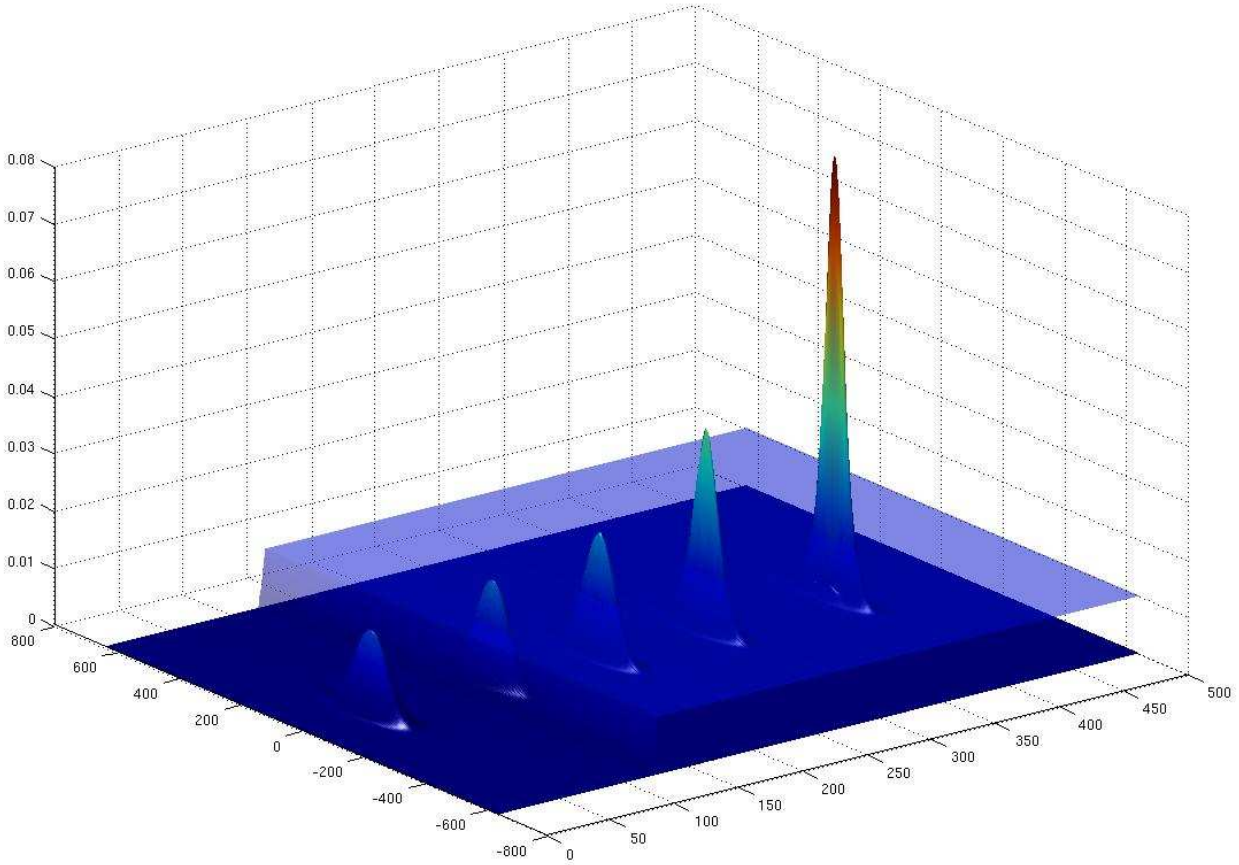


Outline

- Motivation
- Model
- Adaptive Rank
- Numerical Results
- Conclusion

Example in 2d

$$a_{tt} - \Delta a + g(|a|^2)a = 0$$

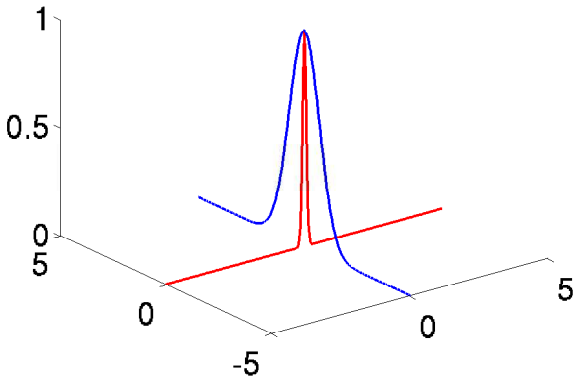


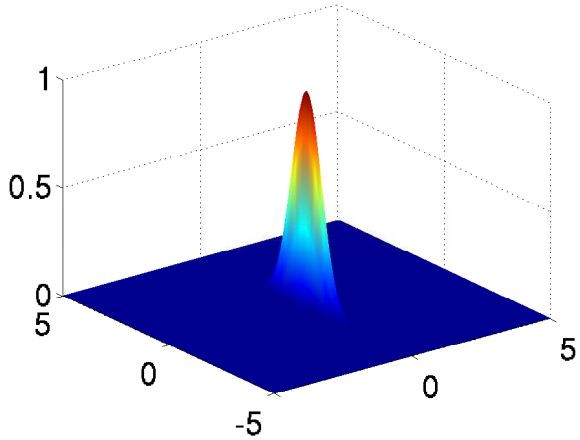
2d simulation in cartesian coordinates
(Gautschi–type method including QEA ...)

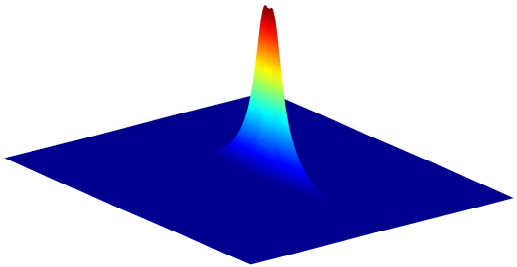
Ch. Karle

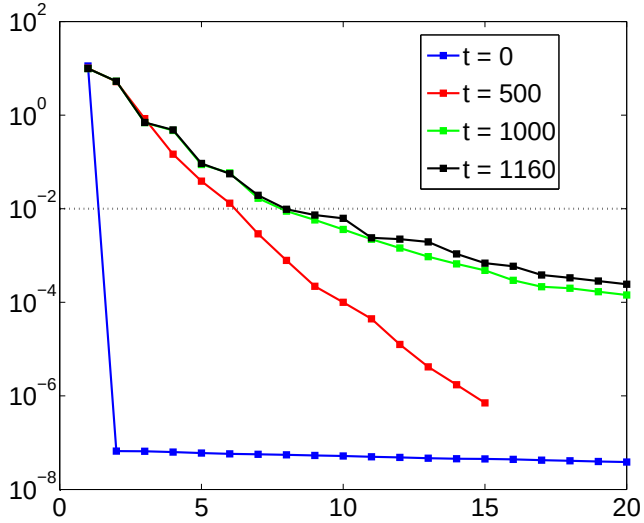
Properties of the solution

spatial discretization on uniform grid $\Rightarrow$ large matrix



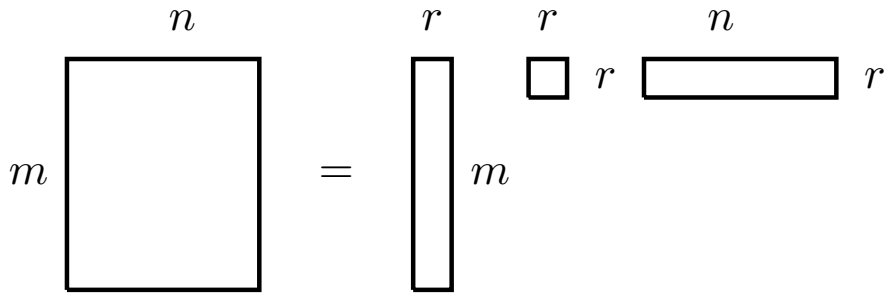






Low-rank representation

$$A(x, y, t) \approx Y(x, y, t) = U(x, t)S(t)V(y, t)^H \in \mathbb{C}^{m,n}$$



$$U \in \mathbb{C}^{m,r}, \quad V \in \mathbb{C}^{n,r}, \quad S \in \mathbb{C}^{r,r},$$

- U and V with orthonormal columns
- S invertible
- A: $m \cdot n$ complex entries
  (example: $m = 2048$, $n = 800 \Rightarrow 1\,638\,400$)
- U, S and V: $m \cdot r + n \cdot r + r^2$ complex entries
  (example: $r = 10 \Rightarrow 28\,580$)

Best approximation

- solve full system in each time step
- after every time step compute singular value decomposition
- save first r singular values as well as right and left singular vectors

Problem: required in each step

- full matrix
- singular value decomposition

Goal: new system of equations for U, S and V $\Rightarrow$
Dynamical Low-Rank approximation

Physical motivation

- total energy of a system described by $a(t, r)$

$$E = \frac{1}{2} \int_\Omega \left(|a_t|^2 + \|\nabla a\|^2 + G(|a|^2) - G(0) \right) \, dr$$

$$G'(x) = g(x)$$

- energy conservation

$$\frac{d}{dt} E = \mathrm{Re} \int_\Omega \bar{a}_t \left(a_{tt} - \Delta a + g(|a|^2) a \right) \, dr \stackrel{!}{=} 0$$

- energy remains conserved if nonlinear wave equation is fulfilled

$$a_{tt} - \Delta a + g(|a|^2) a =: a_{tt} - F(a) = 0$$

Formulation on manifolds

- energy conservation

$$\mathrm{Re}\,\langle \mathrm{a_t}, \mathrm{a_{tt}} - \mathrm{F(a)} \rangle = 0$$

- since wave equation is fulfilled

$$\langle \delta\mathrm{a}, \mathrm{a_{tt}} - \mathrm{F(a)} \rangle = 0 \quad \forall \delta\mathrm{a}$$

- a weaker model
  - let Y be in a manifold $\mathcal{M}$ and $\mathrm{Y} \approx \mathrm{a}$
  - let $\delta\mathrm{Y}$ be an element of the tangential space $\mathcal{T}_{\mathrm{Y}}\mathcal{M}$ of $\mathcal{M}$
  - $\mathrm{Y_{tt}} - \mathrm{F(Y)} = 0$ doesn't hold any more, but

$$\langle \delta\mathrm{Y}, \mathrm{Y_{tt}} - \mathrm{F(Y)} \rangle = 0 \quad \forall \delta\mathrm{Y} \in \mathcal{T}_{\mathrm{Y}}\mathcal{M}$$

Choice of the manifold

- shape functions
  - in physics: Variation of Action
  - Gauß-Hermite wave packets
  - Hagedorn wave packets

  for first order systems: Lubich, Faou, Gradinaru
- low-rank matrices

  for first order systems: Lubich, Koch, Nonnenmacher
- extension to threedimensional tensors for first order systems

  Lubich, Koch
- application to chemical master equation

  Jahnke

Our choice of the manifold

- manifold of rank r matrices

$$\begin{aligned}\mathcal{M} &= \{Y \in \mathbb{C}^{m,n} : \ \mathrm{rank}(Y) = r\} \\ &= \{U \in \mathbb{C}^{m,r}, S \in \mathbb{C}^{r,r} \text{ inv.}, V \in \mathbb{C}^{n,r} : \ U^H U = I_r = V^H V\}\end{aligned}$$

- S not necessarily diagonal $\Rightarrow$ decomposition not unique
- unique decomposition in tangent space

$$\delta Y = \delta U S V^H + U \delta S V^H + U S \delta V^H$$
$$\delta U^H U = 0 = \delta V^H V$$

- choice of norm on the manifold
  - relation to physical back ground
  - approximation of the integral over Ω for discretized function

$$\langle A, B \rangle = \sum_{i,j} \overline{a_{ij}} b_{ij} \ , \quad \|A\|^2 = \sum_{i,j} |a_{ij}|^2 = \|A\|_F^2$$

DLR–equations

$$\langle \delta \mathrm{Y}, \mathrm{Y}_{\mathrm{tt}} - \mathrm{f}(\mathrm{Y}) \rangle = 0 \quad \forall \delta \mathrm{Y} \in \mathcal{T}_{\mathrm{Y}} \mathcal{M}$$

is equivalent to a system of equations for U, S and V:

$$\begin{aligned}
\mathrm{S}'' &= \mathrm{U}^{\mathrm{H}} \mathrm{f}(\mathrm{Y}) \mathrm{V} + \mathrm{U}'^{\mathrm{H}} \mathrm{U}' \mathrm{S} + \mathrm{S} \mathrm{V}'^{\mathrm{H}} \mathrm{V}' \\
\mathrm{U}'' &= (\mathrm{I} - \mathrm{U}\mathrm{U}^{\mathrm{H}}) \mathrm{f}(\mathrm{Y}) \mathrm{V} \mathrm{S}^{-1} - \mathrm{U}\mathrm{U}'^{\mathrm{H}} \mathrm{U}' - 2\mathrm{U}' \mathrm{S}' \mathrm{S}^{-1} \\
\mathrm{V}'' &= (\mathrm{I} - \mathrm{V}\mathrm{V}^{\mathrm{H}}) \mathrm{f}(\mathrm{Y})^{\mathrm{H}} \mathrm{U} \mathrm{S}^{-\mathrm{H}} - \mathrm{V}\mathrm{V}'^{\mathrm{H}} \mathrm{V}' - 2\mathrm{V}' \mathrm{S}'^{\mathrm{H}} \mathrm{S}^{-\mathrm{H}}
\end{aligned}$$

the properties

$$\mathrm{U}^{\mathrm{H}} \mathrm{U} = \mathrm{I} = \mathrm{V}^{\mathrm{H}} \mathrm{V} \text{ and } \mathrm{U}'^{\mathrm{H}} \mathrm{U} = 0 = \mathrm{V}'^{\mathrm{H}} \mathrm{V}$$

are conserved

Computational aspects

- numerical time integration scheme: standard scheme
- time step selection, error estimation — Lubich, Nonnenmacher
- orthogonality constraints
- inverse of S in case of singularity

$$\mathrm{U}'' = (\mathrm{I} - \mathrm{U}\mathrm{U}^{\mathrm{H}})\mathrm{f}(\mathrm{Y})\mathrm{V}\mathrm{S}^{-1} - \mathrm{U}\mathrm{U}'^{\mathrm{H}}\mathrm{U}' - 2\mathrm{U}'\mathrm{S}'\mathrm{S}^{-1}$$

- evaluation of $\mathrm{f}(\mathrm{Y})$:
  $\mathrm{f}(\mathrm{Y})$ not required but only $\mathrm{f}(\mathrm{Y})\mathrm{V}$ or $\mathrm{f}(\mathrm{Y})^{\mathrm{H}}\mathrm{U}$

Example: Cubic Wave Equation

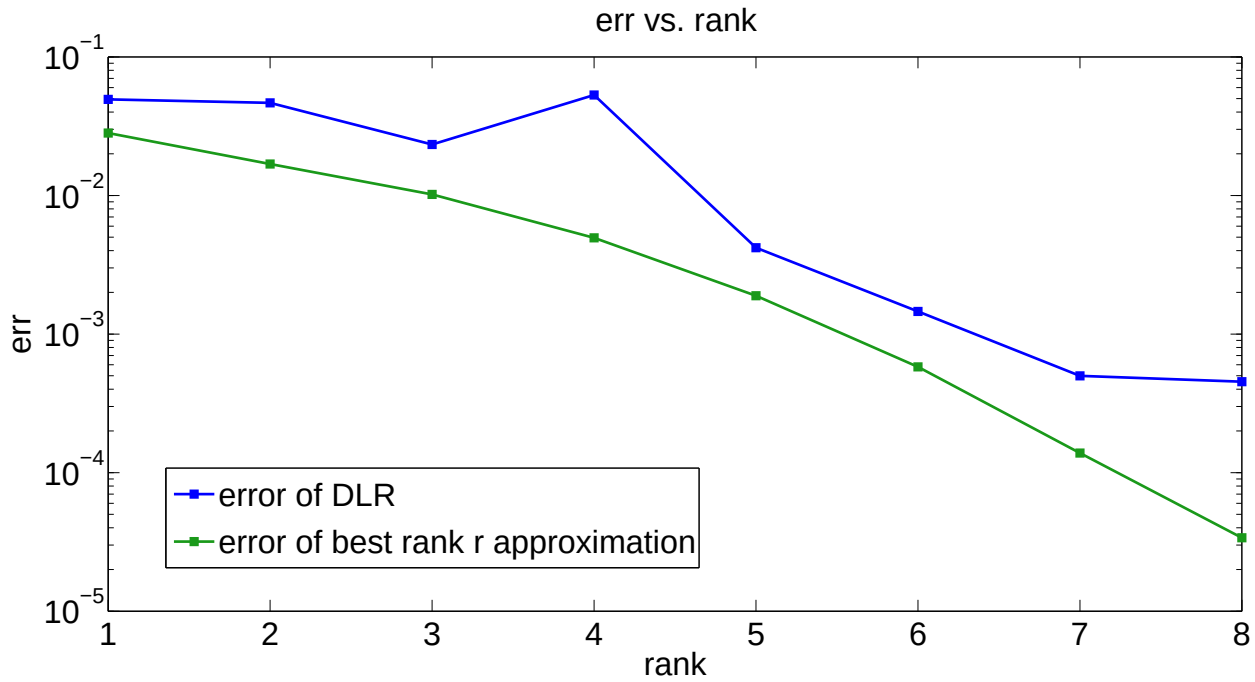
$$a_{tt} - \Delta a = |a|^2 a$$

- initial condition: Gaußian pulse (slim in direction of transport, wide in perpendicular direction)
- periodic boundary conditions (compute spatial derivatives via `fft`)
- small example ($n = m = 256$)
- comparison with Störmer–Verlet / leap–frog method

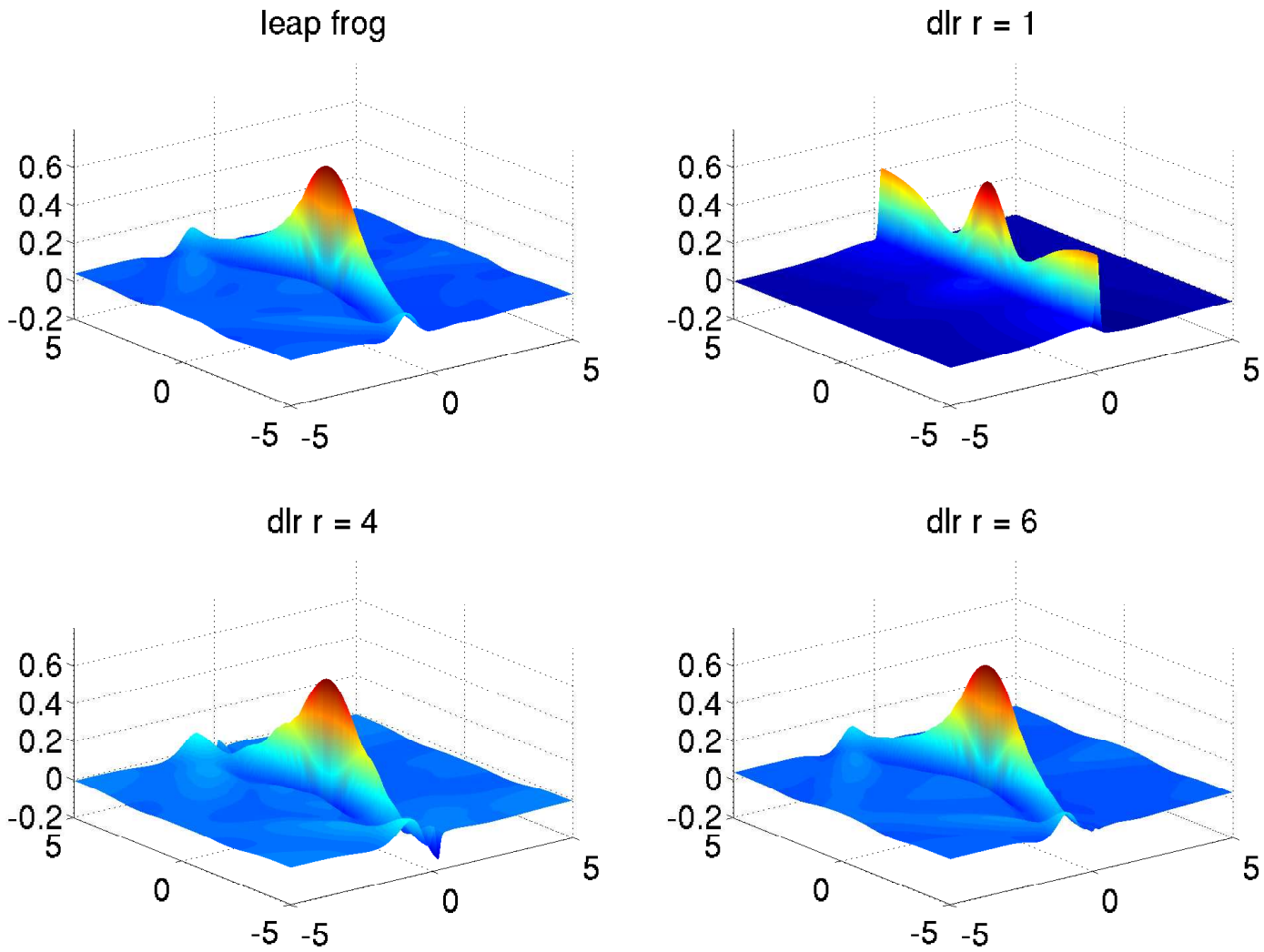
Results

rank	3	4	5	6	7	8
storage	1545	2064	2585	3108	3633	4160
error DLR	0.023	0.053	0.041	0.014	0.0049	0.0045
error BA	0.010	0.004	0.001	0.0005	0.0001	0.00003

storage for Y: 65536 matrix entries



Results



Rank control

Why is this important?

- theory for first order equations: regularization does not affect the error considerably Lubich, Koch
- But: system is not very stable and time steps are chosen too small

Solution: variable rank

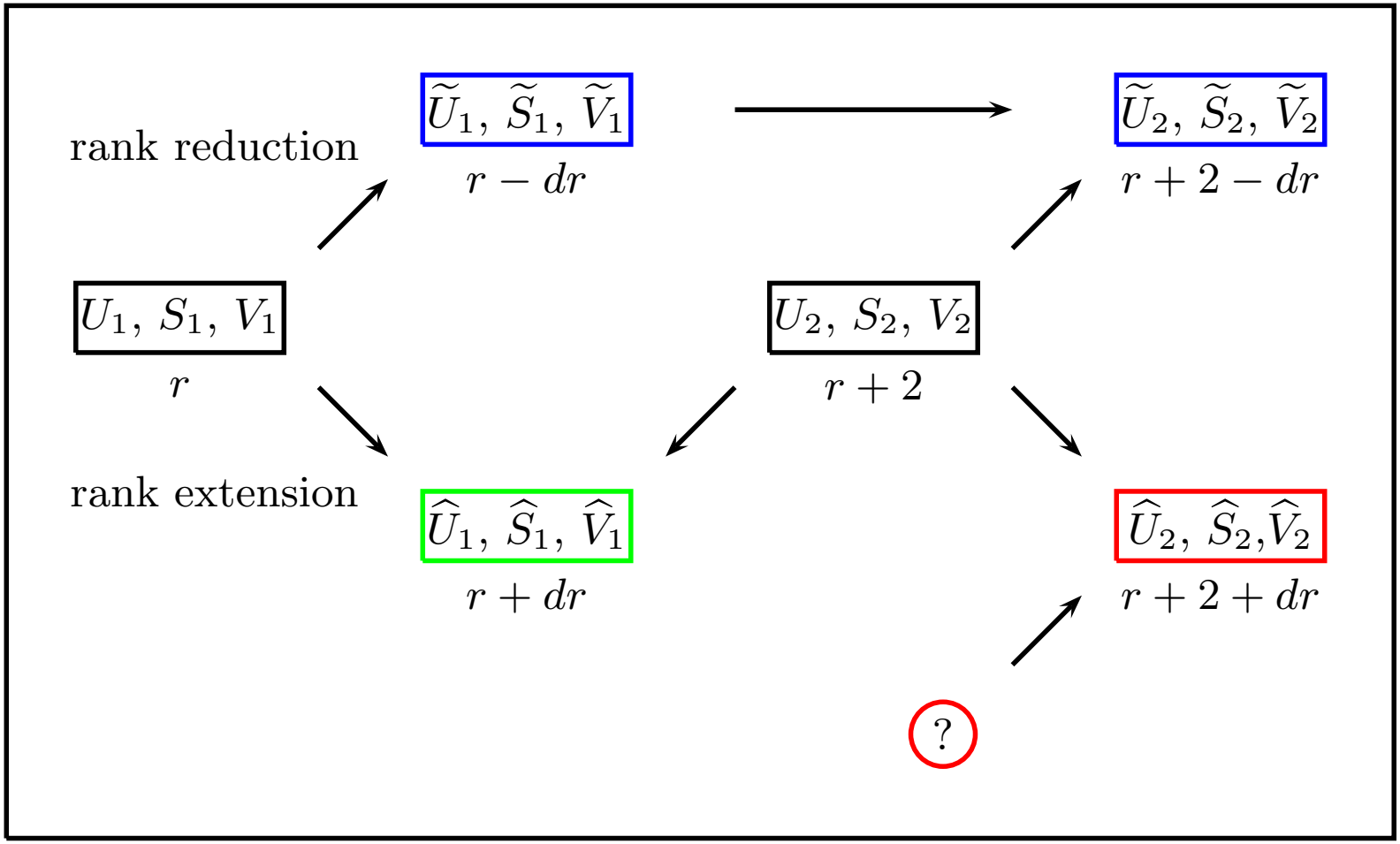
- S too large: easy!
  - S nearly singular $\Rightarrow$
    remove small singular values and corresponding vectors
- S too small: not so easy
  - indicator for rising rank
  - initial condition for additional singular vectors

“Embedded” method

integrate two sets of matrices:

- 1st set: $U_1 \in \mathbb{C}^{n,r_1}$, $S_1 \in \mathbb{C}^{r_1,r_1}$ and $V_1 \in \mathbb{C}^{m,r_1}$
  - S_1 invertible
  - can be integrated in stable way
  - contains relevant information
- 2nd set: $U_2 \in \mathbb{C}^{n,r_2}$, $S_2 \in \mathbb{C}^{r_2,r_2}$ and $V_2 \in \mathbb{C}^{m,r_2}$
  - $r_2 = r_1 + 2$
  - S_2 not necessarily invertible
  - regularization not too bad
  - indicator for rising rank
  - extract initial conditions for 1st set in case of rising rank

Rank change


rank reduction
$\widetilde{U}_1,\ \widetilde{S}_1,\ \widetilde{V}_1$
$r - dr$
$\widetilde{U}_2,\ \widetilde{S}_2,\ \widetilde{V}_2$
$r + 2 - dr$
$U_1,\ S_1,\ V_1$
r
$U_2,\ S_2,\ V_2$
$r + 2$
rank extension
$\widehat{U}_1,\ \widehat{S}_1,\ \widehat{V}_1$
$r + dr$
$\widehat{U}_2,\ \widehat{S}_2,\widehat{V}_2$
$r + 2 + dr$
?

Rank extension

- project 2nd set onto orthogonal complement of 1st set

$$(\mathrm{I} - \mathrm{U}_1\mathrm{U}_1^{\mathrm{H}})\mathrm{U}_2\mathrm{S}_2\mathrm{V}_2^{\mathrm{H}}(\mathrm{I} - \mathrm{V}_1\mathrm{V}_1^{\mathrm{H}}) = \overline{\mathrm{U}}\ \overline{\mathrm{S}}\ \overline{\mathrm{V}}^{\mathrm{H}}$$

- keep only dominant parts

$$\overline{\mathrm{U}} = \overline{\mathrm{U}}(:, 1:\mathrm{dr}) \quad \overline{\mathrm{S}} = \overline{\mathrm{S}}(1:\mathrm{dr}, 1:\mathrm{dr}) \quad \overline{\mathrm{V}} = \overline{\mathrm{V}}(:, 1:\mathrm{dr})$$

- combine with old data

$$\widehat{\mathrm{S}}_1 = \begin{bmatrix} \mathrm{S}_1 & 0 \\ 0 & \overline{\mathrm{S}} \end{bmatrix} \quad \begin{aligned} \widehat{\mathrm{V}}_1 &= [\mathrm{V}_1\ \overline{\mathrm{V}}] \\ \widehat{\mathrm{U}}_1 &= [\mathrm{U}_1\ \overline{\mathrm{U}}] \end{aligned}$$

- for derivatives use variation of 1st order system — Lubich, Koch

$$\overline{\mathrm{S}}' = \overline{\mathrm{U}}^{\mathrm{H}}\mathrm{Y}'\overline{\mathrm{V}} \qquad \overline{\mathrm{U}}' = (\mathrm{I} - \widehat{\mathrm{U}}\widehat{\mathrm{U}}^{\mathrm{H}})\mathrm{Y}'\overline{\mathrm{V}}\ \overline{\mathrm{S}}^{-1}$$

$$\overline{\mathrm{V}}' = (\mathrm{I} - \widehat{\mathrm{V}}\widehat{\mathrm{V}}^{\mathrm{H}})\mathrm{Y}'^{\mathrm{H}}\overline{\mathrm{US}}^{-\mathrm{H}}$$

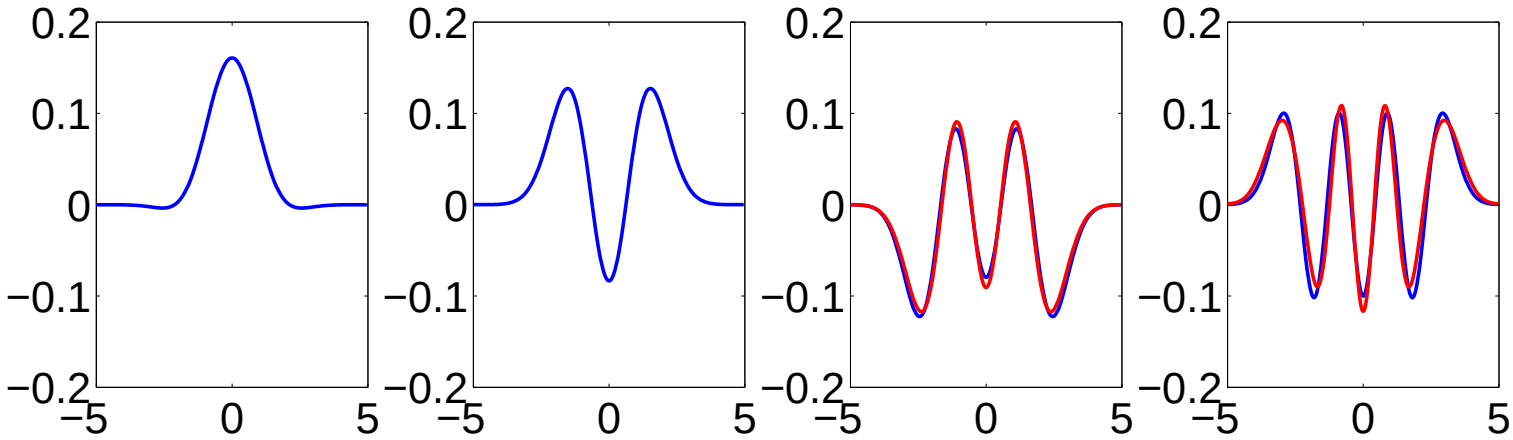
  - $\mathrm{Y}' = \mathrm{U}_2'\mathrm{S}_2\mathrm{V}_2^{\mathrm{H}} + \mathrm{U}_2\mathrm{S}_2'\mathrm{V}_2^{\mathrm{H}} + \mathrm{U}_2\mathrm{S}_2\mathrm{V}_2'^{\mathrm{H}}$
  - projection with respect to the complete new space

Initial conditions for particular applications

Guess initial values for 2. set in case of the moving wave:

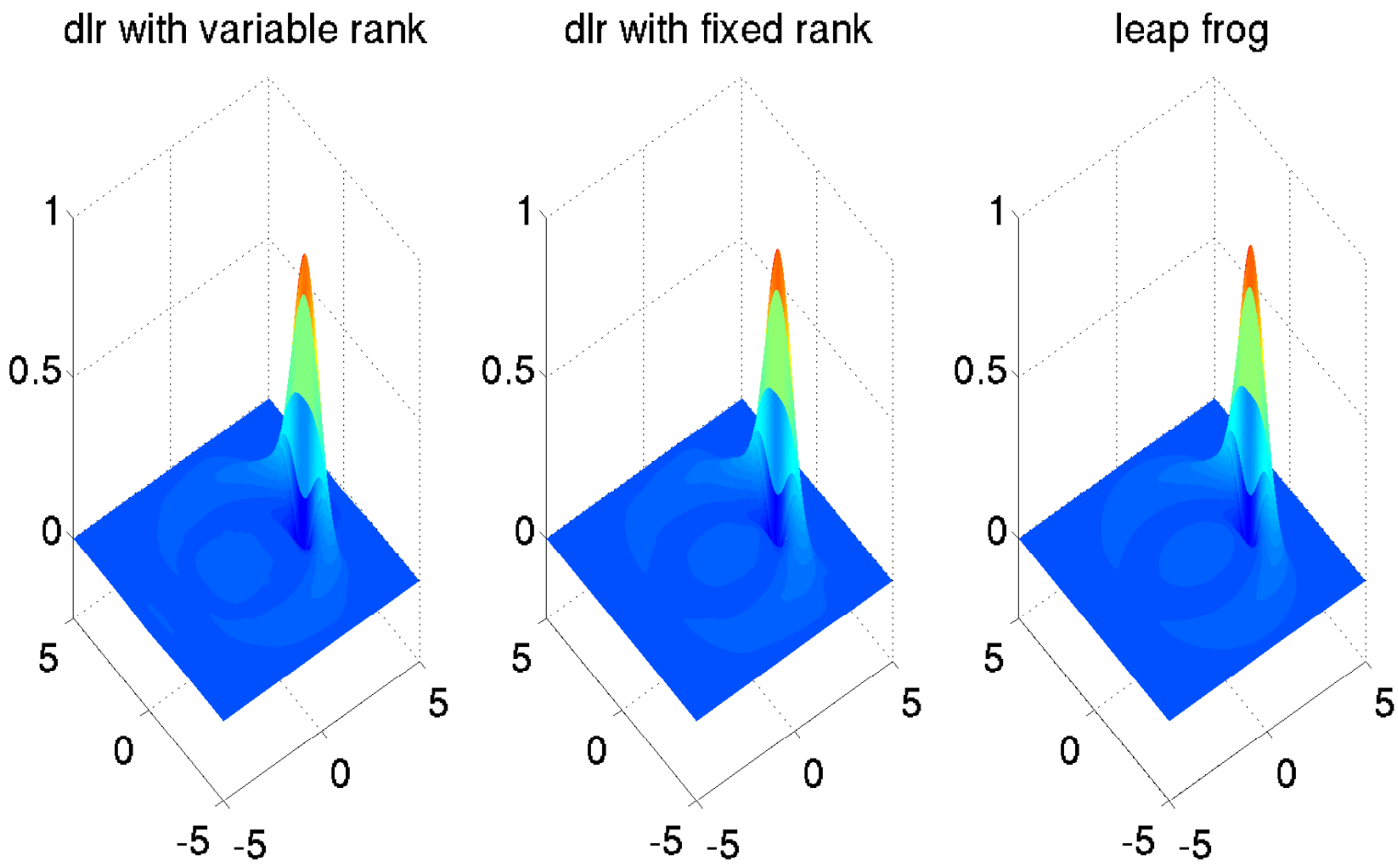
- S, S′ are set to zero
- transversal direction U:

$$\widetilde{U}\widetilde{S}\widetilde{V}^{H} = (I - U_2 U_2^{H}) D_y^2 U_2 \ , \quad \widetilde{U}' = 0$$



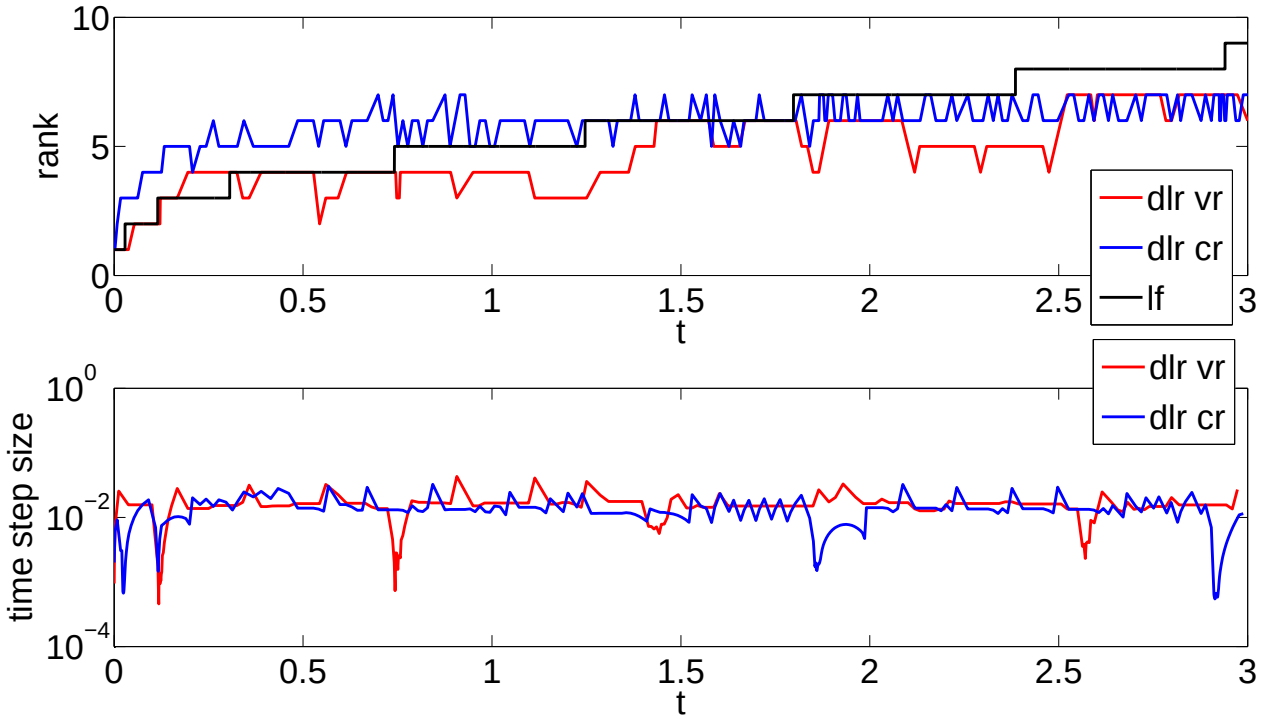
- parallel direction V:
  V either random and orthogonalized or by the same scheme as U
  V′ such that it resembles the speed of the pulse

Results



fixed rank = 7 = max rank of variable rank

Results



variable rank fixed rank

Conclusion

Up to now:

- equations for DLR approximation for 2. order equations
- error estimator
- adaptive rank

Goals:

- more sophisticated time integration scheme
- application to real laser-plasma problem
- extension to 3d problems