MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Symplectic Krylov Subspace Methods for Hamiltonian Systems

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joint work with:
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XXI Householder Symposium on Numerical Linear Algebra
June 12–17, 2022
Selva di Fasano (Br), Italy

Introduction

Consider nonlinear dynamical system:

$$\dot{y} = F(y), \quad y(0) = y_0$$

$$F(y) = \underbrace{Ay + c}_{\text{linear}} + \underbrace{g(y)}_{\text{nonlinear}}, \quad A = \mathrm{D}F(y_0)$$

Exponential Integrator

$$\widehat{y}(t) = e^{tA} y_0 + t\,\varphi(tA)\,(c + g(\widehat{y}))$$

$$\varphi(z) = \frac{e^z - 1}{z}$$

Large-scale Hamiltonian systems

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Let

$$J := J_n := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}.$$

Definition

- $H \in \mathbb{R}^{2n \times 2n}$ Hamiltonian iff $JH = (JH)^T$.
- $S \in \mathbb{R}^{2n \times 2k}$ symplectic (J-isometric/-orthogonal) iff $S^J S = I$, where $S^J := J^T S^T J$.

Corollary

H Hamiltonian, S symplectic $\Rightarrow$ $S^J H S$ Hamiltonian.

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Hamiltonian and Symplectic Matrices

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$$\dot{y} = J^{-1}\nabla\mathcal{H}(y), \quad \mathcal{H}: \mathbb{R}^{2n} \to \mathbb{R} \quad \text{"the Hamiltonian"} \tag{1}$$

$$\Updownarrow \quad y = \begin{bmatrix} p \\ q \end{bmatrix}$$

$$\dot{p}_i = -\frac{\partial\mathcal{H}}{\partial q_i}(p,q), \quad \dot{q}_i = \frac{\partial\mathcal{H}}{\partial p_i}(p,q), \quad i = 1,\dots,n$$

$$\mathcal{H}: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$$

Conservative System

For initial condition $y(t_0) = y_0$, the Hamiltonian (loosely speaking, the "total energy" of the system) is preserved along solution trajectories:

$$\mathcal{H}(y(t)) \equiv \mathcal{H}(y_0) \quad \forall\, t \geq t_0 \quad \text{if } y(t) \text{ solves (1)}$$

⇝ numerical approximation should satisfy $\mathcal{H}(y(t)) \approx \mathcal{H}(y_0) \quad \forall\, t \geq t_0$.
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Linearization of $\dot{y} = J^{-1}\nabla\mathcal{H}(y)$ at y_0

$$\dot{y} = F(y) = Ay + c + g(y), \qquad g(y_0) = 0$$

Hamiltonian system $\implies$ A Hamiltonian.

$$\dot{y} = F(y) := Ay + c + g(y)$$
$$y(0) = y_0, \quad A = \mathrm{D}F(y_0)$$

Exponential Integrators

- exponential(ly fitted) Euler method (EE)

$$y_1 = \Phi_h^{\mathrm{EE}}(y_0) := e^{hA} y_0 + h\,\varphi(hA)\,(c + g(y_0)) = y_0 + h\,\varphi(hA)\,F(y_0)$$

- explicit exponential midpoint rule (EEMP)

$$y_1 = \Phi_h^{\mathrm{EEMP}}(y_0) := y_0 + e^{hA}(y_{-1} - y_0) + 2h\varphi(hA)g(y_0)$$

- implicit exponential midpoint rule (IEMP)

$$0 = e^{\frac{h}{2}A}(y_0 - \hat{y}) + \frac{h}{2}\varphi(\frac{h}{2}A)g(\hat{y})$$
$$y_1 = \Phi_h^{\mathrm{IEMP}}(y_0) := \hat{y} + e^{hA}(y_0 - \hat{y}) + h\varphi(hA)g(\hat{y})$$

Recall the phi function: $\varphi(z) = \frac{e^z - 1}{z}$.

Definition (Hairer/Lubich/Wanner 2006, Chapter VI, Def. 3.1)

$y_1 = \Phi_h(y_0)$ is *symplectic* iff $\mathrm{D}\Phi_h(y_0)$ is symplectic for Hamiltonian Systems.

Examples:

- symplectic Euler,
- leap frog/(Störmer-)Verlet,
- symplectic Runge-Kutta methods,
- splitting methods,
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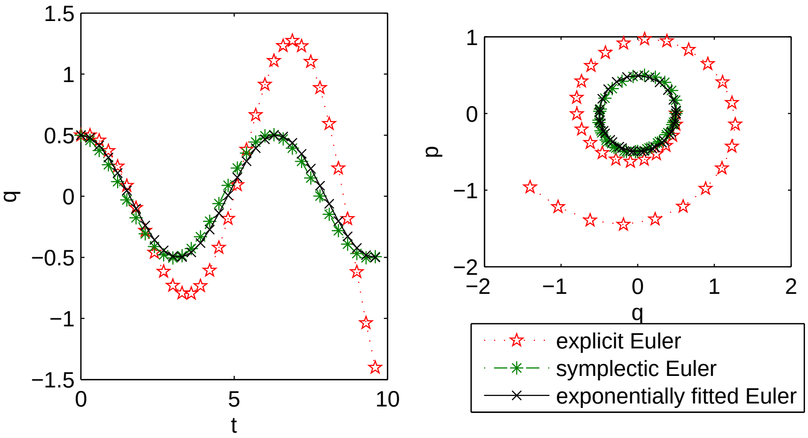
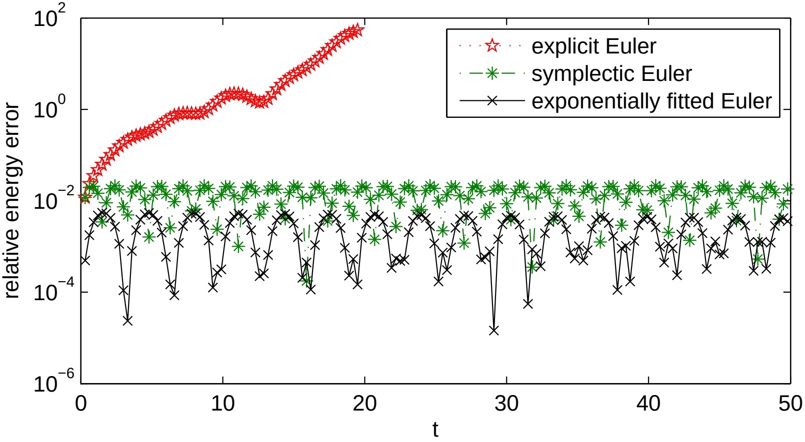


Idea for picture taken from [Hairer/Lubich/Wanner 2006].

Symplectic vs. Non-Symplectic Integrators



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For an efficient application of exponential integrators to large-scale Hamiltonian systems, we need:

1. efficient evaluation of matrix function applied to a vector $f(A)v$, where $f \in \{\exp,\ \varphi\}$

   $\rightsquigarrow$ approximation of $f(A)v$ using (rational) Krylov subspaces;

2. a symplectic flow to ensure preservation of the Hamiltonian, to guarantee this for the approximation of $f(A)v$, one should use

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1. Numerical Approximation of $f(A)v$

Given a function $f : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$, we are interested in approximating

$$f(A)v$$

for a large and sparse matrix A and a vector v (where we assume that f is sufficiently regular so that $f(A)$ is well defined).

Typical approach for large-scale computations:
find a matrix $V \in \mathbb{R}^{n\times k}$ with orthonormal columns so that

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- As $A_k = V^T AV \in \mathbb{R}^{k\times k}$, the evaluation of $V f(A_k)V^T v$ should be much faster than that of $f(A)v$.
- **Note:** The problem of approximating the action of $f(A)$ to a vector is significantly different from that of approximating $f(A)$ (see seminal Higham book).

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Use, e.g., Arnoldi method to compute V as an orthogonal basis of Krylov subspace

$$\mathcal{K}_k(A, v) = \mathrm{span}\{v, Av, A^2v, \dots, A^{k-1}v\}.$$

As $Ve_1 = v/\|v\|_2$, (2) simplifies to

$$f(A)v \approx \|v\|_2 Vf(V^TAV)e_1.$$

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[Druskin/Knizhnerman 1998] suggest to use orthogonal basis of the extended Krylov subspace

$$\mathcal{K}_k(A, v) + \mathcal{K}_k(A^{-1}, A^{-1}v) = \operatorname{span}\{A^{-k}v, \ldots, A^{-2}v, A^{-1}v, v, Av, A^2v, \ldots, A^{k-1}v\}.$$

(. . . and later on also rational Krylov subspaces, see also Güttel, Beckermann, Simoncini, . . .)

Hamiltonian Lanczos Method [B./Faßbender 1997, Ferng et al 1997]

- Symplectic basis of Krylov subspace $\mathcal{K}_{2r}(H, u_1) = \operatorname{span}\{u_1, Hu_1, \ldots, H^{2r-1}u_1\}$.
- Generates $S = [U_r \;\; V_r]$ with $U_r, V_r \in \mathbb{R}^{2n \times r}$ with J-orthogonal columns such that

$$H[U_r \; V_r] = [U_r \; V_r] \begin{bmatrix} G^{(r)} & T^{(r)} \\ D^{(r)} & -G^{(r)} \end{bmatrix} + u_{r+1} t_{r+1,r} e_{2r}^T$$

  where $G^{(r)}, D^{(r)} \in \mathbb{R}^{r \times r}$ are diagonal and $T^{(r)} \in \mathbb{R}^{r \times r}$ is tridiagonal.
- Short recurrence to compute the next vectors u_{r+1} and v_{r+1} of the basis involving only the three preceding vectors v_r, u_r, u_{r-1}.
- Requires $2r$ matrix-vector products and $3r$ inner products.
- Classical Arnoldi method requires $2r$ matrix-vector products and r^2 inner products.
- $f(H)u_1 \approx \|u_1\|_2 S f(J_r^T S^T J_n H S) e_1$ as $J_r^T(S^T(J_n u_1)) = \|u_1\|_2 e_1$.

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Let a Hamiltonian matrix $H \in \mathbb{R}^{2n \times 2n}$ and a vector $u_1 \in \mathbb{R}^{2n}$ be given.

Construct $S_{r+s} \in \mathbb{R}^{2n \times 2(r+s)}$ with J-orthonormal columns such that the columns of S_{r+s} span the same subspace as $\mathcal{K}_{2r}(H, u_1) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$.

Assume that dim $\mathcal{K}_{2r}(H, u_1) = 2r$ and dim $\mathcal{K}_{2s}(H^{-1}, H^{-1}u_1) = 2s$.

In [Meister 2011], it is suggested to construct S_{r+s} in the following way:

- Step 1: Start with the two vectors in $\mathcal{K}_2(H, u_1)$ and construct

$$S_1 = [u_1 \mid v_1] \in \mathbb{R}^{2n \times 2}$$

  with $S_1^T J_n S_1 = J_1$ and span$\{S_1\} = \mathcal{K}_2(H, u_1)$. $(r = 1, s = 0)$

- Step 2: Take the two vectors in $\mathcal{K}_2(H^{-1}, H^{-1}u_1)$ and construct

$$S_2 = [y_1 \quad u_1 \mid x_1 \quad v_1] = [Y_1 \quad U_1 \mid X_1 \quad V_1] \in \mathbb{R}^{2n \times 4}$$

  with $S_2^T J_n S_2 = J_2$ and span$\{S_2\} = \mathcal{K}_2(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1)$. $(r = s = 1)$

Proceed in this fashion by alternating between $\mathcal{K}_{2r}(H, u_1)$ and $\mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$.

Let a Hamiltonian matrix $H \in \mathbb{R}^{2n \times 2n}$ and a vector $u_1 \in \mathbb{R}^{2n}$ be given.

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$$S_2 = [y_1 \quad u_1 \mid x_1 \quad v_1] = [Y_1 \quad U_1 \mid X_1 \quad V_1] \in \mathbb{R}^{2n \times 4}$$

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Observation:

In case $r = s = k$, $H_{2k} = J_{2k} S_{2k}^T J_n H S_{2k} \in \mathbb{R}^{4k \times 4k}$ has the form (Hamiltonian)

$$
\left[\begin{array}{cccc|cccc||cccc|cccc}
0 &&&& &&&& \lambda_k &&&& &&& \gamma_k \\
& \ddots &&& &&&& & \ddots &&& && \iddots & \mu_k \\
&& \ddots && &&&& && \ddots && & \iddots & \iddots & \\
&&& 0 & &&&& &&& \lambda_1 & \gamma_1 & \mu_2 && \\
\hline
&&&& 0 &&& & &&& \gamma_1 & \alpha_1 & \beta_2 && \\
&&&& & \ddots && & && \iddots & \mu_2 & \beta_2 & \ddots & \ddots & \\
&&&& && \ddots & & & \iddots & \iddots & & & \ddots & \ddots & \beta_k \\
&&&& &&& 0 & \gamma_k & \mu_k && & && \beta_k & \alpha_k \\
\hline\hline
\delta_k &&&& &&&& 0 &&&& &&& \\
& \ddots &&& &&&& & \ddots &&& &&& \\
&& \ddots && &&&& && \ddots && &&& \\
&&& \delta_1 & &&&& &&& 0 & &&& \\
\hline
&&&& \vartheta_1 &&& & &&&& 0 &&& \\
&&&& & \ddots && & &&&& & \ddots && \\
&&&& && \ddots & & &&&& && \ddots & \\
&&&& &&& \vartheta_k & &&&& &&& 0
\end{array}\right]
$$

Observation:
In case $r = s + 1 = k + 1$, the special form of the Hamiltonian matrix $H_{2k+1} = J_{2k+1} S_{2k+1}^T J_n H S_{2k+1}$ is given by

$$
\left[\begin{array}{cccc|ccccc||cccc|ccccc}
0 & & & & & & & & & \lambda_k & & & & & & & \gamma_k & \mu_{k+1} \\
 & \ddots & & & & & & & & & \ddots & & & & & \iddots & \mu_k & \\
 & & \ddots & & & & & & & & & \ddots & & & \iddots & \iddots & & \\
 & & & 0 & & & & & & & & & \lambda_1 & \gamma_1 & \mu_2 & & & \\
\hline
 & & & & 0 & & & & & & & & \gamma_1 & \alpha_1 & \beta_2 & & & \\
 & & & & & \ddots & & & & & & \iddots & \mu_2 & \beta_2 & \alpha_2 & \beta_3 & & \\
 & & & & & & \ddots & & & & \iddots & \iddots & & & \beta_3 & \ddots & \beta_k & \\
 & & & & & & & 0 & & \gamma_k & \mu_k & & & & & \ddots & \ddots & \beta_{k+1} \\
 & & & & & & & & 0 & \mu_{k+1} & & & & & & & \beta_{k+1} & \alpha_{k+1} \\
\hline\hline
\delta_k & & & & & & & & & 0 & & & & & & & & \\
 & \ddots & & & & & & & & & \ddots & & & & & & & \\
 & & \ddots & & & & & & & & & \ddots & & & & & & \\
 & & & \delta_1 & & & & & & & & & 0 & & & & & \\
\hline
 & & & & \vartheta_1 & & & & & & & & & 0 & & & & \\
 & & & & & \ddots & & & & & & & & & \ddots & & & \\
 & & & & & & \ddots & & & & & & & & & \ddots & & \\
 & & & & & & & \vartheta_k & & & & & & & & & 0 & \\
 & & & & & & & & \vartheta_{k+1} & & & & & & & & & 0
\end{array}\right]
$$

Yields algorithm with short recurrences, about 1 page long.

Efficient implementation requires

- 4 matrix-vector-multiplications with H,
- 3 linear solves with H,
- 14 scalar products.

Theorem (B./Faßbender/Senn, arXiv:2202.12640)

Let $H \in \mathbb{R}^{2n\times 2n}$ be a Hamiltonian matrix. Let $r+s=n$ and either $r=s+1$ or $r=s$. Then in case the procedure sketched does not break down for $u_1 \in \mathbb{R}^{2n}$ with $\|u_1\|_2 = 1$, there exists a symplectic matrix $S \in \mathbb{R}^{2n\times 2n}$ such that $Se_{s+1} = u_1$,

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Hamiltonian Extended Krylov Subspace (HEKS) Method

- HEKS recursion for $r = s = k$

$$HS_{2k} = S_{2k}H_{2k} + u_{k+1}(\mu_{k+1}e_{2k+1}^T + \beta_{k+1}e_{4k}^T).$$

In case $\mu_{k+1} = \beta_{k+1} = 0$ or $u_{k+1} = 0$, we have a lucky breakdown as

$$\text{span}\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$$

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- HEKS recursion for $r = s + 1 = k + 1$

$$HS_{2k+1} = S_{2k+1}H_{2k+1} + (\gamma_{k+1}y_{k+1} + \beta_{k+2}u_{k+2})e_{4k+2}^T.$$

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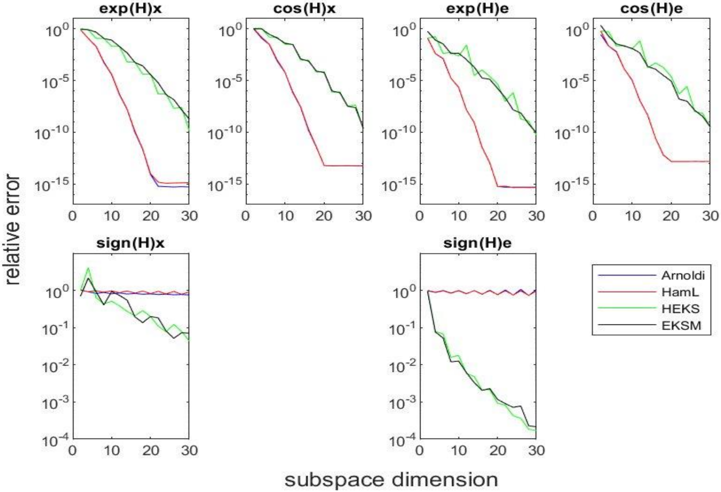
$$H \in \mathbb{R}^{1998\times 1998}, \quad x = \mathrm{randn}\,(2n,1); \quad e = \mathrm{ones}\,(2n,1);$$



Compare

- Classical *Arnoldi* (A) and *unsymmetric Lanczos* (UL) methods (non-symplectic basis),
- *symplectic Lanczos* (SL) method [B./Faßbender 1997],
- *symplectic Arnoldi* (SA) method (range $S = \mathcal{K}_{2r}(H, u_1) + J\mathcal{K}_{2r}(H, u_1)$) [Eirola/Koskela 2019],
- *isotropic Arnoldi* (IA) method ($S = [\, U_r, \; -JU_r \,]$) [Mehrmann/Watkins 2000],
- *block J-orthogonal* (BJ) method ($S = W_r \oplus W_r$) [Li/Celledoni 2019],
- *Hamiltonian extended Krylov subspace* (HEKS) method [Meister 2011, B./Faßbender/Senn 2022].

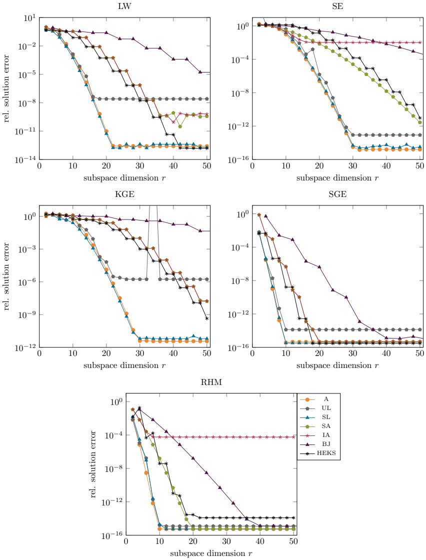
for the approximation of $\exp(H)v$, $\varphi(H)v$ using four semi-discretized 1D Hamiltonian PDE examples:

- **linear wave equation** (LW),
- **nonlinear Schrödinger equation** (SE),
- **nonlinear Klein-Gordon equation** (KGE),
- **sine-Gordon equation** (SGE),

and a random Hamiltonian matrix (RHM). All Hamiltonian matrices are of size $2,500 \times 2,500$.

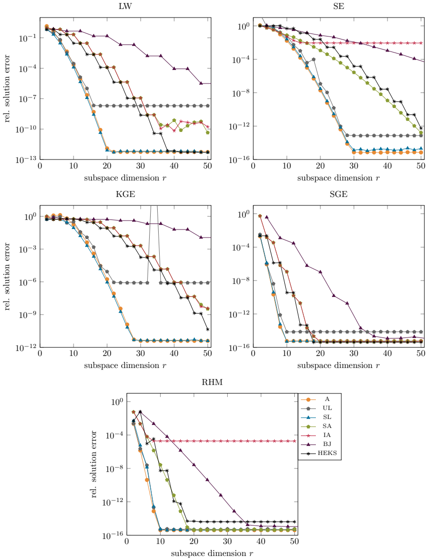
Numerical Experiments

Relative solution error for the approximation of $\exp(H)v$



Numerical Experiments

Relative solution error for the approximation of $\varphi(H)v$



Observations from previous experiment:

- Both, classical Arnoldi and symplectic Lanczos are accurate for all considered examples.
- All other methods need higher-dimensional subspace, or do not reach full precision at all, for at least one example.
- Thus, **for testing exponential integrators for Hamiltonian systems,** we employ classical Arnoldi (non-symplectic) and symplectic Lanczos (symplectic).

Using the same examples as before, we test the (approximated) exponential integrators

- exponential(ly fitted) Euler (EE),
- explicit exponential midpoint rule (EEMP),
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- exponential(ly fitted) Euler (EE),
- explicit exponential midpoint rule (EEMP),
- implicit exponential midpoint rule (IEMP),
- a fourth-order method (EI4) from [Hochbruck et al 1998].

Numerical Experiments

Observations from previous experiment:

- Both, classical Arnoldi and symplectic Lanczos are accurate for all considered examples.
- All other methods need higher-dimensional subspace, or do not reach full precision at all, for at least one example.
- Thus, **for testing exponential integrators for Hamiltonian systems,** we employ classical Arnoldi (non-symplectic) and symplectic Lanczos (symplectic).

Using the same examples as before, we test the (approximated) exponential integrators

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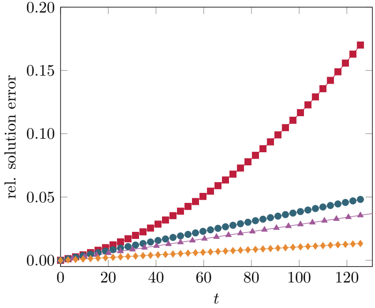
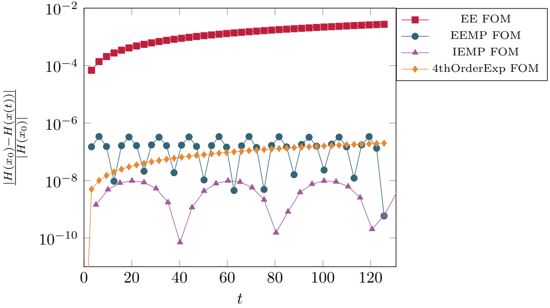
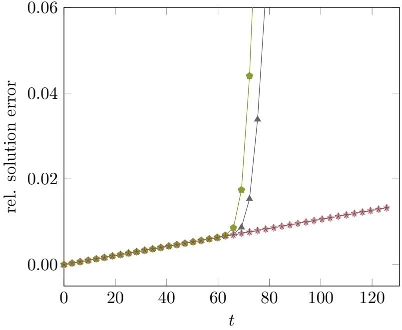
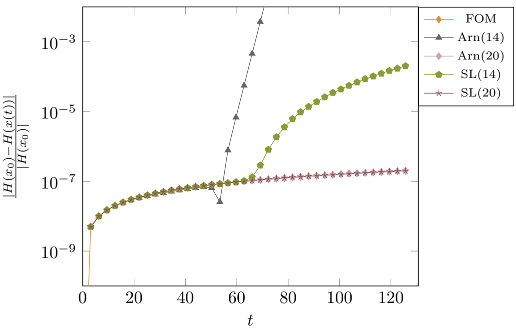
Numerical Experiments: nonlinear 1D Schrödinger equation from [Eirola/Koskela 2019]

Relative solution error and preservation of Hamiltonian for full-order models

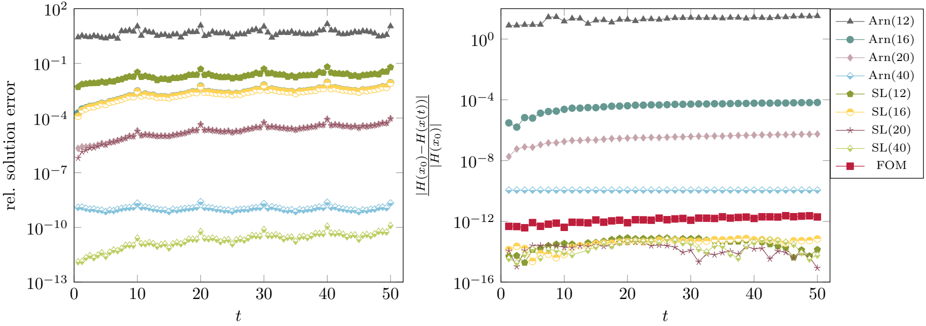





0.06
0.04
0.02
0.00
rel. solution error
0
20
40
60
80
100
120
t


10^{-3}
10^{-5}
10^{-7}
10^{-9}
$\frac{|H(x_0)-H(x(t))|}{|H(x_0)|}$
0
20
40
60
80
100
120
t
FOM
Arn(14)
Arn(20)
SL(14)
SL(20)

Relative solution error and preservation of Hamiltonian for reduced-order models (EE)



Conclusions

- Symplectic Lanczos method appears to be a reliable method for approximating the action of a matrix function to a vector in exponential integrators for Hamiltonian systems.
- The Hamiltonian extended Krylov subspace method (HEKS) has interesting numerical properties (sparse structure of matrix Rayleigh quotient, short recurrence), but has to prove its merits in other areas.
- Further applications:
  - model order reduction for linear (port?-)Hamiltonian systems,
  - efficient generation of snapshots for symplectic POD-like model order reduction methods.

Thank you for your attention!

Conclusions

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Thank you for your attention!

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