Flattening the error curve of predictor algorithms for implicit methods in IVP

PinT 2022: 11th Conference on Parallel-in-Time Integration (CIRM, Marseille, France)

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July 11-15, 2022

Initial value problems (IVPs)

We consider initial value problems for example for ordinary differential equations (ODEs)

$$\frac{d}{dt}x = f(t, x), \qquad x(t_0) = x_0$$

where

$$f \in \mathcal{C}^{M \geq 1},$$

e.g., with $M = \infty$.

We could in fact consider differential-algebraic equations (DAEs), time-dependent partial differential equations (PDEs), or any other type of deterministic time-dependent equations.

Implicit methods

We consider for example implicit Runge-Kutta (IRK) methods

$$x_{n+1} = x_n + h_n \sum_{i=1}^{s} b_i f(t_n + c_i h, X_{n+1,i}) \quad \text{for } n = 0, 1, 2, \ldots$$

where at each step the s internal stages $X_{n+1,1}, \ldots, X_{n+1,s}$ must satisfy the system of nonlinear equations

$$X_{n+1,i} - x_n - h_n \sum_{j=1}^{s} a_{ij} f(t_n + c_j h, X_{n+1,j}) = 0 \quad \text{for } i = 1, \ldots, s.$$

We can consider any other type of implicit methods: multistep methods, general linear methods, the generalized-α method, etc.

Example: the 2-stage IRK Gauss method

The 2-stage Gauss IRK method of order 4:

$$\begin{array}{c|cc} c_1 & a_{11} & a_{12} \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array} \equiv \begin{array}{c|cc} 1/2-\sqrt{3}/6 & 1/4 & 1/4-\sqrt{3}/6 \\ 1/2+\sqrt{3}/6 & 1/4+\sqrt{3}/6 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}$$

Main assumption

Assumption: Constant stepsizes: $h_n = h$

Advantages:

- Asymptotic expansion of global error
- Backward error analysis (ODEs: $x_n \approx \widetilde{x}(t_0 + nh)$, $\dot{\widetilde{x}} = f_h(t, \widetilde{x})$)
- Global (componentwise!) error estimation (at $nh = \widehat{n}\widehat{h}$)
- Extrapolation (at $nh = \widehat{n}\widehat{h}$)
- No "local error estimates"/stepsize control needed
- No need to recompute Jacobian decompositions due to stepsize changes

Main disadvantage:

- May be inefficient.
  This can be addressed by time-rescaling

Goal of predictor algorithms

To obtain accurate guesses of implicitly defined unknowns in order to reduce the number of fixed point/Newton-type (FN) iterations needed.

- An overlooked problem with great potential for improvements
- Before the first FN iteration: starting approximation algorithms
- New proposed methodology can also be applied after the first FN iteration

$$X^0_{n+1,k+1} := \Phi_{h,n+1,k+1}(X_{n+1,k}), \qquad k = 0, 1, \ldots, K_{n+1} - 1.$$

and which introduces nonlinearity in the new predictor algorithm

Implicit discrete dynamical systems

More generally, we consider

$$R(h, X_n, X_{n+1}) = 0, \qquad X_n, X_{n+1} \in \mathbb{R}^d$$

where

- X_0 given
- h a small parameter
- we suppose local existence and uniqueness of X_{n+1} for $|h|$ sufficiently small

For example for IRK methods we have

$$X_n := (X_{n,1}, \ldots, X_{n,s})$$

and h is the stepsize.

A new predictor algorithm

Notation $X^{l}_{n+1,k}$

- l: correction level
- $n+1$: new time step
- k: index of FN iteration ($k = 0$ for a starting approximation)

$\underline{k = 0}$: $X^{0}_{n+1,0}$ any initial starting approximation of order r_0

$$X_{n+1} - X^{0}_{n+1,0} = O(h^{r_0+1}) \quad \text{for } h \to 0$$

Examples for IRK methods:

- $X^{0}_{n+1,0} := (x_n, \ldots, x_n)$ (order $r_0 = 0$)
- additional function evaluations (M.P. Laburta, 1997)
- continuous output (I. Higueras, T. Roldán, 2005)

Initial starting approximation for the 2-stage Gauss method

$$X_{n+1} := (X_{n+1,1}, X_{n+1,2})$$

Initial starting approximation of order $r_0 = 2$ given by the extrapolated values

$$X^0_{n+1,1,0} := p_n(t_n + c_1 h), \quad X^0_{n+1,2,0} := p_n(t_n + c_2 h)$$

where $p_n(t)$ is the degree 2 interpolation/collocation polynomial through

$$(t_{n-1}, x_{n-1}), \quad (t_{n-1} + c_1 h, X_{n,1}), \quad (t_{n-1} + c_2 h, X_{n,2}), \quad (t_n, x_n).$$

A new predictor algorithm

Based on error corrections

$$X^{l+1}_{n+1,k} := X^{l}_{n+1,k} + E^{l}_{n+1,k} \qquad \text{for } l = 0, \ldots, L_{n+1,k} - 1$$

where

$$E^{l}_{n+1,k} := e^{l}_{k}(t_{n+1})$$

and $e^{l}_{k}(t)$ is the interpolation polynomial of degree d^{l}_{k} of exact errors of previous predicted values

$$e^{l}_{k}(t_{n-\ell}) := X_{n-\ell} - X^{l}_{n-\ell,k} \qquad \text{for } \ell = 0, \ldots, d^{l}_{k} \geq 0.$$

The final predictor/terminizer at FN iteration k:

$$X_{n+1,k} := X^{L_{n+1,k}}_{n+1,k} = X^{0}_{n+1,k} + \sum_{l=0}^{L_{n+1,k}-1} E^{l}_{n+1,k}$$

A new predictor algorithm

- $E^l_{n+1,k}$ are embarrassingly parallel across:
  - the component indices $j = 1, \ldots, d$
  - the correction levels l
  - even the FN iterations k
- Computational cost is minimal, no evaluation of f needed. IVPs (ODEs, DAEs, etc.) are all treated in the same way, it is a universal approximation algorithm.
- Unifies and extends different approaches,.
- Trades time for memory, here function evaluations in FN iterations, requiring also communication, with embarrassingly parallel extrapolation procedures. In summary: less FN iterations, more memory use, but only local communication.
- the choice $d^l_k = 0$ leads to a simple implementation

Error estimate of new starting algorithm ($k = 0$)

Consider any initial starting algorithm $X^0_{n+1,0}$ of order $r_0 \leq M-1$ with asymptotic expansion in h

$$X_{n+1} - X^0_{n+1,0} = \sum_{m=r_0+1}^{M} h^m a_0^{m,0}(t_{n+1}) + o(h^M) \quad \text{for } h \to 0$$

with $a_0^{m,0}(t) \in \mathcal{C}^{M-m} \Longrightarrow$ for $h \to 0$ we have

$$X_{n+1} - X^{l+1}_{n+1,0} = \begin{cases} O(h^{p_0^{l+1}+1}) & \text{if } p_0^{l+1} \leq M-1, \\ o(h^M) & \text{if } M \leq p_0^{l+1}. \end{cases}$$

where $p_0^{l+1} := r_0 + l + 1 + d_0^0 + \ldots + d_0^l$

Error estimate of new predictor algorithm ($k = 1$)

Under the assumptions of Theorem (1) $\Longrightarrow$ *for* $h \to 0$ *we have*

$$X_{n+1} - X^{l+1}_{n+1,1} = \begin{cases} O(h^{p_1^{l+1}+1}) & \text{if } p_1^{l+1} \leq M-1, \\ o(h^M) & \text{if } M \leq p_1^{l+1}. \end{cases}$$

where $p_1^{l+1} := r_1 + l + 1 + d_1^0 + \ldots + d_1^l$ *and*
$r_1 := 1 + \min_{j=1,\ldots,d} p_0^{L_{\cdot,0}}$

etc. for $k = 2, 3, \ldots, K_{n+1} - 1$. But remember that our goal is to have K_{n+1} small!

A stopping criterion of FN iterations for IRK methods

For $k \geq 1$ (at least one FN iteration per time-step)

$$\max_{j=1,\ldots,s} (\Psi_{\mathrm{Tol}}(X^0_{n+1,j,k}, \Delta X^0_{n+1,j,k})) \leq 1$$

where

$$\Psi_{\mathrm{Tol}}(y, \Delta y) := \max_{i=1,\ldots,d} \left(\frac{|\Delta y_i|}{\max(\mathtt{RTol}_i \cdot |y_i|, \mathtt{ATol}_i)} \right)$$

here with $\mathtt{RTol}_i = 10^{-10}$, $\mathtt{ATol}_i = 10^{-14}$.

On the stopping criterion

Consider $\texttt{rtol} > 0$ *and* $\texttt{atol} > 0$. *Then*

$$|r - q| \leq \max(\texttt{rtol} \cdot |r|, \texttt{atol})$$

$$\iff \quad |r - q| \leq \frac{\texttt{rtol}}{1 + \texttt{rtol}} \cdot \max(|q|, p)$$

where

$$p := \frac{\texttt{atol}}{\texttt{rtol}}(1 + \texttt{rtol}).$$

Hence, when $|q| \geq p$ we have

$$\frac{|r - q|}{|r|} \leq \texttt{rtol}$$

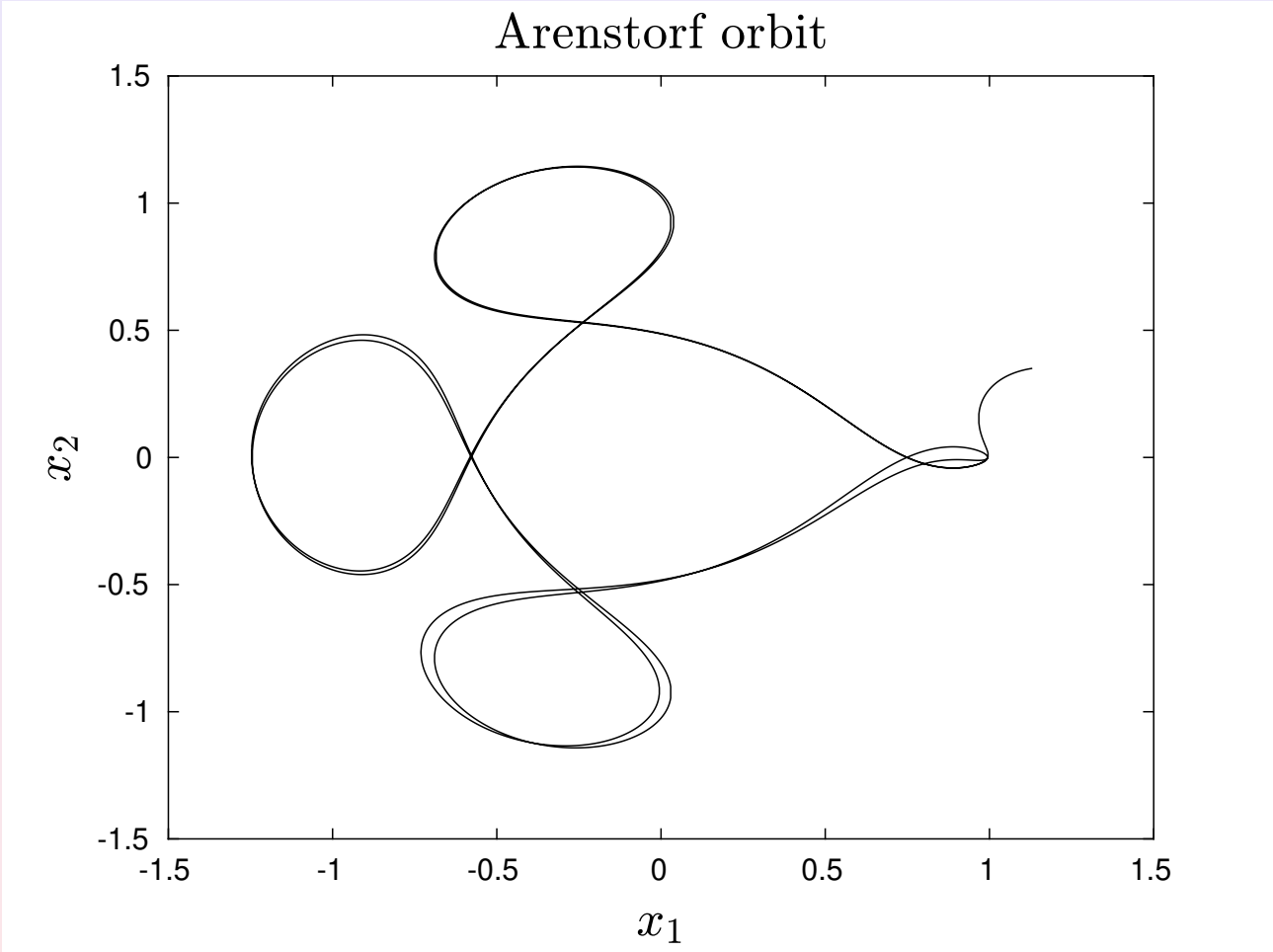
and when $|q| \leq p$ we have $|r - q| \leq \texttt{atol} = p(1 + \texttt{rtol})/\texttt{rtol}$.

The periodic Arenstorf orbit

$$
\begin{aligned}
\frac{d}{dt}x_1 &= x_3, \qquad x_1(0) = 0.994,\\
\frac{d}{dt}x_2 &= x_4, \qquad x_2(0) = 0,\\
\frac{d}{dt}x_3 &= x_1 + 2x_4 + (\mu-1)\frac{(x_1+\mu)}{D_1} - \mu\frac{(x_1+\mu-1)}{D_2}, \qquad x_3(0) = 0,\\
\frac{d}{dt}x_4 &= x_2 - 2x_3 + (\mu-1)\frac{x_2}{D_1} - \mu\frac{x_2}{D_2}, \; x_4(0) = -2.001585106379082 5\ldots\\
D_1 &= ((x_1+\mu)^2 + x_2^2)^{3/2}, \qquad D_2 = ((x_1+\mu-1)^2 + x_2^2)^{3/2},\\
\mu &= 0.012277471.
\end{aligned}
$$

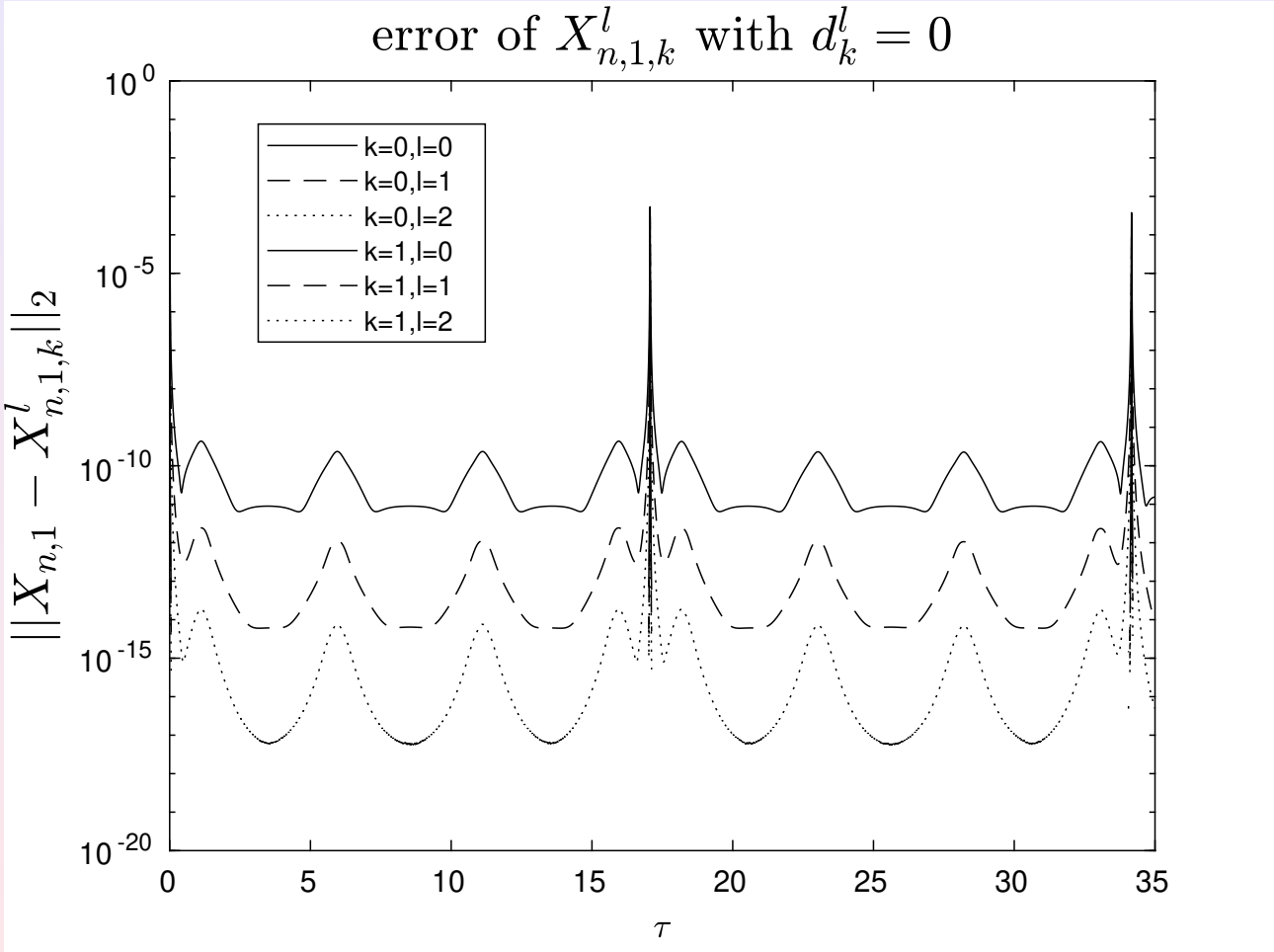
The solution is periodic with period $T = 17.06521656015796 2\ldots$

The periodic Arenstorf orbit and the 2-stage Gauss method



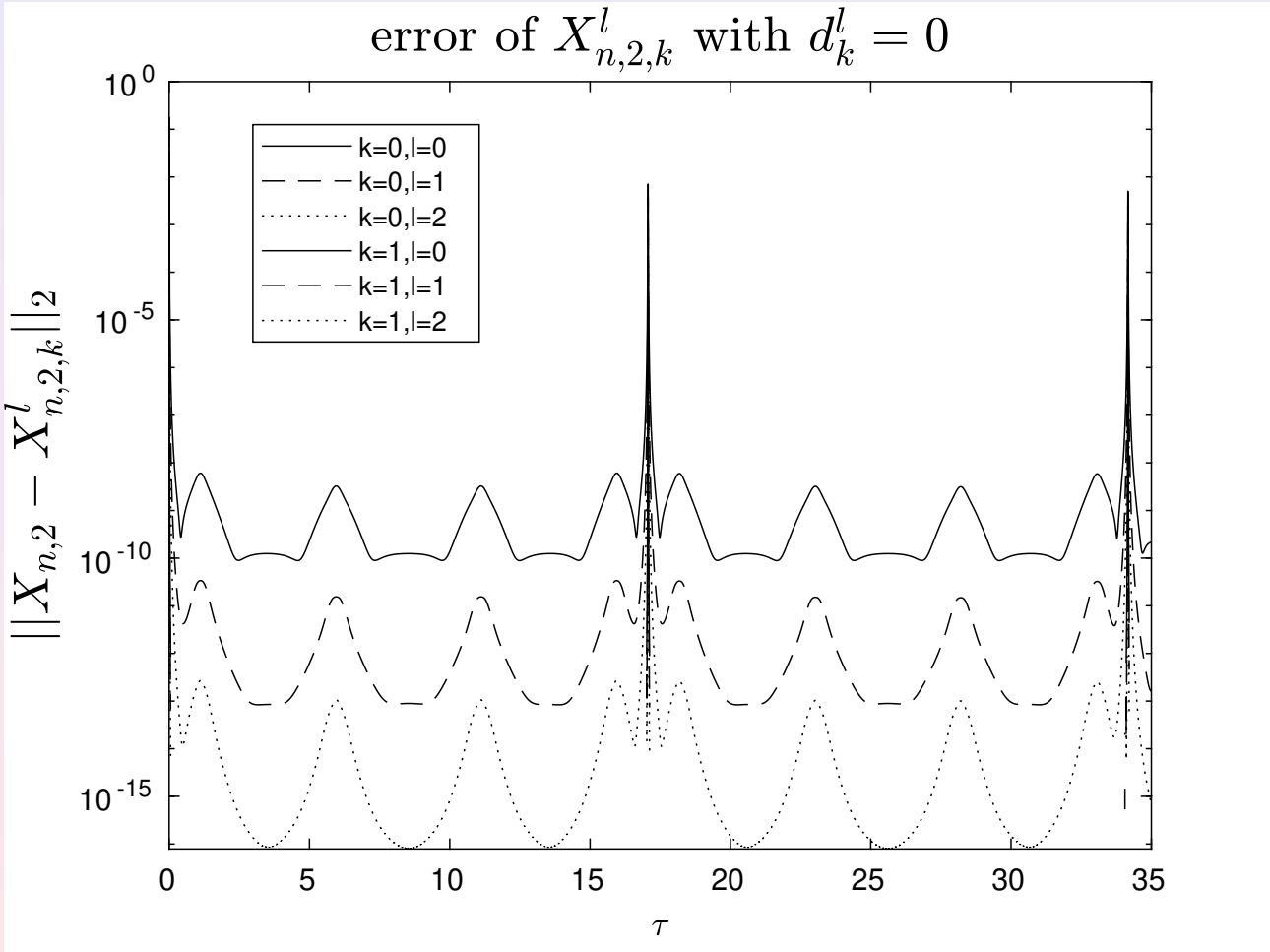
50000 time steps on the time interval $[0, 35]$, $h = 0.0007$.

The periodic Arenstorf orbit and the 2-stage Gauss method



Fixed-point iterations, $h = 0.0007$.

The periodic Arenstorf orbit and the 2-stage Gauss method



Fixed-point iterations, $h = 0.0007$.

A perturbed Kepler problem

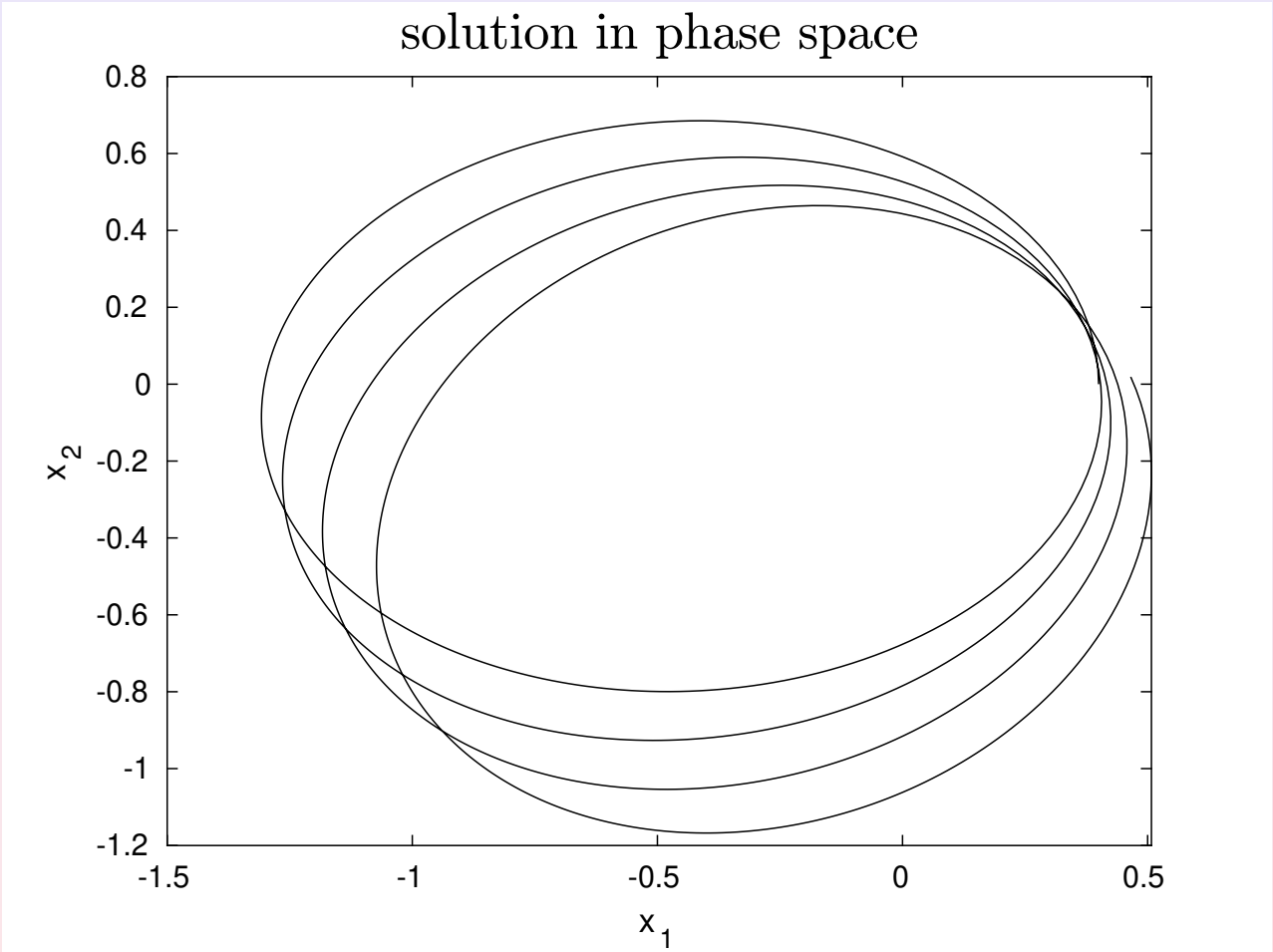
A perturbed Kepler problem with eccentricity $e = 0.6$ and perturbation $\delta = 0.015$:

$$\begin{aligned}
\frac{d}{dt}x_1 &= x_3 & x_1(0) &= 1 - e \\
\frac{d}{dt}x_2 &= x_4 & x_2(0) &= 0 \\
\frac{d}{dt}x_3 &= -x_1\left(\frac{1}{(x_1^2+x_2^2)^{3/2}} + \frac{\delta}{(x_1^2+x_2^2)^{5/2}}\right) & x_3(0) &= 0 \\
\frac{d}{dt}x_4 &= -x_2\left(\frac{1}{(x_1^2+x_2^2)^{3/2}} + \frac{\delta}{(x_1^2+x_2^2)^{5/2}}\right) & x_4(0) &= \sqrt{\frac{1+e}{1-e}}
\end{aligned}$$

corresponding to the Hamiltonian:

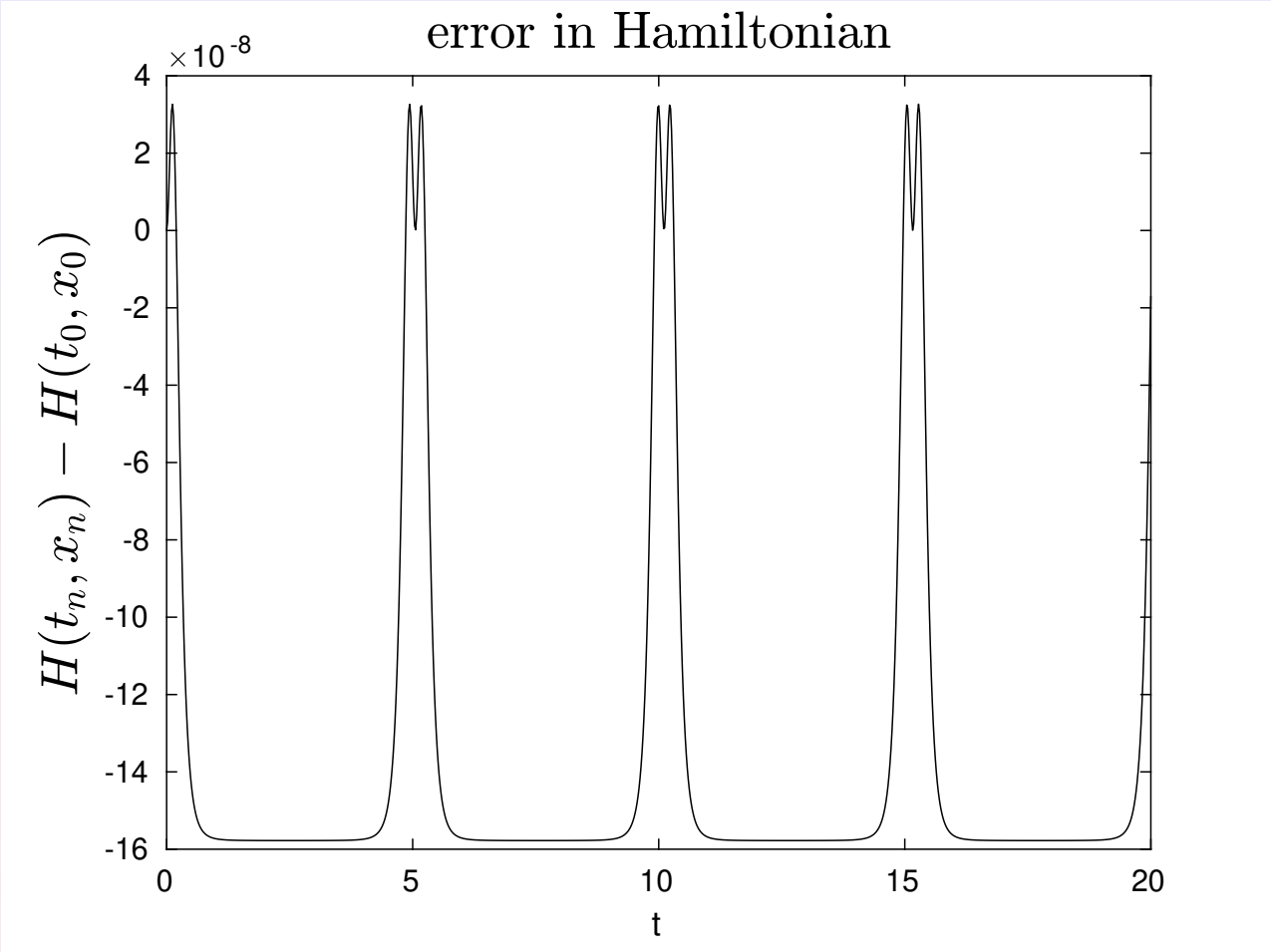
$$H(x) = \frac{x_3^2 + x_4^2}{2} - \frac{1}{(x_1^2+x_2^2)^{1/2}} - \frac{\delta}{3(x_1^2+x_2^2)^{3/2}}$$

A perturbed Kepler problem and the 2-stage Gauss method



1000 time steps on the time interval $[0, 20]$, $h = 0.02$.

A perturbed Kepler problem and the 2-stage Gauss method



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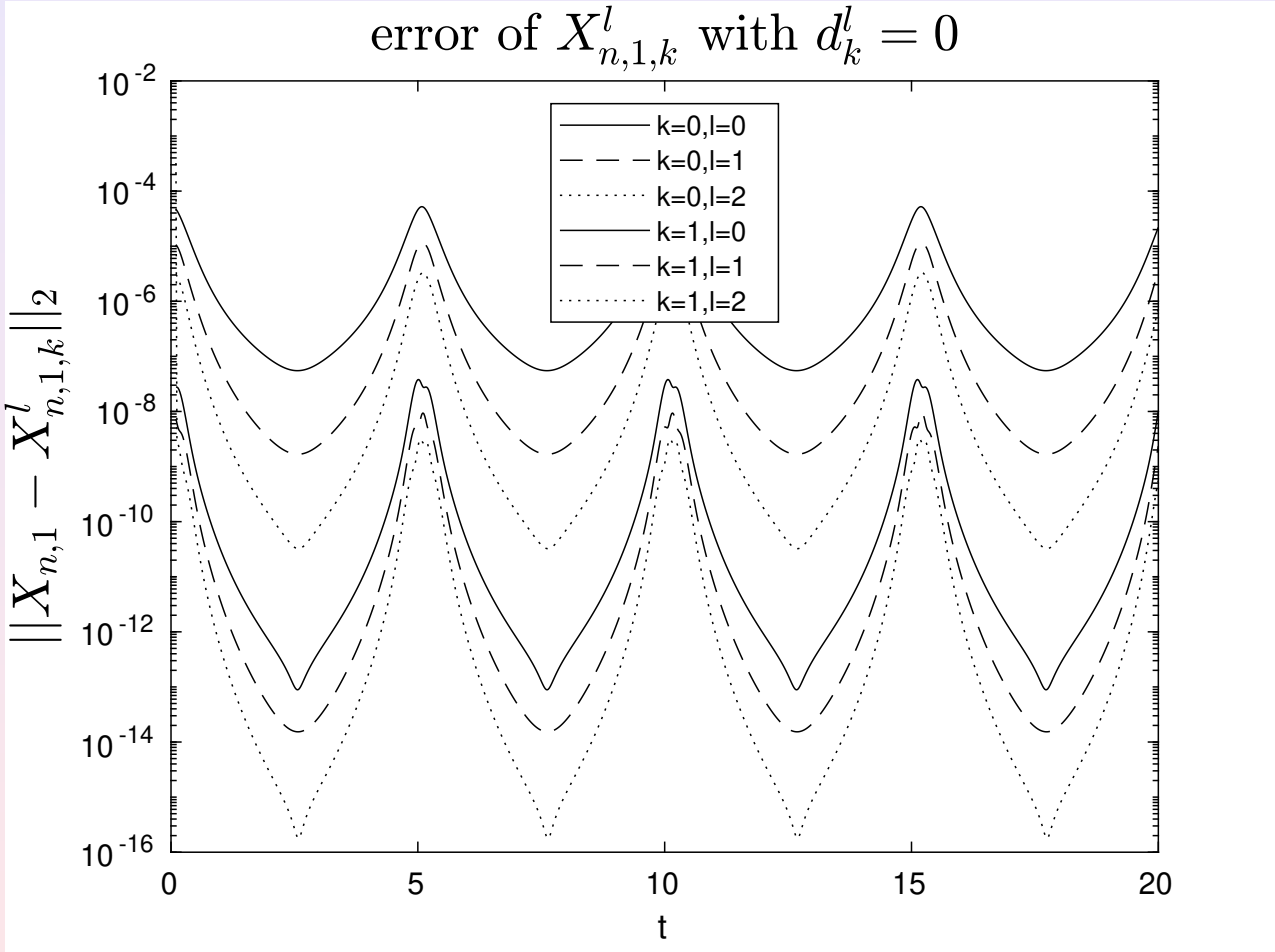

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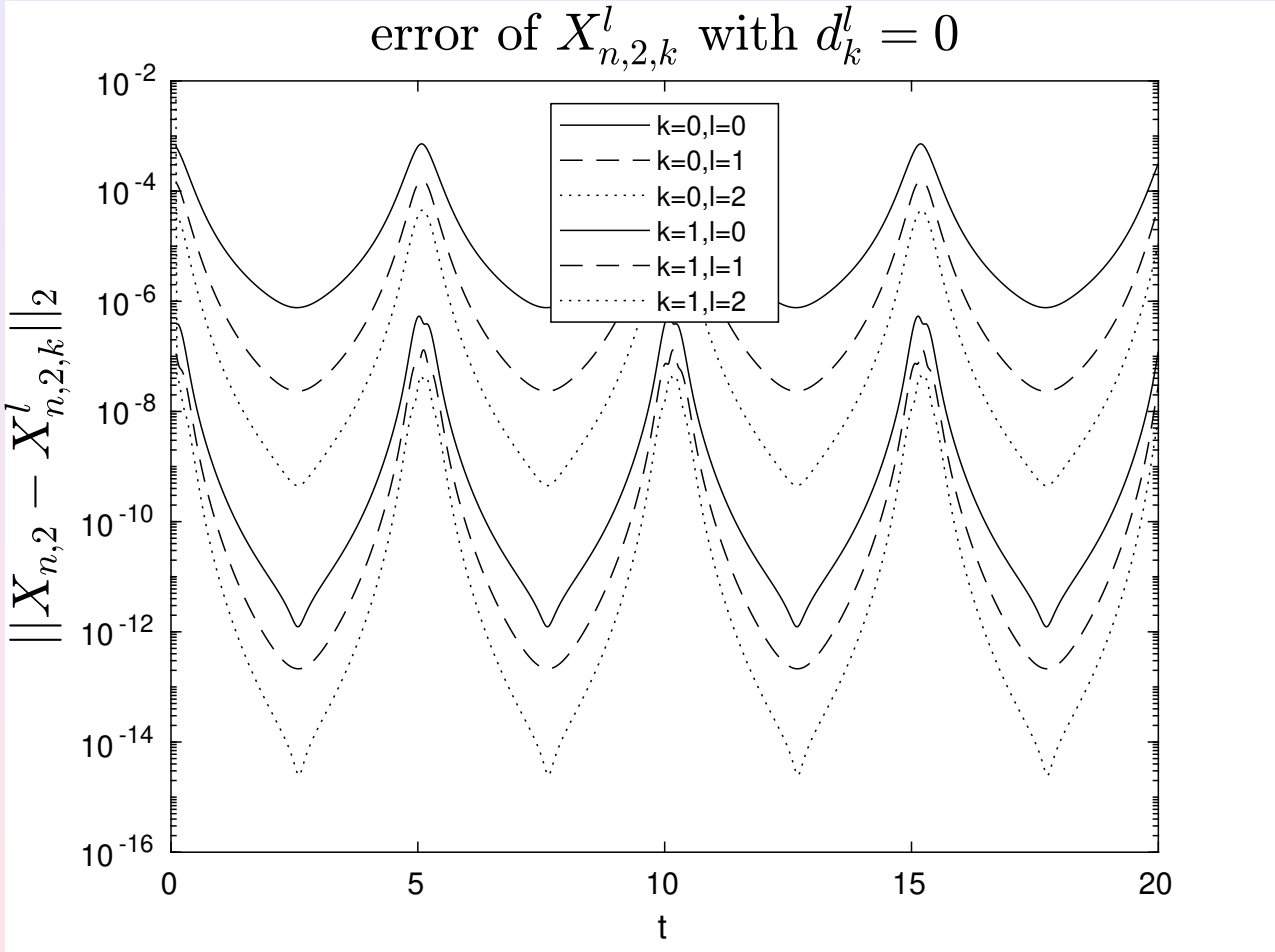


Fixed-point iterations, $h = 0.02$.

Time-rescaling

Variable stepsizes trick: use constant stepsizes h after time-rescaling

$$\frac{d}{d\tau}t = \rho(t,x), \qquad \frac{d}{d\tau}x = \rho(t,x)f(t,x)$$

which is autonomous in τ with $\rho \in \mathcal{C}^M(\mathbb{R}\times\mathbb{R}^d,\mathbb{R}^+)$ when $f \in \mathcal{C}^M$, for example

$$\rho(t,x) := \frac{1}{(\alpha + \|Bf(t,x))\|_q^r)^p}$$

with $\alpha > 0$, $q = 2m$ even, $r = jq$ with $j \in \mathbb{N}$, $p > 0$, and B nonsingular. In the original time t the value of $\alpha > 0$ is such that

$$\frac{h}{\alpha^p} = h_{\max}$$

Example: Time-rescaling with the mipoint rule

$$
\begin{aligned}
t_{n+1} &= t_n + h_n \\
x_{n+1} &= x_n + h_n f\left(t_n + \frac{h_n}{2}, \frac{x_n + x_{n+1}}{2}\right) \\
h_n &= h\rho\left(t_n + \frac{h_n}{2}, \frac{x_n + x_{n+1}}{2}\right)
\end{aligned}
$$

Time-rescaling of Hamiltonian systems

We consider Hamiltonian systems

$$\frac{d}{dt}x = J\nabla_x H(t,x)$$

where J is skew-symmetric. Even for $H = H(x)$

$$\frac{d}{d\tau}x = \rho(x)J\nabla_x H(x)$$

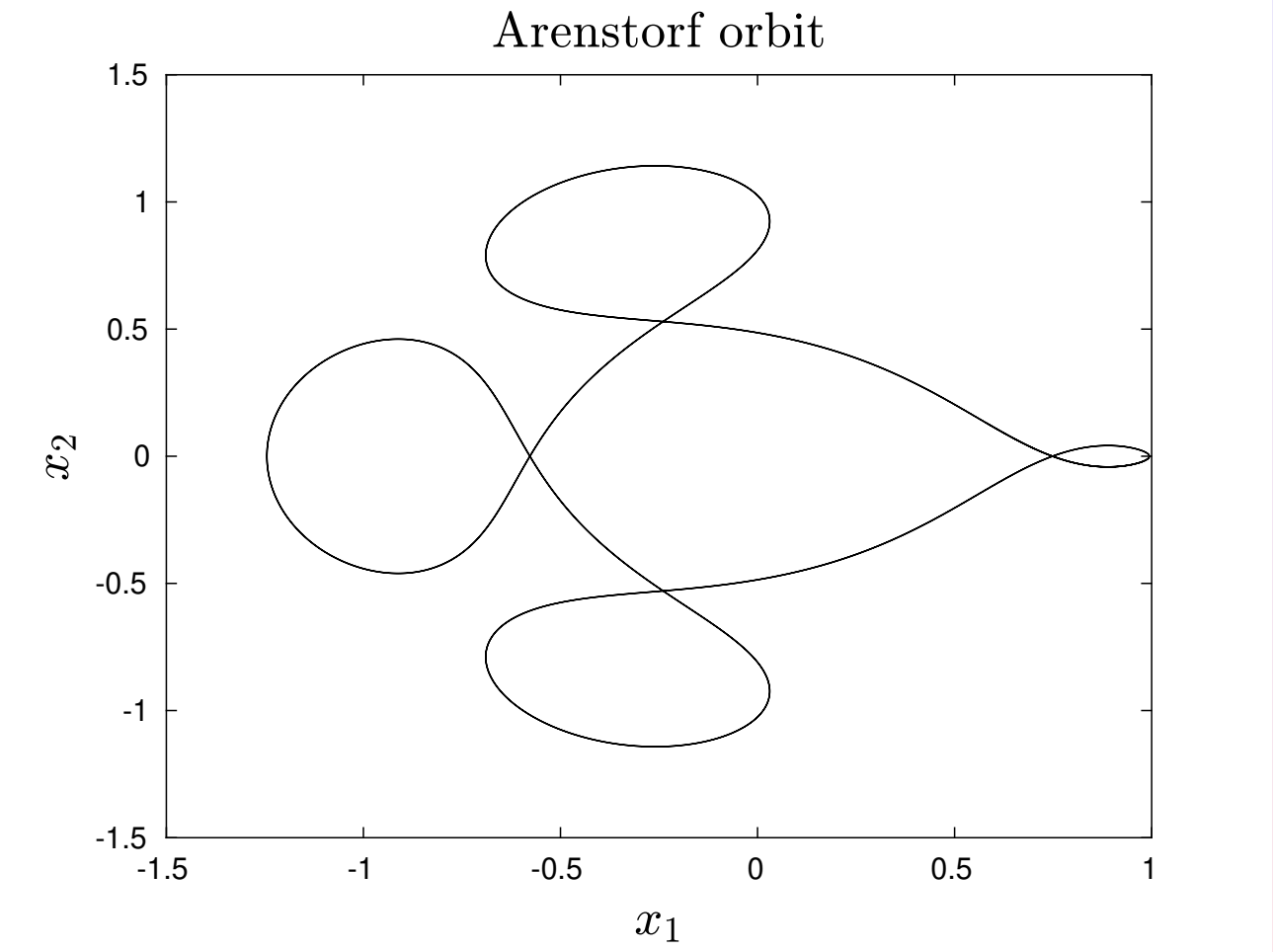
is not Hamiltonian. Introducing (u,s) $(s(\tau) = t, u(\tau) = H(t,x(t))$,

$$\mathbf{H}(x,u,s) := \rho(s,x)(H(s,x) - u)$$

we obtain the extended autonomous Hamiltonian system

$$\begin{aligned}
\frac{d}{d\tau}x &= \rho(s,x)J\nabla_x H(s,x) + (H(s,x) - u)J\nabla_x \rho(s,x) \\
\frac{d}{d\tau}u &= \rho(s,x)\partial_t H(s,x) + (H(s,x) - u)\partial_t \rho(s,x) \\
\frac{d}{d\tau}s &= \rho(s,x)
\end{aligned}$$

The periodic Arenstorf orbit and the 2-stage Gauss method



4000 time steps on the rescaled time interval $[0, 50]$ in τ,
Fixed-point iterations, $h_\tau = 0.0125$, $s(\tau = 50) \approx 34.81$.
$\rho(t, x)$: $B = I$, $\alpha = 0$, $q = 2$, $r = 2$, $p = 1/2$.

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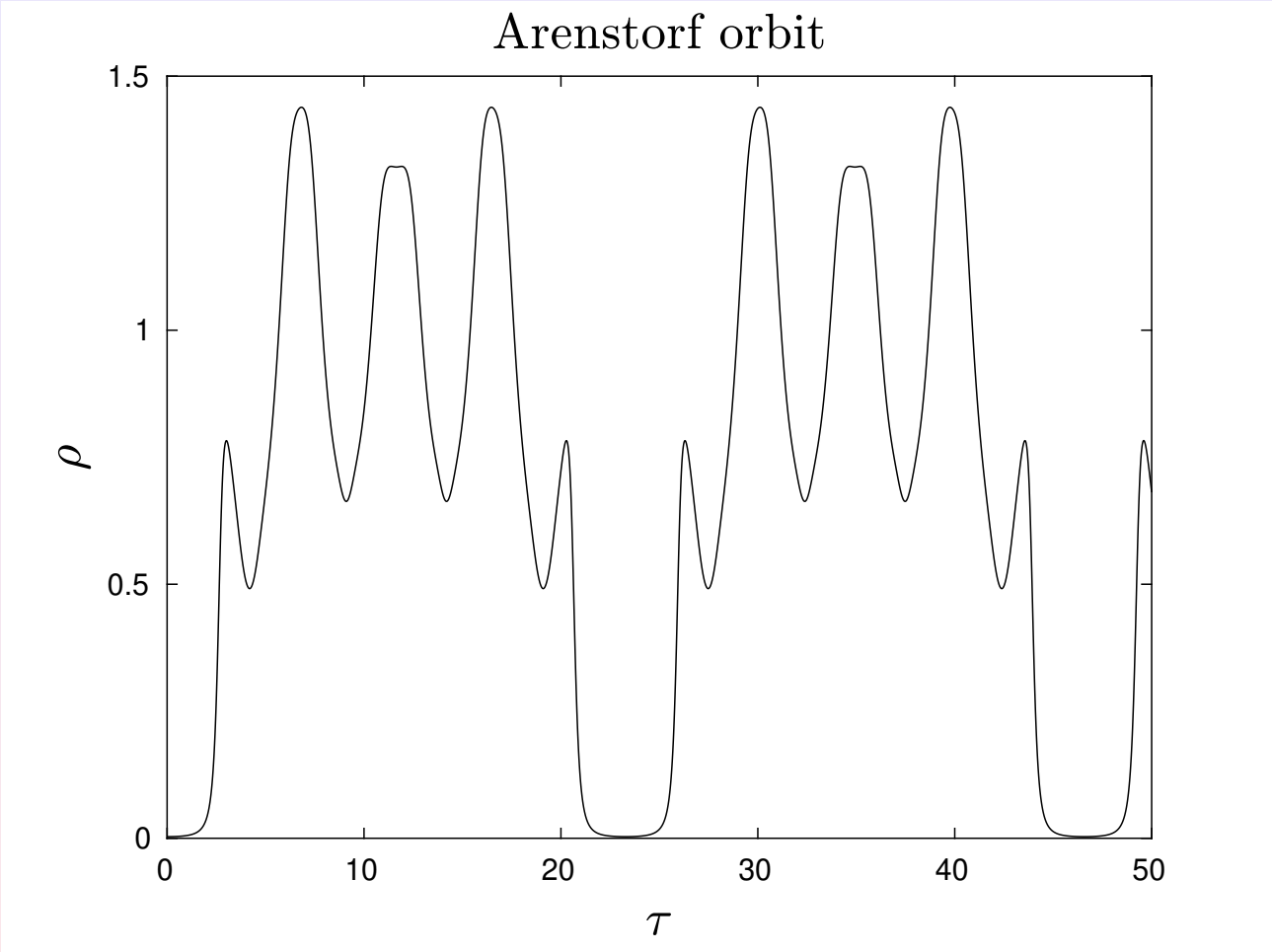

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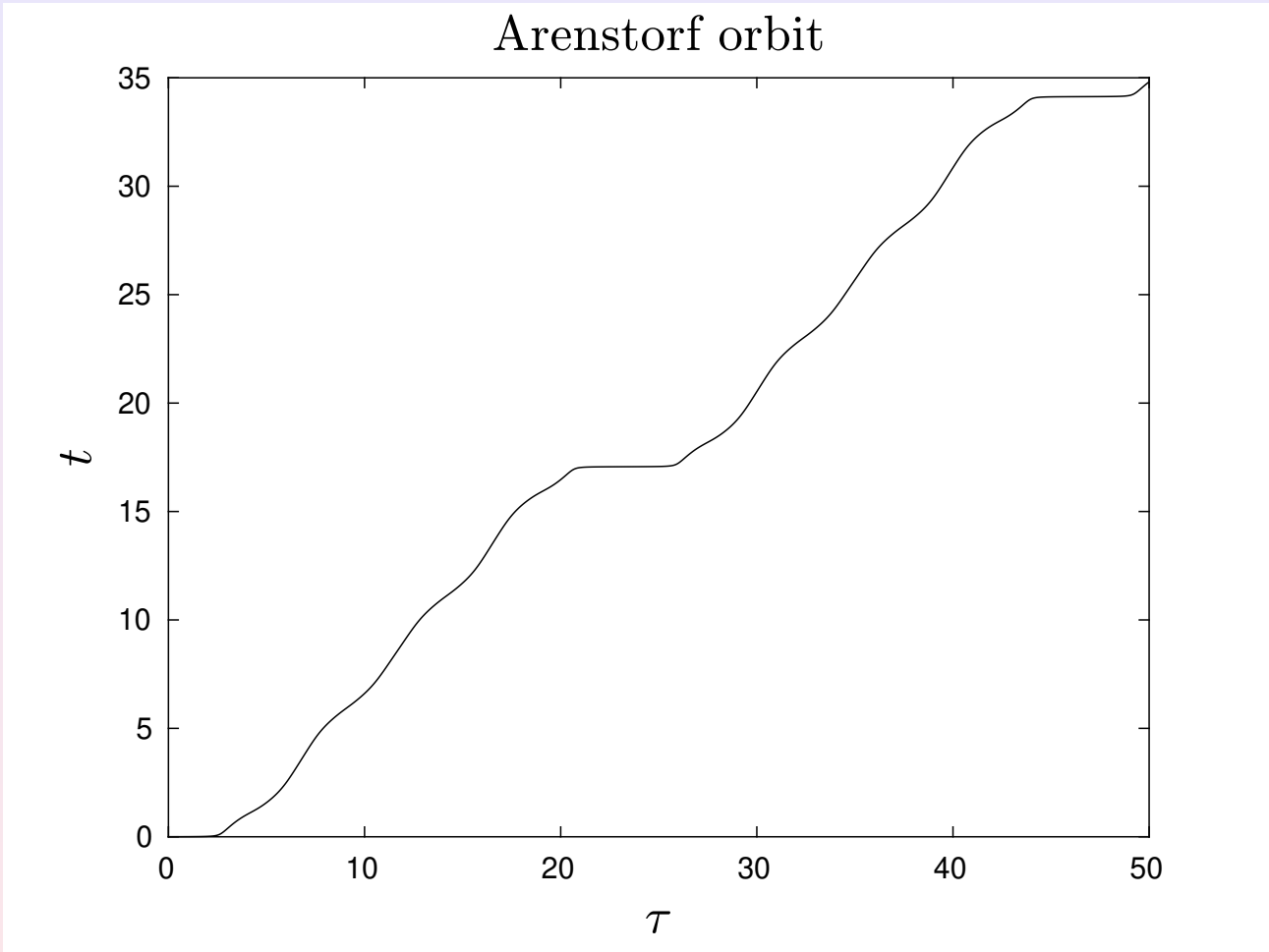

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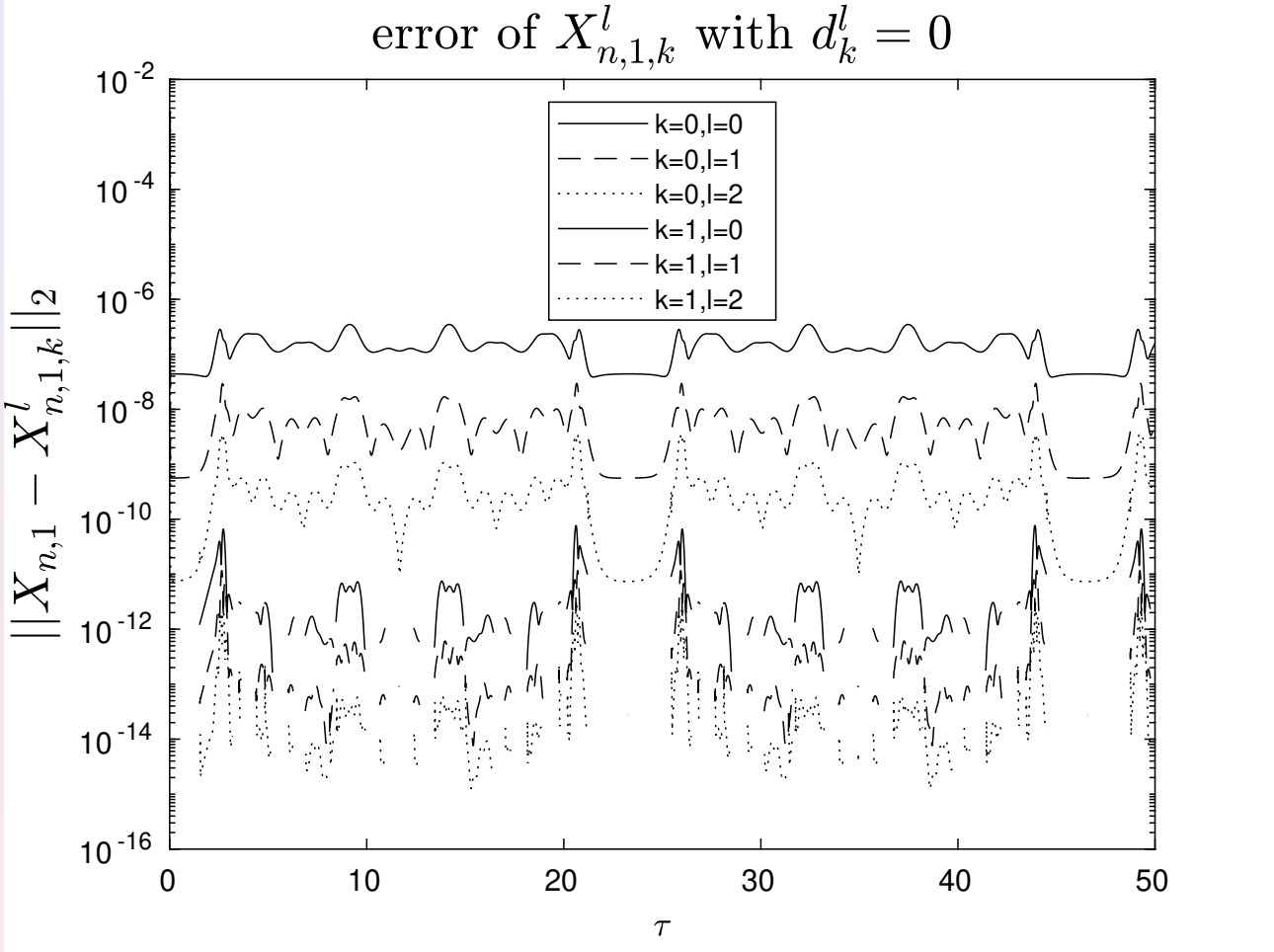

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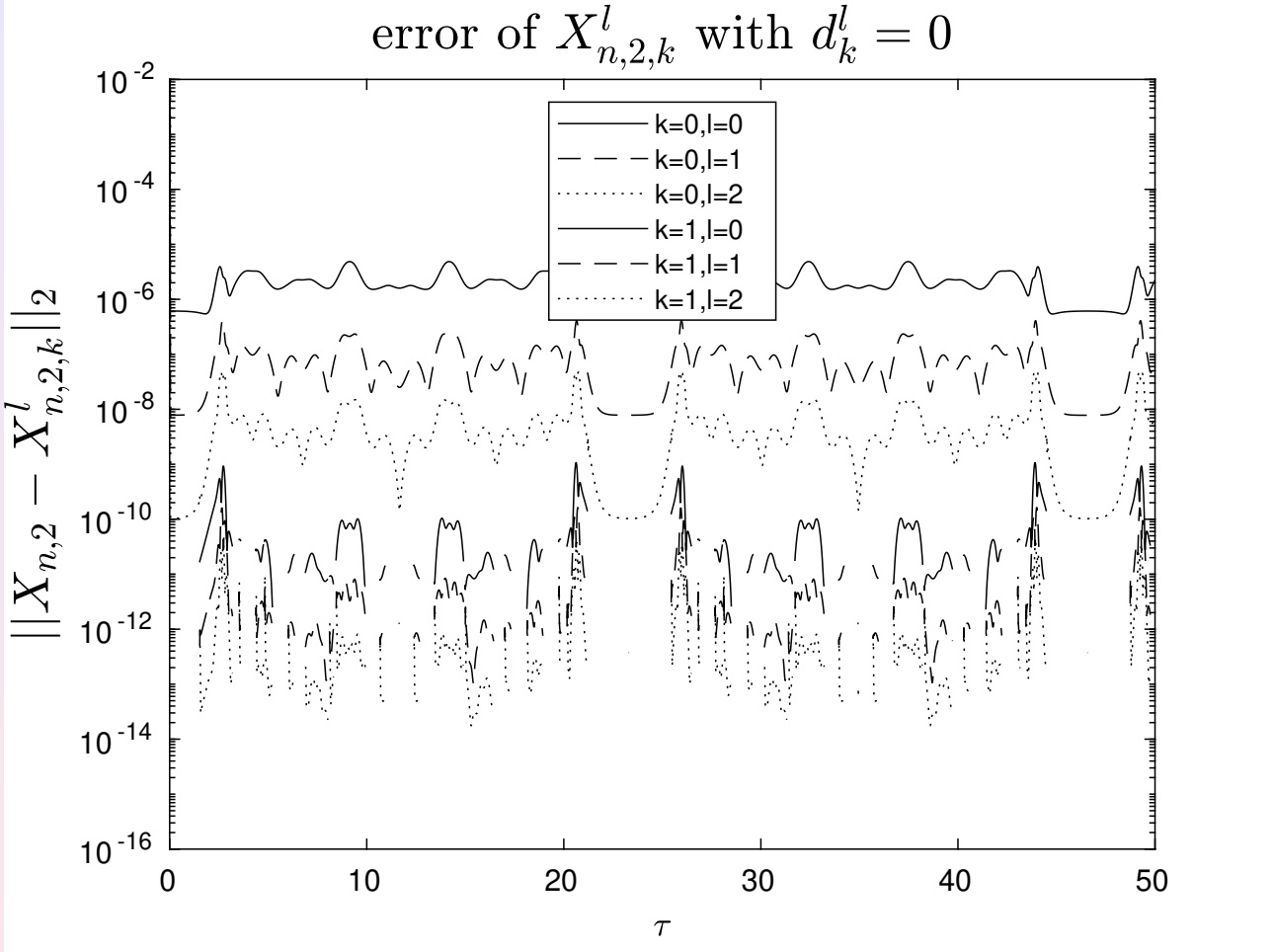

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The periodic Arenstorf orbit and the 2-stage Gauss method

Number of fixed-point iterations using:

- only $X^0_{n+1,j,0} = x_n$ as the initial starting approximation: 18394.
- only the collocation polynomial as initial starting approximation, i.e., $L_{n+1,k=0} = 0$: 11326.
- the new predictor with $L_{n+1,k=0} = 1$ and $d^I_{n+1,k=0} = 0$: 8248.
- the new predictor with $L_{n+1,k=0} = 2$ and $d^I_{n+1,k=0} = 0$: 5977.

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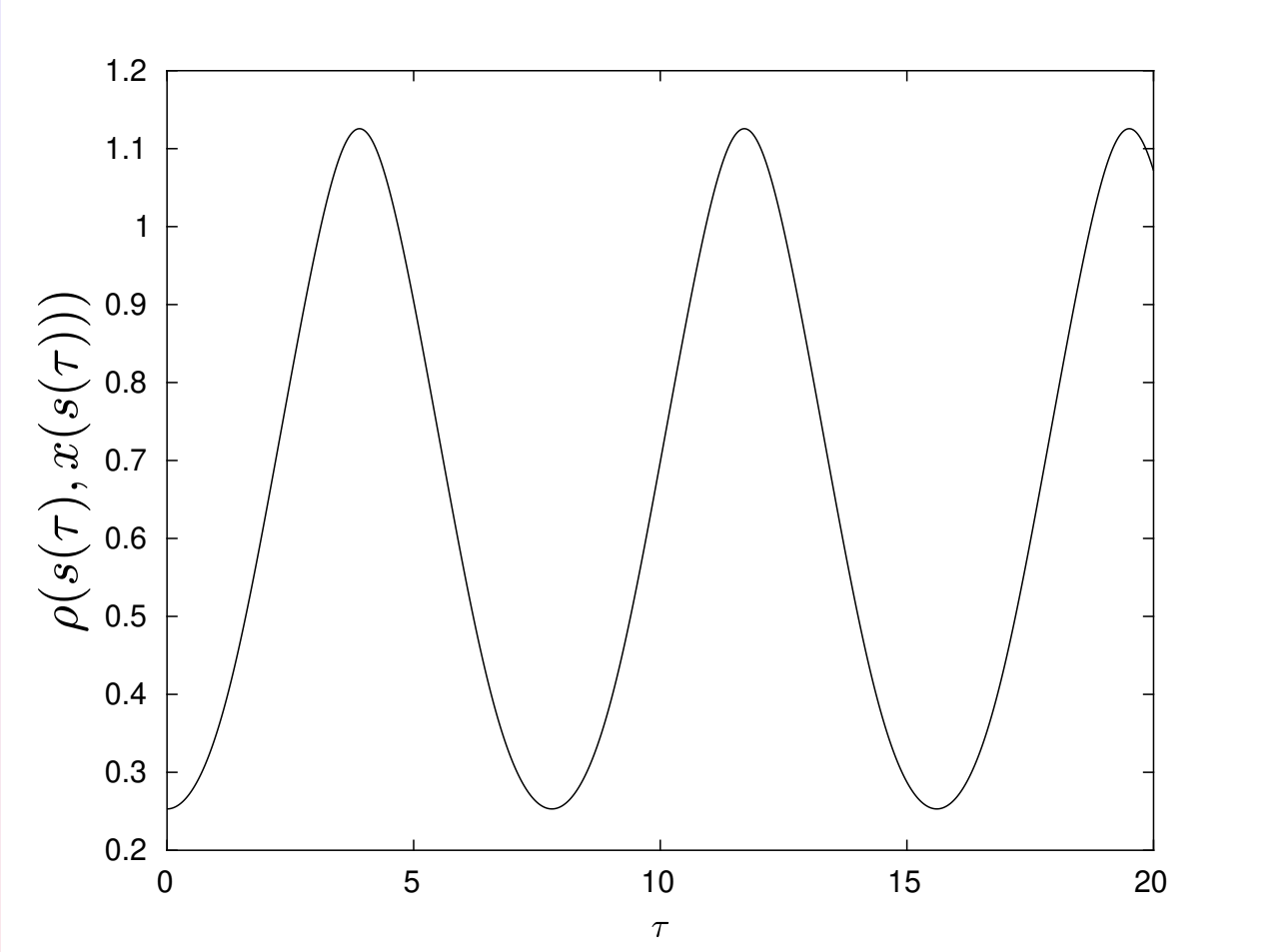
A perturbed Kepler problem and the 2-stage Gauss method



4000 time steps on the rescaled time interval $[0, 20]$ in τ.
Fixed-point iterations, $h_\tau = 0.02$, $s(\tau = 20) \approx 13.182$.
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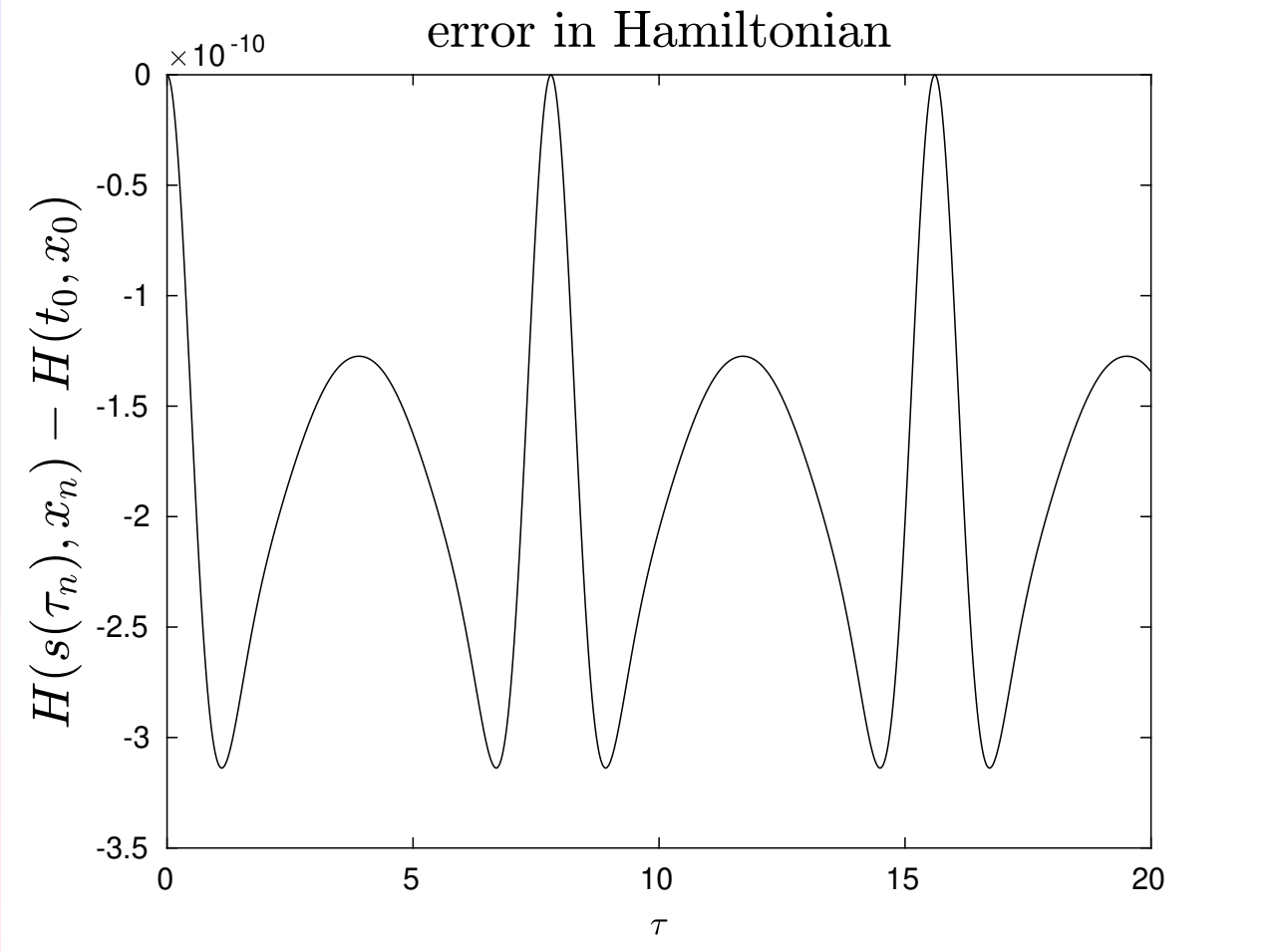

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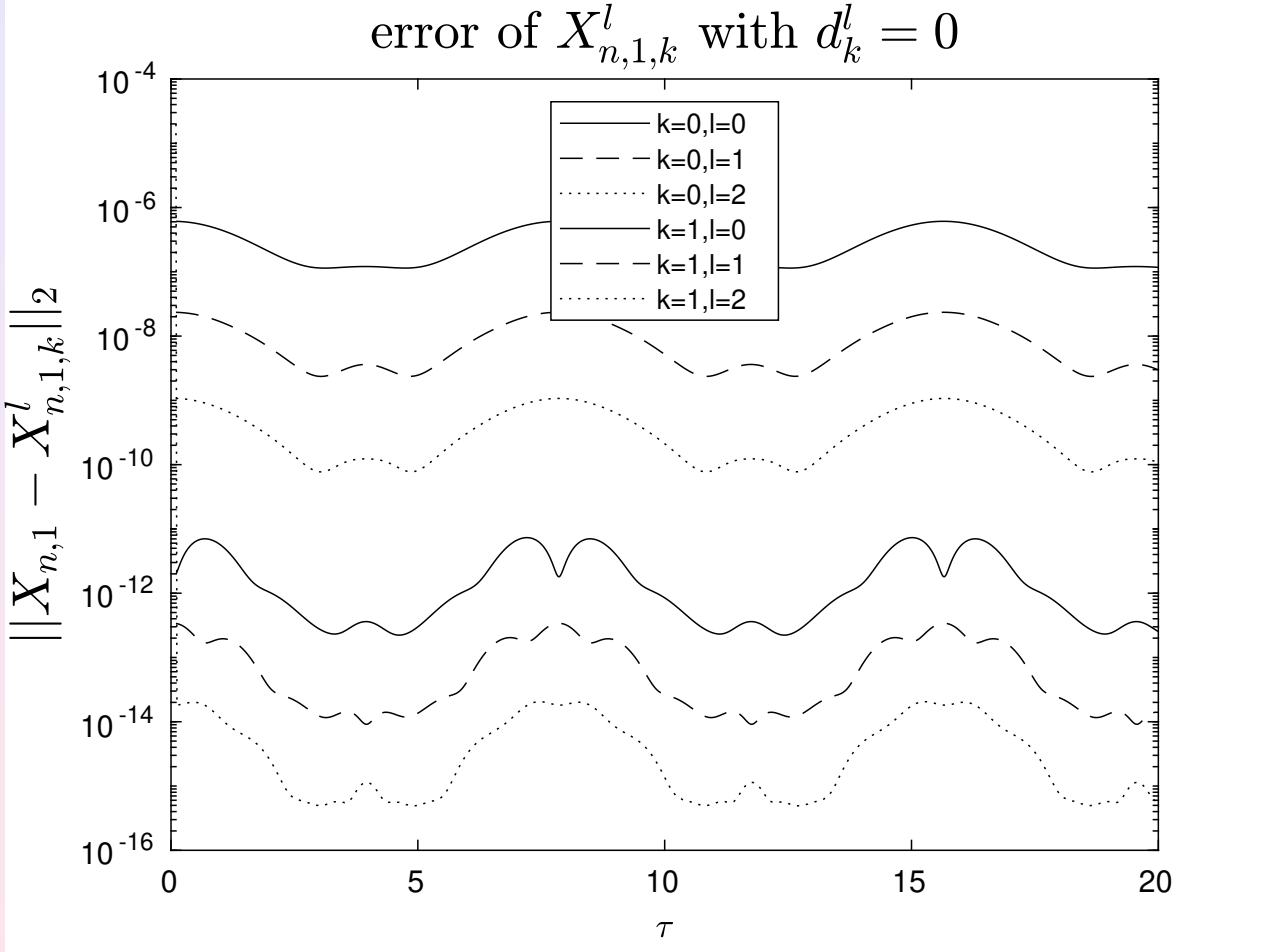

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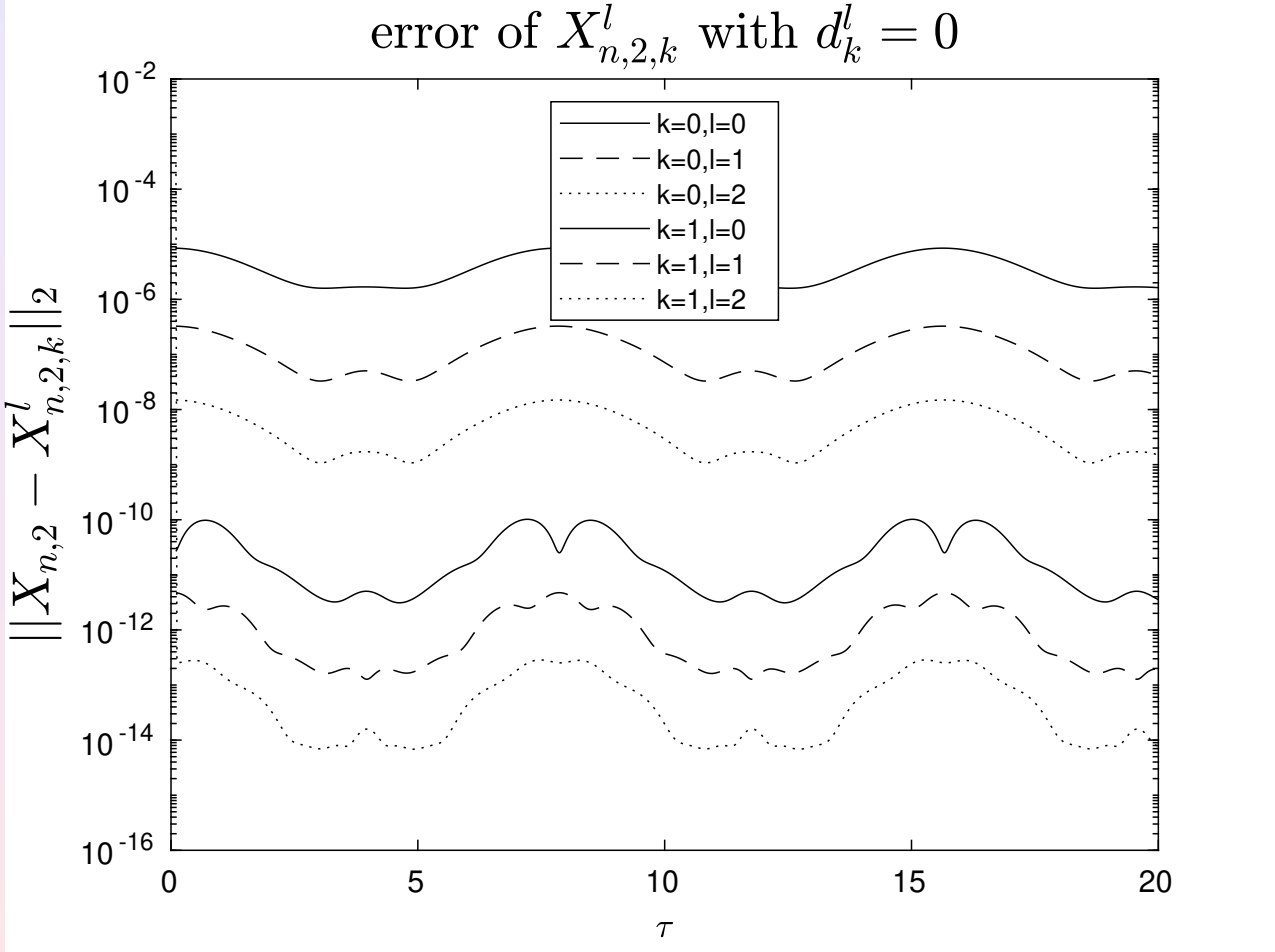

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Conclusion

A new general predictor algorithm is proposed:

- unifies, complements, and improves on current starting approximation algorithms
- can also improve FN iterates leading to a new mixed type of prediction/FN correction iterations
- uses exact errors of approximations from previous steps
- universal since applicable to any

$$R(h, X_n, X_{n+1}) = 0$$

- of arbitrarily high order
- embarrassingly parallel
- time-rescaling of the differential equations can address the efficiency issue

Current/future work to be investigated/implemented

- adaptivity of highest levels $L_{n+1,k}$
- comparison of implicit versus explicit methods: implicit methods have high potential for parallelism and may be more efficient than explicit methods using fixed-point iteration or quasi-Newton methods such as Broyden iterations
- stiff ODEs, parabolic PDEs, DAEs, integral equations, etc.
- parallel implementation
- other time-rescaling functions $\rho(t, x)$
- application to nonlinear optimization: $\min_{x \in X} f(x)$, $\dot{x} = -B(x)\nabla f(x)$ ("descent ODEs")

THANK YOU FOR YOUR ATTENTION

MERCI POUR VOTRE ATTENTION