Numerical Methods in Engineering and Applied Science

Lecture 6. Initial value problems for ODEs.

Explicit ordinary differential equation of order n:

$$x^{(n)} = F(t, x, x', \ldots, x^{(n-1)})$$

It can be reduced to a system of first-order explicit ODEs:

Note that

$$y(t) = \left(y_0(t), \ldots, y_{n-1}(t)\right) \qquad y_0(t) = x(t), \ldots, y_{n-1}(t) = x^{(n-1)}(t)$$

The equation becomes

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f\left(t, y\right) \qquad \text{with}$$

$$f(t, y) = \left(y_1, \ldots, y_{n-2}, F(t, y_0, \ldots, y_{n-1})\right)$$

Initial value problem (Cauchy problem)

For a function $f:[0,T]\times\mathbb{R}^N \to \mathbb{R}^N$ and for $u_0 \in \mathbb{R}^N$

Find a differentiable function $u(t)$ defined over $t\in[0,T]$ such that

- $u(0) = u_0$
- $u' = f\left(t, u(t)\right)$ for all $t \in [0,T]$

Cauchy theorem

Let $f(t,u)$ be a continuous function of t and Lipschitz continuous with respect to u at any $t\in[0,T]$
(i.e., $\exists L > 0$ such that $\|f(t,u) - f(t,v)\| \le L\|u-v\|$ for $\forall u, v \in \mathbb{R}^N, t\in[0,T]$)
Then there exist only one differentiable function $u(t)$ that satisfies the initial value problem.

Example: nonlinear pendulum

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2}+\frac{g}{l}\sin\theta=0$$

Initial condition

$$\theta(0)=\theta_0; \qquad \theta'(0)=\omega_0$$

Some important properties

- Periodicity: $\exists P>0$ such that $\theta(t+P)=\theta(t)$

$$P=4\sqrt{\frac{l}{g}}K\left(\sin\frac{\theta_0}{2}\right)$$

- Conservation of energy:

$$E(t)-E(0)=0 \quad\Rightarrow\quad \frac{(\theta')^2}{2}+\frac{g}{l}(\cos\theta_0-\cos\theta)=0$$

- On can choose the time unit such that $g/l=1$

Note that

$$\omega = \theta' \qquad u(t) = (\theta(t), \omega(t)) \qquad u_0 = (\theta_0, \omega_0)$$

$$f(u) = (\omega, -\sin\theta)$$

Let us solve numerically

$$\begin{cases} u' = f(u) \\ u(0) = u_0 \end{cases}$$

over $t \in [0, T], \quad T = 4P$

with $\theta_0 = \pi / 3, \;\; \omega_0 = 0$

We know that $\theta(\;T\;) = \theta_0, \;\; \omega(\;T\;) = \omega_0$

We are interested in numerical methods capable of solving any initial value problem that has a unique solution.

We will consider methods of three different types:

- Taylor series methods
- Multistep methods
- Runge-Kutta methods

<u>Discretization:</u>

Given N+1 points t_0, t_1, …, $t_{N\text{-}1}$, t_N=T

$u(t_k)$ is the exact solution

u_k is the numerical solution

Uniform grid: $t_k = t_0+kh$, $k = 0, \ldots, N$

Euler method (explicit)

Derivation: use Taylor series expansion at t_k

$$u(t_{k+1}) = u(t_k) + h\,u'(t_k) + R_k$$

Where R_k is the local truncation error,

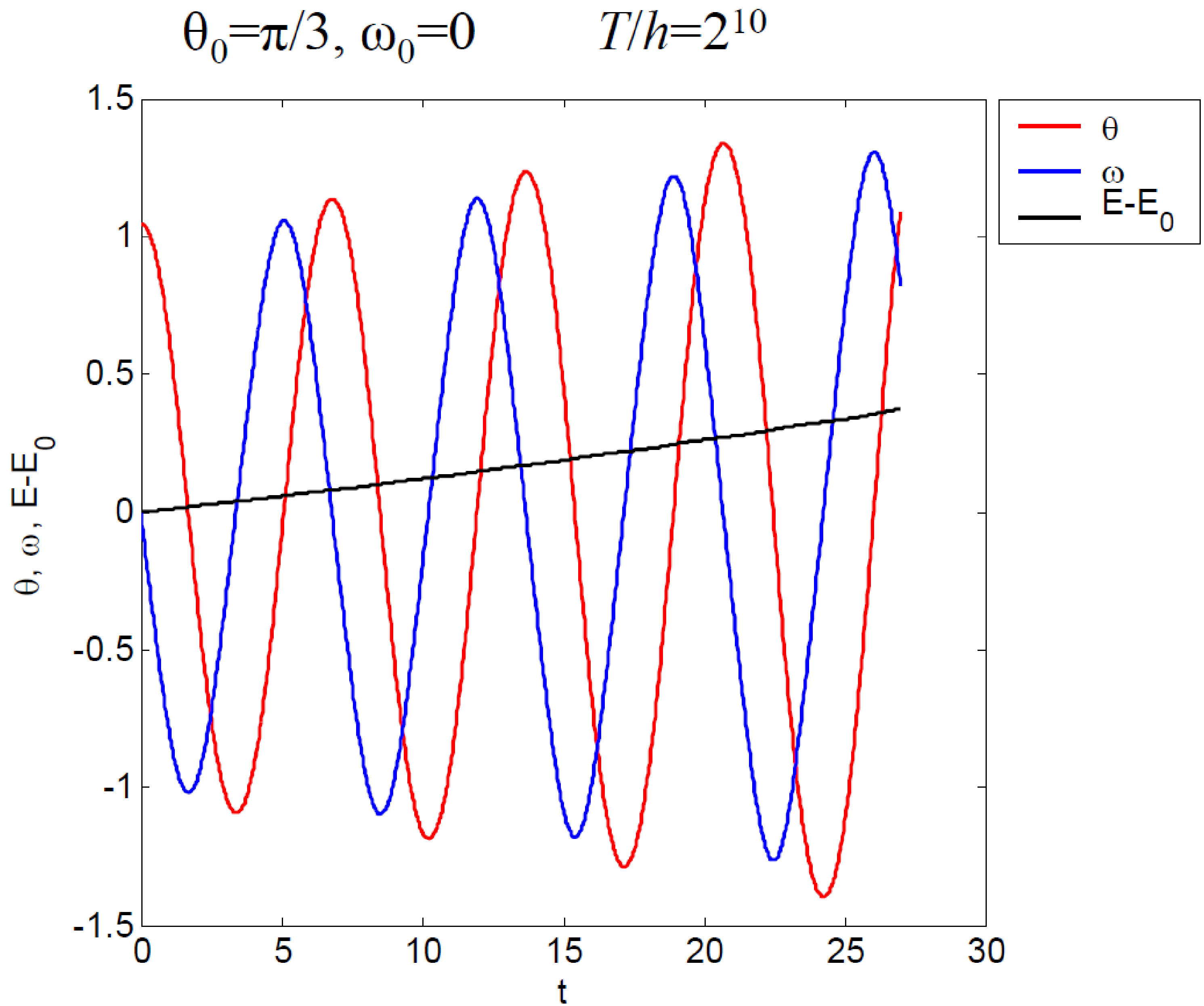
$$R_k = \frac{1}{2} h^2 u''(\xi) = \mathcal{O}(h^2) \qquad \xi \in [t_k, t_{k+1}]$$

Replace $u'(t_k)$ by $f(t_k, u(t_k))$

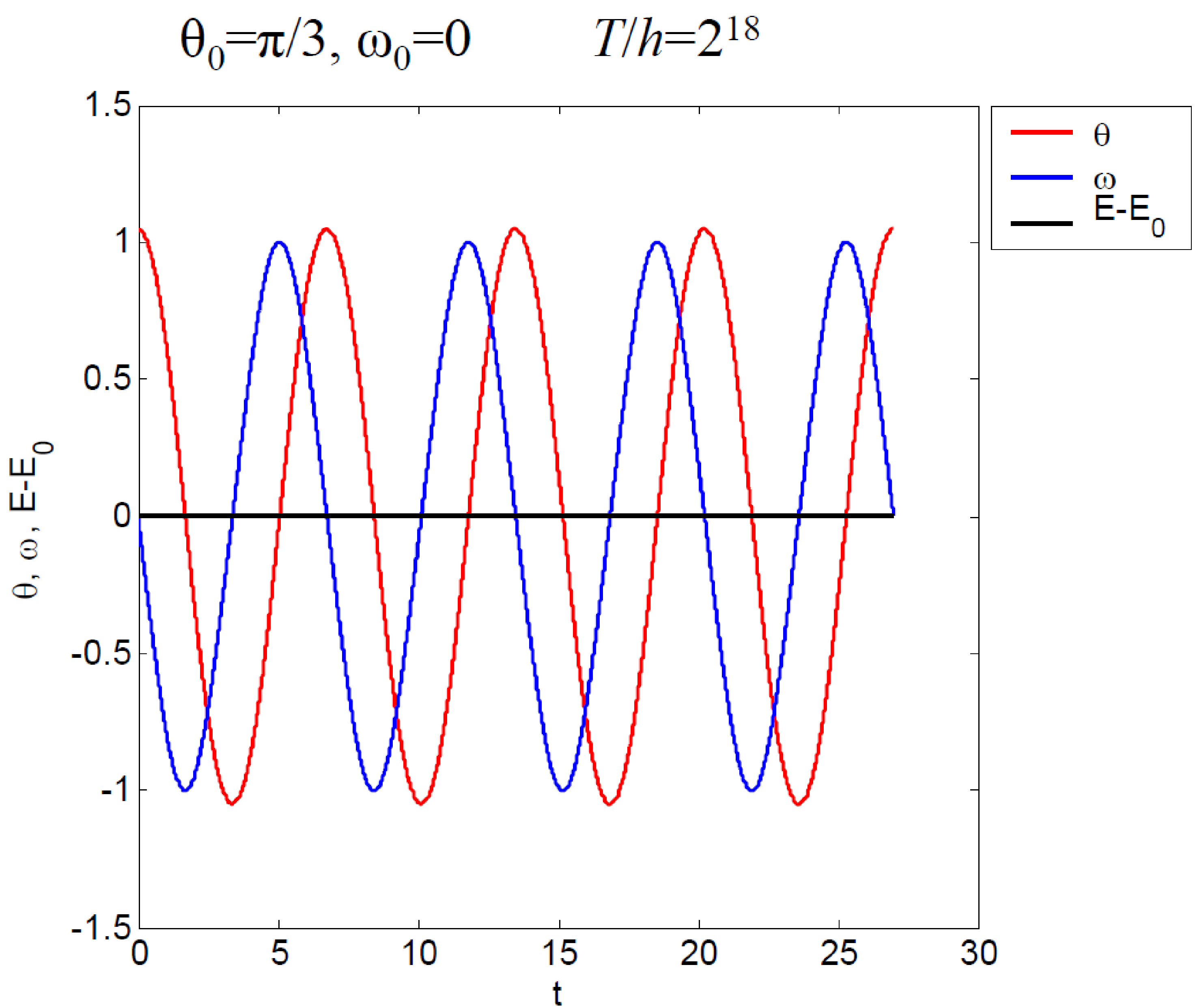
Neglect higher order terms in h and obtain

$$\underline{u_{k+1} = u_k + h\, f(t_k, u_k)}$$

with u_0 being the initial condition

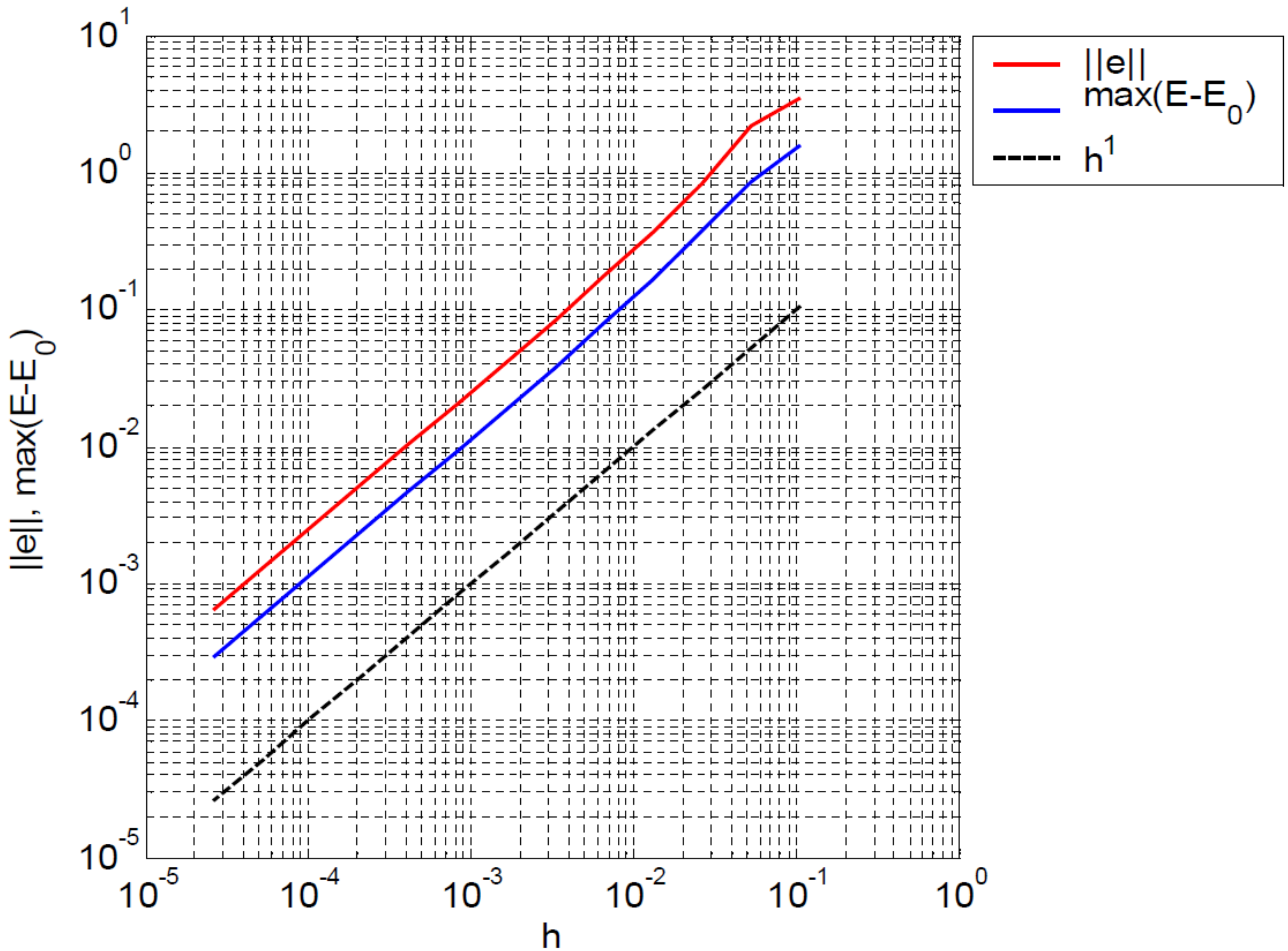


$\theta_0=\pi/3$, $\omega_0=0$ $T/h=2^{10}$
1.5
1
0.5
0
-0.5
-1
-1.5
0
5
10
15
20
25
30
t
θ, ω, $E-E_0$
θ
ω
$E-E_0$

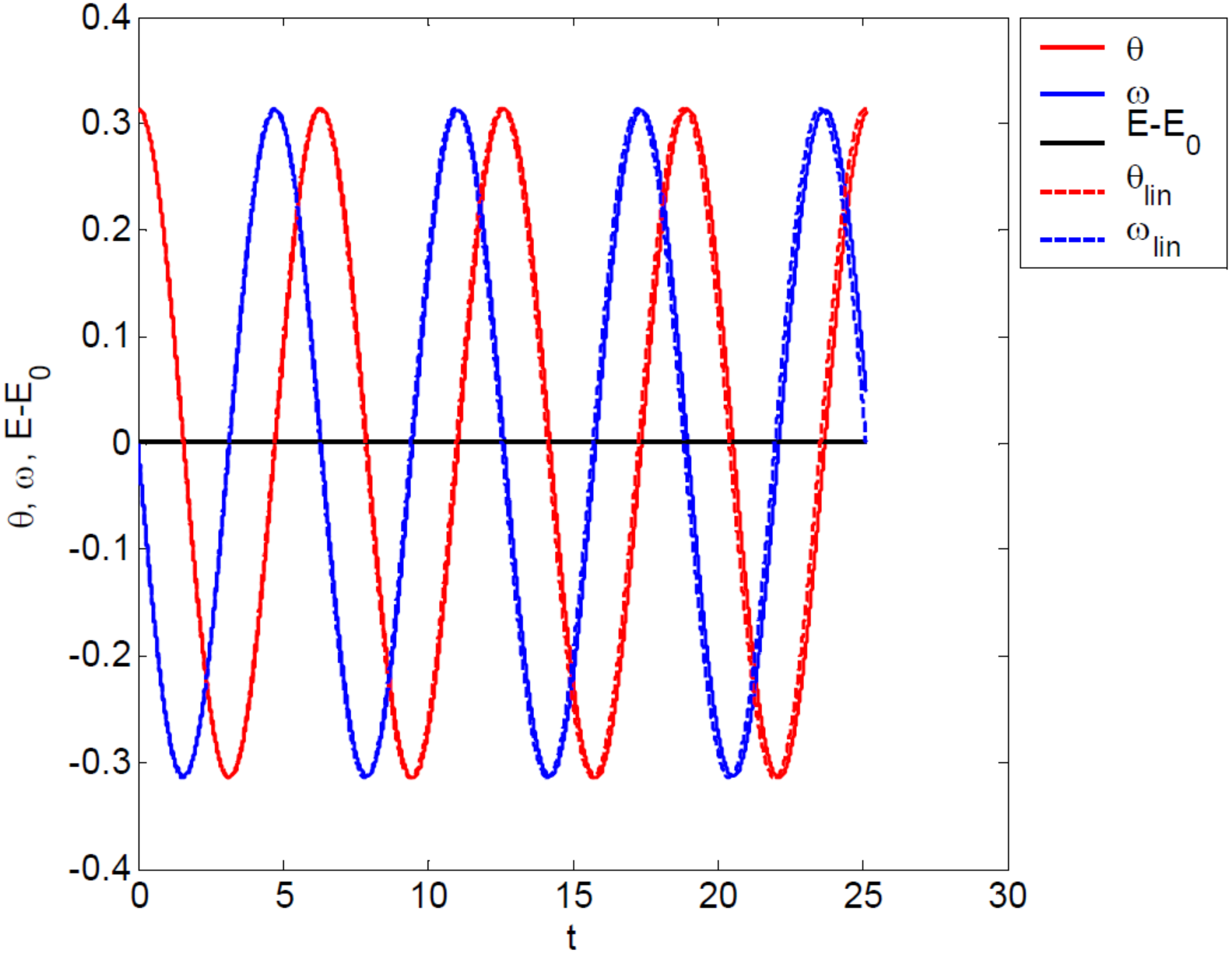


θ0=π/3, ω0=0 T/h=2^18
θ, ω, E-E0
t
θ
ω
E-E0
1.5
1
0.5
0
-0.5
-1
-1.5
0
5
10
15
20
25
30

$$\|e\| = \sqrt{(\theta(T)-\theta_0)^2 + (\omega(T)-\omega_0)^2}$$



$$\theta_{lin}(t) = \cos(\sqrt{\frac{g}{l}}t),\ \ \omega_{lin}(t) = -\sqrt{\frac{g}{l}}\sin(\sqrt{\frac{g}{l}}t)$$



$T/h = 2^{18}$

$\theta_0 = \pi/10$

Global discretization error analysis

$$
\begin{aligned}
e_k &:= u(t_k) - u_k \\
&= \left(u(t_{k-1}) + hf(t_{k-1}, u(t_{k-1})) + R_{k-1}\right) - \left(u_{k-1} + hf(t_{k-1}, u_{k-1})\right) \\
&= u(t_{k-1}) - u_{k-1} + h\left[f(t_{k-1}, u(t_{k-1})) - f(t_{k-1}, u_{k-1})\right] + R_{k-1}
\end{aligned}
$$

- Since f is uniformly Lipschitz continuous with respect to u,

$$\exists L > 0 \text{ t.q. } \left|f(t_{k-1}, u(t_{k-1})) - f(t_{k-1}, u_{k-1})\right| \leq L\left|u(t_{k-1}) - u_{k-1}\right| = L\left|e_{k-1}\right|$$

- Note that $R = \max\limits_{k=0\ldots N} |R_k|$, $\quad R \leq \dfrac{Mh^2}{2}$ where $\quad M = \max\limits_{t\in[0,T]} |u''(t)|$

- Using triangle inequality, we obtain

$$\left|e_k\right| \leq \left|e_{k-1}\right| + hL\left|e_{k-1}\right| + h^2 M / 2$$

with $\quad e_0 = 0 \quad$ because $\quad u_0 = u(t_0)$

Consequently,

$$
\begin{aligned}
|e_k| &\le (1+hL)\Big((1+hL)|e_{k-2}| + h^2M/2\Big) + h^2M/2 \\
&= (1+hL)^2|e_{k-2}| + \Big((1+hL)+1\Big)h^2M/2 \\
&\le (1+hL)^3|e_{k-3}| + \Big((1+hL)^2 + (1+hL)+1\Big)h^2M/2 \\
&\le \ldots \le \Big((1+hL)^{k-1} + (1+hL)^{k-2} + \ldots + (1+hL)+1\Big)h^2M/2 \\
&= \frac{(1+hL)^k - 1}{hL}h^2M/2 \le hM\frac{e^{hLk}-1}{2L} \\
&= h\frac{M(e^{Lt_k}-1)}{2L} \le h\frac{M(e^{LT}-1)}{2L} = \mathcal{O}(h)
\end{aligned}
$$

<u>The solution converges and it is first-order accurate.</u>

Second-order Taylor series method (for scalar equations)

Derivation: use Taylor series expansion at t_k

$$u(t_{k+1}) = u(t_k) + h\,u'(t_k) + \frac{h^2}{2}u''(t_k) + R_k \qquad\qquad R_k = \mathcal{O}(h^3)$$

The ODE that we consider is

$$u'(t) = f(t, u(t))$$

Its derivative is

$$u''(t) = f_t(t,u) + u'(t) f_u(t,u) = f_t(t,u(t)) + f(t,u(t)) f_u(t,u(t))$$

By substituting it in the Tayler expansion, we obtain

$$u(t_{k+1}) = u(t_k) + h\,f(t_k, u(t_k))$$
$$+\frac{h^2}{2}\big(f_t(t_k,u(t_k)) + f(t_k,u(t_k)) f_u(t_k,u(t_k))\big) + R_k$$

Since $R_k = \mathcal{O}(h^3)$, we obtain the following scheme:

$$u_{k+1} = u_k + h\,f(t_k, u_k) + \frac{h^2}{2}\big(f_t(t_k, u_k) + f(t_k, u_k) f_u(t_k, u_k)\big)$$

Taylor series method for systems of ODEs

Let us consider a system of two first-order equations,

$$\begin{cases} u' = f(t,u,v) \\ v' = g(t,u,v) \end{cases}$$

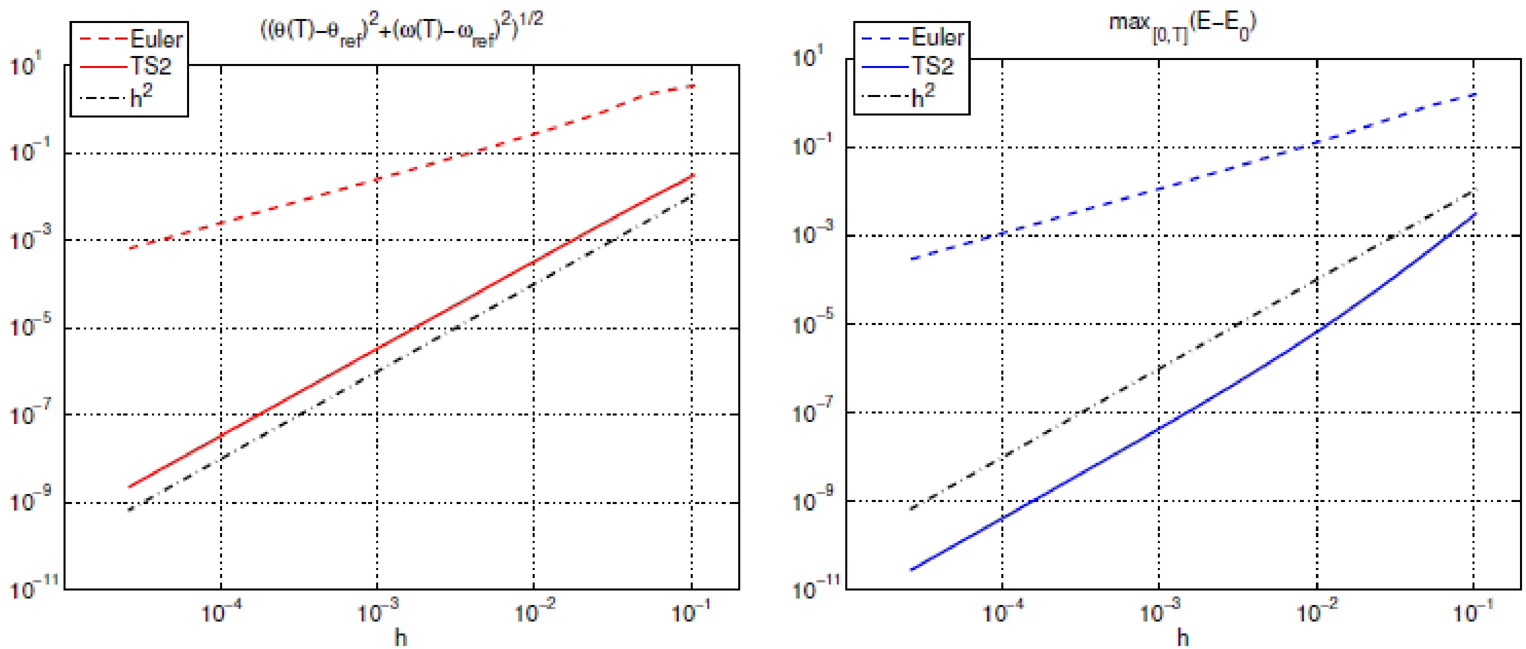
The second-order Taylor series scheme is:

$$u_{n+1} = u_n + hf(t_n,u_n,v_n) + \frac{h^2}{2}\left(f_t + ff_u + gf_v\right)\big|_{t=t_n,u=u_n,v=v_n}$$
$$v_{n+1} = v_n + hg(t_n,u_n,v_n) + \frac{h^2}{2}\left(g_t + fg_u + gg_v\right)\big|_{t=t_n,u=u_n,v=v_n}$$

Example of the nonlinear pendulum: $u = \theta$, $v = \omega$, $f = \omega$, $g = -\sin\theta$,

$$\theta_{n+1} = \theta_n + h\omega_n - \frac{h^2}{2}\sin\theta_n$$
$$\omega_{n+1} = \omega_n - h\sin\theta_n - \frac{h^2}{2}\omega_n\cos\theta_n$$

Convergence of Euler and second-order Taylor series schemes



By increasing the order of convergence we improve the precision for a given h, but we increase the computational cost. The most expensive operation is the computation of $f(t, u)$ (and its partial derivatives if we consider a Taylor series method). Nevertheless, the passage from order 1 to order 2 is justified. If we divide h by 2, the calculation error is divided by 2 for a method of order 1 and by 4 for a method of order 2. The number of operations becomes twice as large in both cases. So there is h^* (and $e^* = e(h^*)$) such that the second-order method performs better if $h < h^*$ (and $||e|| < ||e^*||$). We conclude that the use of a high-order method is justified if the precision of the computation that we require is high. The use of second-order methods is very often justified, but some problems require higher order schemes (higher than 2).