A stroboscopic numerical method for highly oscillatory problems

M. P. Calvo
Universidad de Valladolid, Spain

with Ph. Chartier, A. Murua, J. M. Sanz-Serna

I. HIGHLY OSCILLATORY PROBLEMS

Example 1: The pendulum

• A material point B is attached to one of the ends of a massless rod, of length ℓ. The other end of the rod can rotate around a point S (the pivot). The system is subjected to gravity.

• If q is the angle between the rod and the UPWARD vertical through S, the equation of motion is

$$\ell \frac{d^2 q}{dt^2} = +g \sin q,$$

or

$$\frac{dp}{dt} = +\frac{g}{\ell} \sin q, \qquad \frac{dq}{dt} = p.$$

Stabilizing effect of vibrations

• The *unstable* position $q \equiv 0$ (bob B *above* pivot S), becomes *stable* if S receives fast, small-amplitude vertical vibrations.

• Many other physical systems may be stabilized by vibrations (Paul's trap, Nobel Prize 1989).

• If $a(t)$ is the (upwards) acceleration of S wrt. laboratory, eqn. of motion is

$$\frac{d^2}{dt^2}q = \ell^{-1}(g + a(t)) \sin q.$$

• Assume that $a(t)$ is sinusoidal

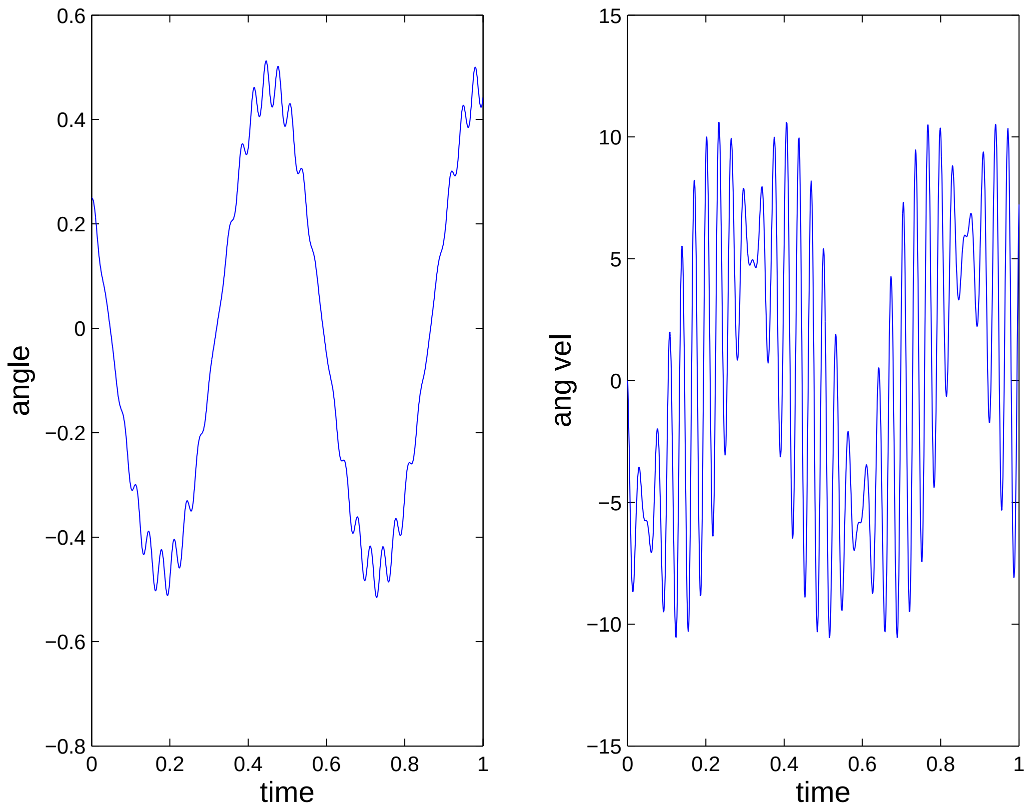
$$a(t) = \frac{1}{\epsilon} v_{max} \cos(\frac{t}{\epsilon} + \theta_0), \qquad v_{max} > 0.$$

• The (vertical) pivot velocity $v(t)$ and pivot displacement $s(t)$ are given by

$$v(t) = v_{max} \sin(\frac{t}{\epsilon} + \theta_0), \qquad s(t) = -\epsilon v_{max} \cos(\frac{t}{\epsilon} + \theta_0).$$

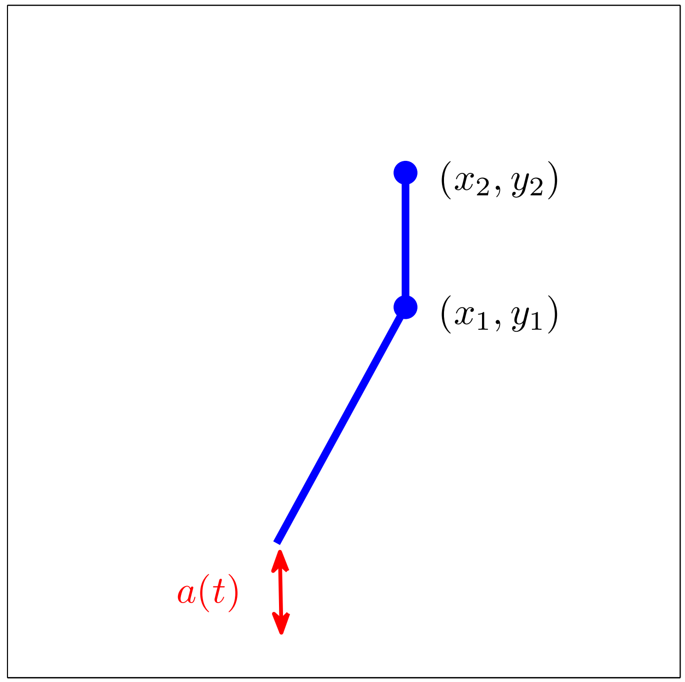
• We are interested in the case where $\epsilon \ll 1$; with respect to this small parameter, a, v and s are therefore of sizes $O(1/\epsilon)$, $O(1)$ and $O(\epsilon)$ respectively. *Direct numerical solution very costly.*

• Next slide shows stabilization for $\epsilon = 1/200$. (Here and later $g = 9.8$, $\ell = 0.2$, $v_{max} = 4$, $\theta_0 = 2$, $q(0) = 0.25$, $p(0) = 0$.)



0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
angle
0
0.2
0.4
0.6
0.8
1
time
15
10
5
0
−5
−10
−15
ang vel
0
0.2
0.4
0.6
0.8
1
time

Example 2: The double pendulum in cartesian coordinates



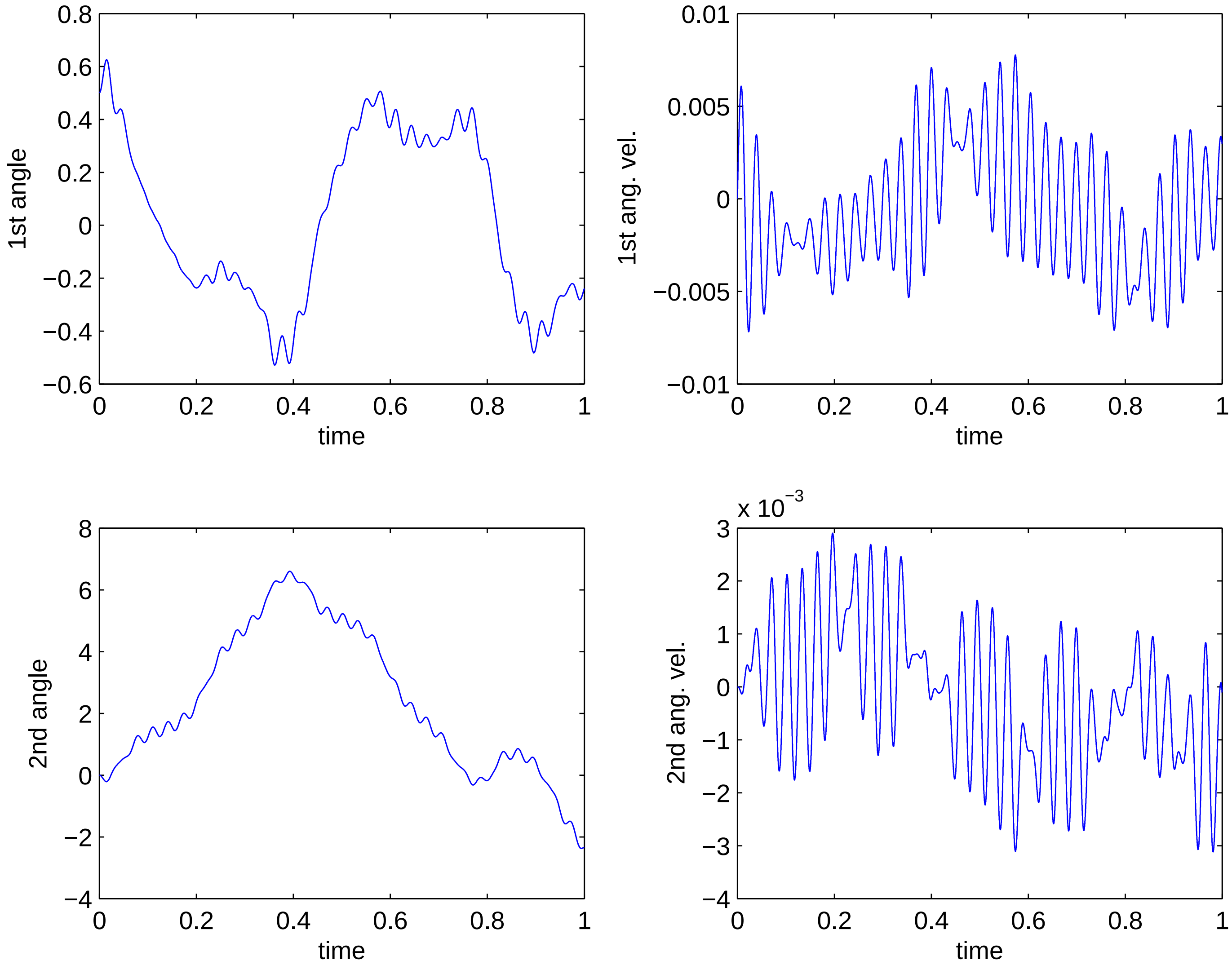
- Here and later $m_1 = 0.01$, $m_2 = 0.005$, $\ell_1 = 0.2$, $\ell_2 = 0.1$, $x_1(0) = \ell_1 \sin(0.5)$, $y_1(0) = \ell_1 \cos(0.5)$, $x_2(0) = x_1(0)$, $y_2(0) = y_1(0) + \ell_2$.

$$
\begin{aligned}
m_1\dot{x}_1 &= m_1u_1 && \boxed{- 2x_1\mu_1 - 2(x_1 - x_2)\mu_2,} \\
m_1\dot{y}_1 &= m_1v_1 && - 2y_1\mu_1 - 2(y_1 - y_2)\mu_2, \\
m_2\dot{x}_2 &= m_2u_2 && - 2(x_2 - x_1)\mu_2, \\
m_2\dot{y}_2 &= m_2v_2 && - 2(y_2 - y_1)\mu_2, \\
m_1\dot{u}_1 &= && - 2x_1\lambda_1 - 2(x_1 - x_2)\lambda_2, \\
m_1\dot{v}_1 &= -m_1(g + a(t)) && - 2y_1\lambda_1 - 2(y_1 - y_2)\lambda_2, \\
m_2\dot{u}_2 &= && - 2(x_2 - x_1)\lambda_2, \\
m_2\dot{v}_2 &= -m_2(g + a(t)) && - 2(y_2 - y_1)\lambda_2,
\end{aligned}
$$

with constraints

$$
x_1^2 + y_1^2 - \ell_1^2 = 0, \quad (x_2 - x_1)^2 + (y_2 - y_1)^2 - \ell_2^2 = 0,
$$

$$
x_1u_1 + y_1v_1 = 0, \quad (x_2 - x_1)(u_2 - u_1) + (y_2 - y_1)(v_2 - v_1) = 0.
$$



1st angle
time
1st ang. vel.
time
2nd angle
time
x 10^−3
2nd ang. vel.
time

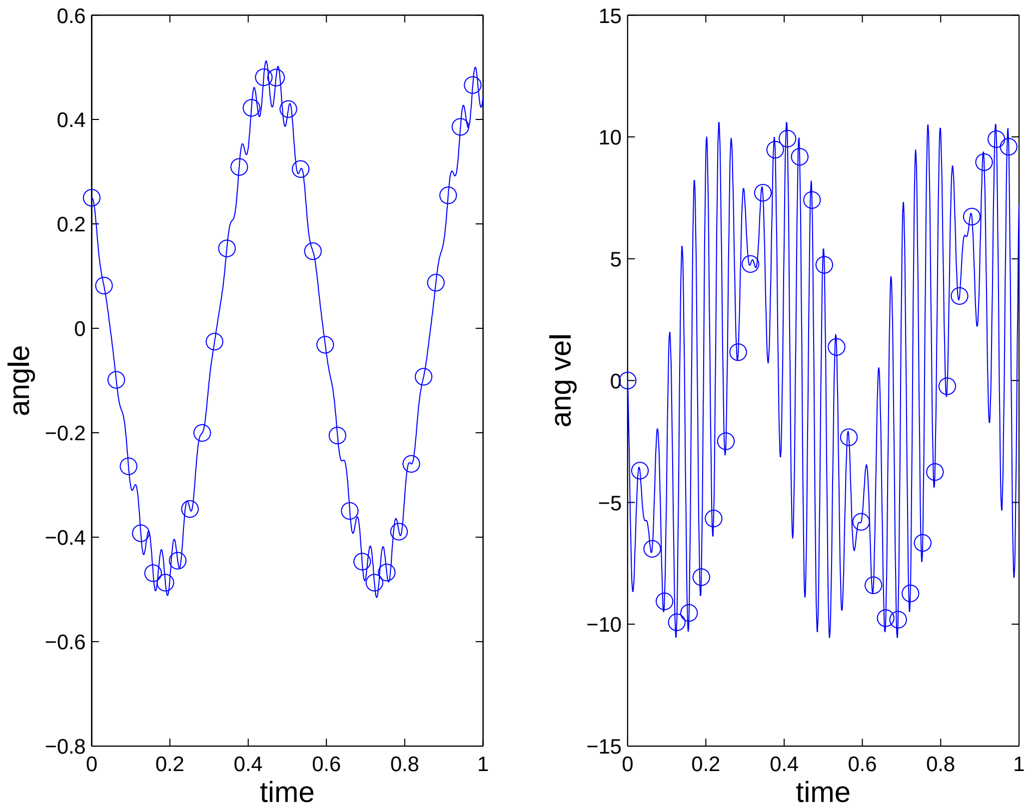
II. STROBOSCOPIC AVERAGING

• Averaging: try to describe the ‘smooth’ evolution of the system without tracking the fast, period $O(\epsilon)$, oscillations of true solution $y(t)$.

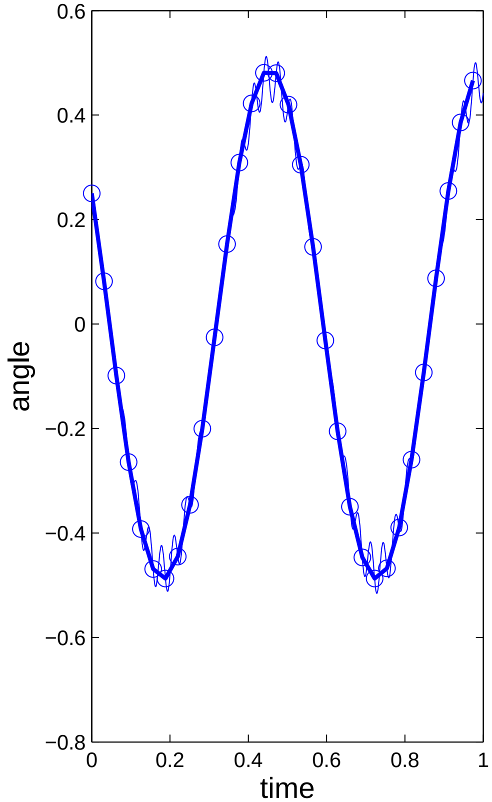
• $y(t)$ approximated by a ‘smooth’ $Y(t)$. Usually Y is understood as average of y over one period of the fast oscillations.

• Here we look at true solution y with a stroboscopic light that flashes every $2\pi\epsilon$ units of time.

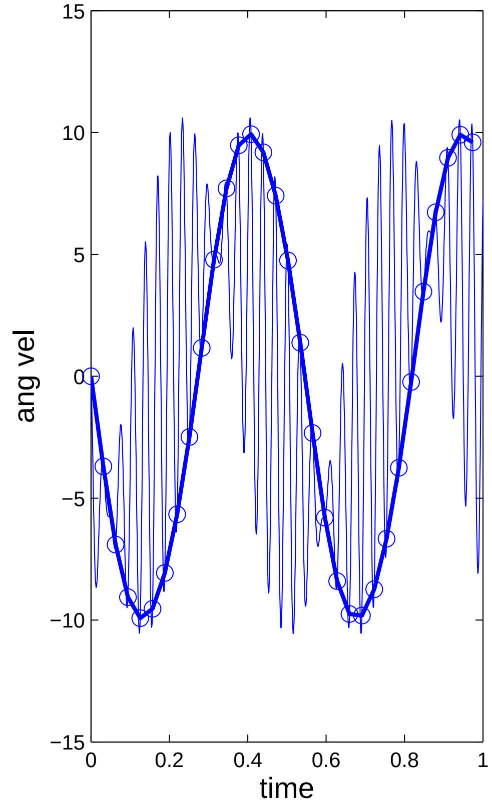
• In the pendulum case this yields (vector solution y has components p and q) . . .



angle
time
ang vel
time



angle
time
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
0
0.2
0.4
0.6
0.8
1



ang vel
time
15
10
5
0
−5
−10
−15
0
0.2
0.4
0.6
0.8
1

• Values appear to come from a smooth function $Y(t)$ that interpolates the values $y(0)$, $y(2\pi\epsilon)$, $y(4\pi\epsilon)$, ...

• Note that the time-derivative of the smooth interpolant of q does not coincide with the smooth interpolant of $p = dq/dt$.

In general:

• Consider the oscillatory IVP

$$\frac{dy}{dt} = f(y, \frac{t}{\epsilon}; \epsilon), \quad 0 \le t \le T, \qquad y(0) = y_0 \in \mathcal{R}^d,$$

where $\epsilon \ll 1$, $f(y, \tau; \epsilon)$ is 2π-periodic in τ.

• To simplify the notation, the initial condition has been imposed at $t = 0$. No loss of generality: other cases reduced to this by considering the new independent variable $t - t_0$.

• Denote by φ_t the solution operator $y_0 \mapsto y(t)$. This is not a flow: if $t_1 \ne 2\pi k\epsilon$, then, in general, $\varphi_t y(t_1) \ne y(t_1 + t)$.

• Under suitable hypoths. $\varphi_{2\pi\epsilon}$ is a near identity map. Then:

• There exists an autonomous modified eqn. $(d/dt)Y = F_\epsilon(Y)$, with t-flow $\Phi_t^{(\epsilon)}$, such that $\varphi_{2\pi\epsilon}$ coincides (formally) with $\Phi_{2\pi\epsilon}^{(\epsilon)}$.

• $\varphi_{2\pi\epsilon} = \Phi_{2\pi\epsilon}^{(\epsilon)}$ and $\varphi_{2\pi n\epsilon} = \varphi_{2\pi\epsilon}^n$, $n = 0, 1, \dots$, (periodicity) imply

$$\varphi_{2\pi n\epsilon} = \Phi_{2\pi n\epsilon}^{(\epsilon)}.$$

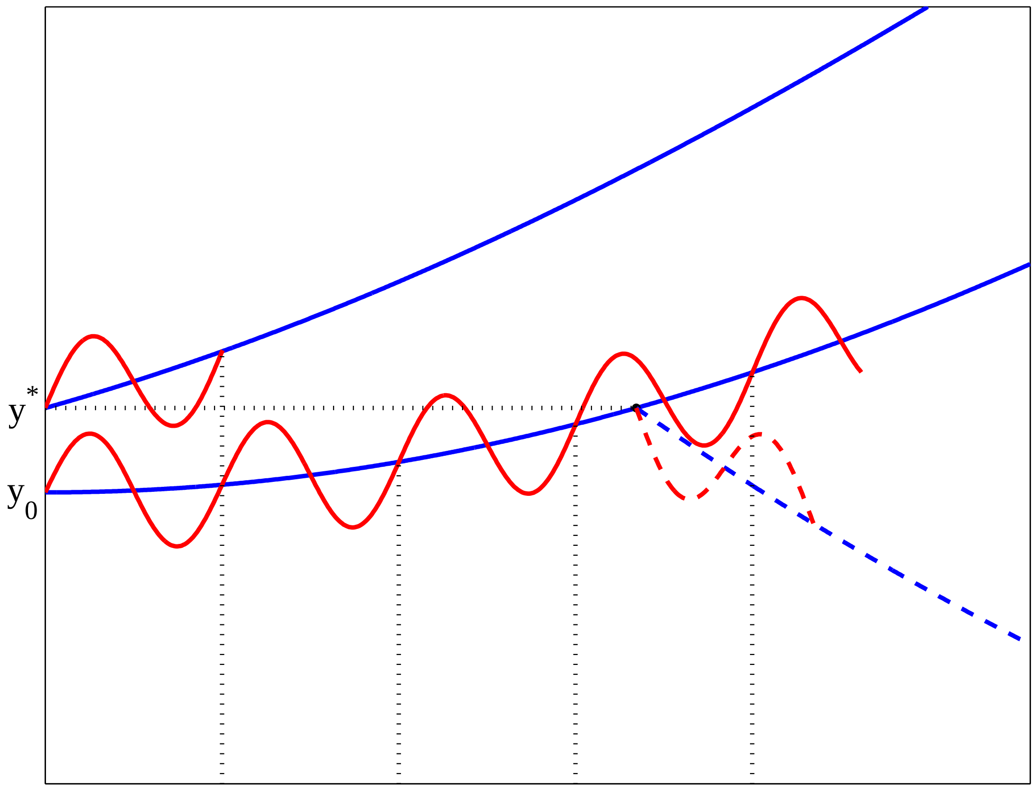
- *Conclusion:* the values

$$y(0), \quad y(2\pi\epsilon), \quad \ldots \quad y(2\pi n\epsilon), \quad \ldots$$

of the highly oscillatory solution of $(d/dt)y = f(y, t/\epsilon; \epsilon)$ coincide (as formal power series in ϵ) with the values

$$Y(0), \quad Y(2\pi\epsilon), \quad \ldots \quad Y(2\pi n\epsilon), \quad \ldots$$

of the solution of $(d/dt)Y = F_\epsilon(Y)$ such that $Y(0) = y(0)$.



Red wiggly lines: solutions of ivp's corresponding to two initial conditions, y_0 and $y*$. Solid blue lines: solutions of $(d/dt)Y = F_\epsilon(Y)$ with same initial data.

Two remarks:

• If the initial condition was prescribed at $t_0 \neq 0$, then the operator $y_0 \mapsto y(t_0+t)$ is not φ_t. The process would have resulted in a different $\Phi_t^{(\epsilon)}$ and therefore in a *different* F_ϵ. (Broken lines in preceding figure.)

• Truncating the formal series of the 'exact' F_ϵ, one obtains averaged systems with $O(\epsilon)$, $O(\epsilon^2)$, ... errors.

In Chartier, Murua & Sanz-Serna, *Higher-order averaging, formal series and numerical integration I: B-series* it is shown:

• Possible to find systematically the explicit analytic expression for F_ϵ in terms of f by using ideas from the modern analysis of numerical methods —trees, B-series, . . . —.

• Such explicit expression is useful on its own right to obtain averaged system of high order of accuracy.

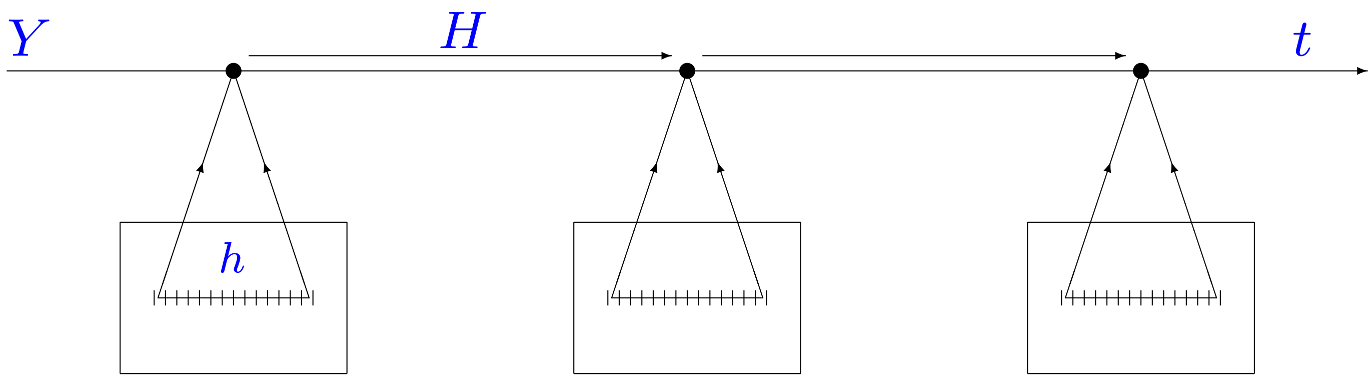
• It may furthermore be used to analyze the multiscale method we shall present next. (However such an analysis will not be covered in this talk.)

III. A MULTISCALE NUMERICAL METHOD

• We shall compute the smooth interpolant $Y(t)$ by integrating the averaged equation $dY/dt = F_\epsilon(Y)$ with a numerical method (macro-solver) with macro-step size H (much) larger than the fast period $2\pi\epsilon$.

• In the spirit of the Heterogeneous Multiscale Methods of E and Engquist, our algorithm does not require the explicit knowledge of the analytic form of F_ϵ. Info. on F_ϵ is gathered on the fly by integrating [with micro-step size h] the original system $dy/dt = f$ in small time-windows of length $O(\epsilon)$.

• There is much freedom in the choice of the macro-solver and micro-solver, including standard variable-step/order codes.


Y
H
t
h

• ¿How to compute F_ϵ at a given value Y^* of its argument?

• Recall that F_ϵ is, by definition, the vector field whose t-flow is $\Phi_t^{(\epsilon)}$. Hence

$$F_\epsilon(Y^*) = \frac{d}{dt}\Phi_t^{(\epsilon)}(Y^*)\Big|_{t=0}.$$

• In algorithm, derivative approximated by differences, such as

$$F_\epsilon(Y^*) = \frac{1}{2\delta}[\Phi_\delta^{(\epsilon)}(Y^*) - \Phi_{-\delta}^{(\epsilon)}(Y^*)] + O(\delta^2).$$

• Choosing $\delta = 2\pi\epsilon$, results in $\Phi_{\pm\delta}^{(\epsilon)} = \varphi_{\pm\delta}$ (stroboscopic effect) and

$$F_\epsilon(Y^*) \approx (1/(4\pi\epsilon))[\varphi_{2\pi\epsilon}(Y^*) - \varphi_{-2\pi\epsilon}(Y^*)].$$

• $\varphi_{\pm 2\pi\epsilon}(Y^*)$ computed by solving the originally given $dy/dt = f(y, t/\epsilon; \epsilon)$, over $-2\pi\epsilon \le t \le 2\pi\epsilon$, with initial condition $y(0) = Y^*$.

• Note lack of synchrony between macro and micro integrations. Starting micro-integrations from current value of t in macro-integration will not do: refer to preceding figure.

• Of course, one may use other finite-difference formulae such as the fourth-order

$$\frac{1}{12\delta}[-\Phi^{(\epsilon)}_{2\delta}(Y^*) + 8\Phi^{(\epsilon)}_{\delta}(Y^*) - 8\Phi^{(\epsilon)}_{-\delta}(Y^*) + \Phi^{(\epsilon)}_{-2\delta}(Y^*)].$$

With $\delta = 2\pi\epsilon$, this requires micro-integrating over $-4\pi\epsilon \le t \le 4\pi\epsilon$. (Our current experience includes formulae of order ≤ 6.)

Error analysis:

- Three sources of errors:

The approximation of the exact values of F_ϵ by finite differences

The replacement in the finite-difference formula of the true values of Φ^ϵ by numerical approximations obtained via micro-integrations.

The discretization error introduced by the macro-integrator.

- Basic error estimate:

$$O\left(\epsilon^d + H^P + \frac{1}{\epsilon}(\frac{h}{\epsilon})^p\right),$$

if the error due to the micro-integration behaves as $\left(\frac{h}{\epsilon}\right)^p$.

- Improved error estimate:

$$O\left(\epsilon^d + H^P + \epsilon^{\nu-1}(\frac{h}{\epsilon})^p\right),$$

if the error due to the micro-integration behaves as $\epsilon^\nu \left(\frac{h}{\epsilon}\right)^p$.

• Algorithm presented evolved from our study of Heterogeneous Multiscale Method (E, Engquist, Tsai, Sharp, Ariel, . . .)

• Basic underlying idea has appeared several times in the literature over the last fifty years (in particular, in astronomy and circuit theory): envelope-following methods, multirevolution methods, . . . Taratynova, Mace and Thomas, Graff and Bettis, Gear/Petzold/Gallivan, Calvo/Jay/Montijano/Rández, . . . (outer integrator has to be built on purpose).

• Kirchgraber 1982, 1988 uses high-order RKs. Recovery of macro-field not from numerical differentiation.

IV. NUMERICAL EXPERIMENTS

IV (A) 'THE' RUNGE-KUTTA METHOD

• 1st block of experiments reported here correspond to 'the' Runge-Kutta method, with constant step-sizes H and h, as macro and micro-integrator.

• H from sequence $2\pi/50 \approx 0.12$, $2\pi/100$, . . . , $2\pi/50/2^{\nu}$, . . .

• h from sequence $2\pi\epsilon/10$, $2\pi\epsilon/20$, . . . , $2\pi\epsilon/10/2^{\nu}$,. . .

• Increasing ν by one unit doubles the number of macro-steps and the work per macro-step, hence multiplies by four the computational effort, which is independent of ϵ, as h and the width of the micro-integration windows are both proportional to ϵ.

Inverted pendulum: Maximum error in q over $0 \leq t \leq 1$, fourth order differencing.

H	Mcrstps	ϵ			
		1/400	1/800	1/1600	1/3200
$\pi/25$	1,120	1.10(-1)	1.09(-1)	1.08(-1)	1.08(-1)
$\pi/50$	4,800	8.12(-3)	7.85(-3)	7.79(-3)	7.76(-3)
$\pi/100$	19,840	7.06(-4)	5.16(-4)	5.01(-4)	4.99(-4)
$\pi/200$	80,640	2.35(-4)	4.71(-5)	3.53(-5)	3.45(-5)
$\pi/400$	325,120	***	1.47(-5)	3.06(-6)	2.32(-6)
$\pi/800$	1,300,480	***	***	9.20(-7)	1.92(-7)
$\pi/1600$	5,212,160	***	***	***	6.08(-8)

• For large H, error $O(H^4)$ (from RK4) uniformly in ϵ. (Much smaller values of ϵ, say $\epsilon = 10^{-9}$, cause no difficulty.)

• For small H, error is clearly $O(\epsilon^4)$ (approximating F_ϵ).

Inverted pendulum: As before, but error in p.

H	Mcrstps	ϵ			
		1/400	1/800	1/1600	1/3200
$\pi/25$	1,120	1.66(0)	1.66(0)	1.66(0)	1.66(0)
$\pi/50$	4,800	1.60(-1)	1.59(-1)	1.58(-1)	1.58(-1)
$\pi/100$	19,840	1.33(-2)	9.80(-3)	9.57(-3)	9.55(-3)
$\pi/200$	80,640	4.45(-3)	9.07(-4)	6.96(-4)	6.83(-4)
$\pi/400$	325,120	***	2.79(-4)	5.96(-5)	4.66(-5)
$\pi/800$	1,300,480	***	***	1.76(-5)	3.78(-6)
$\pi/1600$	5,212,160	***	***	***	1.29(-6)

- Relative errors are similar to those in q, as p takes larger values.

Inverted pendulum: Maximum error in q over $0 \leq t \leq 1$, second order differencing.

H	Mcrstps	ϵ			
		1/400	1/800	1/1600	1/3200
$\pi/25$	560	1.05(-1)	1.08(-1)	1.08(-1)	1.08(-1)
$\pi/50$	2,400	3.00(-2)	1.25(-2)	8.94(-3)	8.05(-3)
$\pi/100$	9,920	2.71(-2)	7.01(-3)	2.07(-3)	8.78(-4)
$\pi/200$	40,320	2.67(-2)	6.61(-3)	1.67(-3)	4.41(-4)
$\pi/400$	162,560	***	6.58(-3)	1.64(-3)	4.10(-4)

- For H small, error clearly behaves as $O(\epsilon^2)$.

- For $H = \pi/50$ and ϵ small, accuracy of 1%, even if number of RK steps is smaller than number of cycles of vibration.

IV (B) ode45 AS MACRO INTEGRATOR

• Micro-problem integrated in the non-dimensional time $\tau = t/\epsilon$.

• Step-points chosen by code in macro-integrator may be totally arbitrary.

• Results for ode45 as macro-integrator combined with splitting as micro-integrator for van der Pol oscillator can be found in Calvo, Chartier, Murua & Sanz-Serna, *Numerical stroboscopic averaging for ODEs and DAEs*

`http://hermite.mac.cie.uva.es/sanzserna`

IV (C) Differential Algebraic Equations

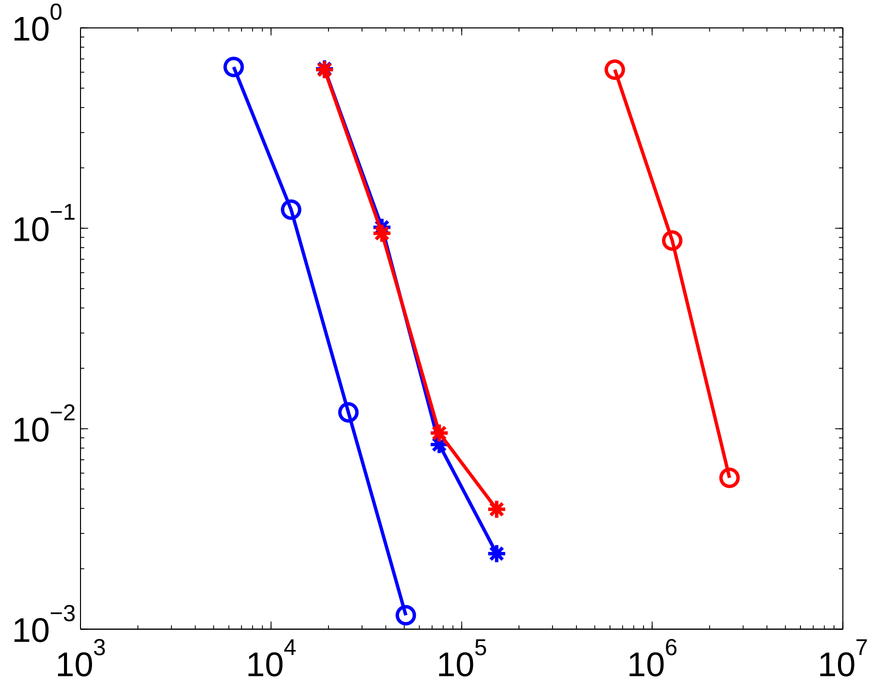
• Approach applies to DAEs, in particular to constrained dynamical systems.

• Index 2 DAEs, if Gear-Gupta-Leimkuhler (GGL) approach used

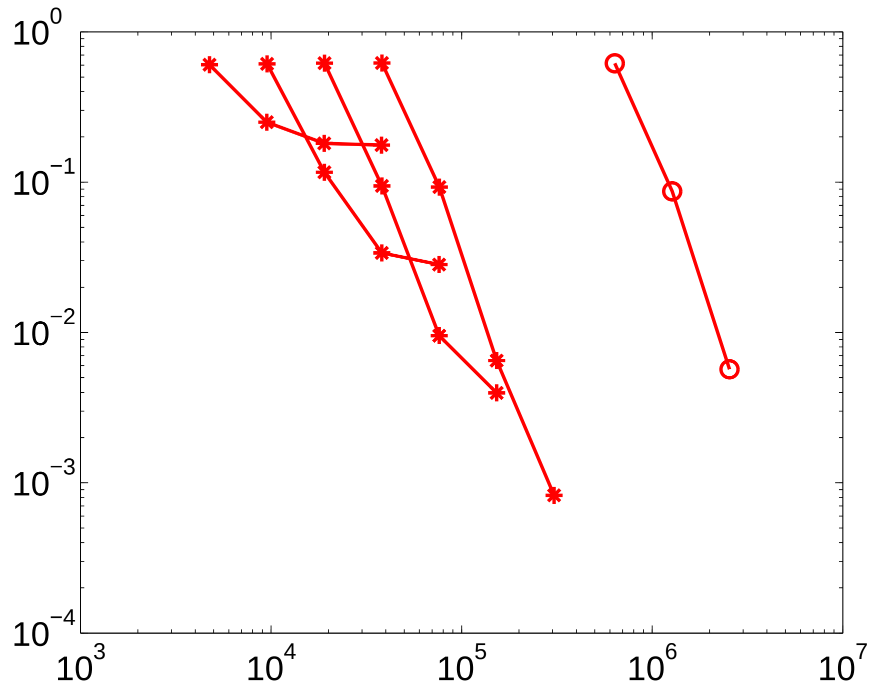
$$\dot{y} = \mathcal{F}(y, z), \qquad \mathcal{G}(y) = 0,$$

• Half-explicit RK method of order 3 (Brasey/Hairer (1993)) successfully implemented.

$$\begin{array}{c|ccc} 0 & & & \\ 1/3 & 1/3 & & \\ 1 & -1 & 2 & \\ \hline & 0 & 3/4 & 1/4 \end{array} .$$



• Error in first angle vs. number of micro-steps, $\epsilon = 10^{-4}$ (blue), 10^{-6} (red), circles correspond to standard integration ($h = 2\pi\epsilon/n$, $n = 2^j, j = 2, 3, 4, 5$) and stars to the stroboscopic method with macro-step-size $H = \pi/2500$.



• Error in first angle vs. number of micro-steps, $\epsilon = 10^{-6}$, circles correspond to standard integration ($h = 2\pi\epsilon/n, n = 2^j, j = 2, 3, 4, 5$) and stars to the stroboscopic method with macro-step-sizes $H = \pi/625, H = \pi/1250, H = \pi/2500, H = \pi/5000$.