Different Differential Equations with the Same Solution

Stephen Lucas* & James Sochacki

Department of Mathematics and Statistics James Madison University, Harrisonburg VA



July 4, 2012 9th AIMS Conference on Dynamical Systems, Differential Equations and Applications Special Session 39

Outline

- What happens: different differential equations, different solutions
- Why it happens: error analysis
- Relations to the Power Series Method
- Symplectic solvers
- Effectively symplectic solver
- Future Work



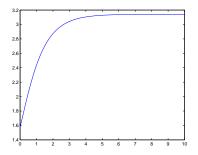
What Happens	Why It Happened	Why PSM
•••••••	0000	0000000
Trig		

Consider
$$y' = \sin y$$
 with $y(0) = \pi/2$.



What Happens	Why It Happened	Why P
00000000		

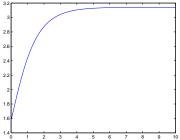
Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious.





What Happens	Why It Happened	Why PSM
0000000	0000	0000000

Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious.

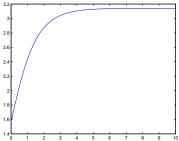


If we let $u_1 = y$, $u_2 = \sin(u_1)$ and $u_3 = \cos(u_2)$, then $u_1' = u_2$, $u_1(0) = \pi/2$;



What Happens	Why It Happened	Why PSM
0000000	0000	0000000

Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious. $y = 2tan^{-1}(e^t)$

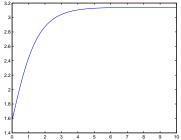


If we let $u_1 = y$, $u_2 = \sin(u_1)$ and $u_3 = \cos(u_2)$, then $u'_1 = u_2$, $u_1(0) = \pi/2$; $u'_2 = u_2u_3$, $u_2(0) = 1$;



Vhat Happens	Why It Happened	Why PSM
0000000	0000	0000000

Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious. $y = 2tan^{-1}(e^t)$

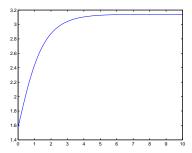


If we let $u_1 = y$, $u_2 = \sin(u_1)$ and $u_3 = \cos(u_2)$, then $u'_1 = u_2$, $u_1(0) = \pi/2$; $u'_2 = u_2u_3$, $u_2(0) = 1$; $u'_3 = -u_2^2$, $u_3(0) = 0$.



Vhat Happens	Why It Happened	Why PSM
0000000		

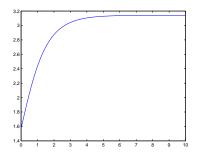
Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious.



If we let $u_1 = y$, $u_2 = \sin(u_1)$ and $u_3 = \cos(u_2)$, then $u'_1 = u_2$, $u_1(0) = \pi/2$; $u'_2 = u_2u_3$, $u_2(0) = 1$; $u'_3 = -u_2^2$, $u_3(0) = 0$. While three first order odes may appear harder than one, compare two multiplications to evaluating a sine.

Vhat Happens	Why It Happened	Why PSM
0000000		

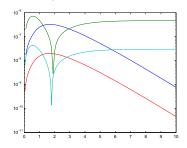
Consider $y' = \sin y$ with $y(0) = \pi/2$. It has solution $y = 2tan^{-1}(e^t)$, which is far from obvious.



If we let $u_1 = y$, $u_2 = \sin(u_1)$ and $u_3 = \cos(u_2)$, then $u'_1 = u_2$, $u_1(0) = \pi/2$; $u'_2 = u_2u_3$, $u_2(0) = 1$; $u'_3 = -u_2^2$, $u_3(0) = 0$. While three first order odes may appear harder than one, compare two multiplications to evaluating a sine. In a numerical solver, do we really need sine to machine precision?

What Happens	Why It Happened	Why PSM
○●○○○○○○○	0000	0000000
Trig Errors		

Equal step RKO4 on [0, 10] with 100, 200 intervals:





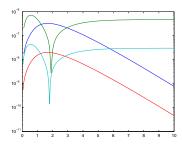
What Happens

Trig Errors

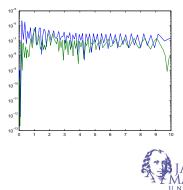
Why It Happened

Why PSM 0000000

Equal step RKO4 on [0, 10] with 100, 200 intervals:



Matlab's ode45 on [0, 10], absolute error 10^{-6} : 85 and 109 function evaluations.



What Happens	Why It Happened	Why PSM
0000000	0000	0000000

PSM

 $u_1' = u_2$, $u_1(0) = \pi/2$; $u_2' = u_2u_3$, $u_2(0) = 1$; $u_3' = -u_2^2$, $u_3(0) = 0$.



What Happens	Why It Happened	Why PSM
⊙⊙●○○○○○○	0000	0000000
PSM		

$$u'_1 = u_2$$
, $u_1(0) = \pi/2$; $u'_2 = u_2u_3$, $u_2(0) = 1$; $u'_3 = -u_2^2$, $u_3(0) = 0$.

Power Series Method: at t = 0, replace variables by power series, explicitly find coefficients using Cauchy products and earlier coefficients (related to AD, Taylor methods).

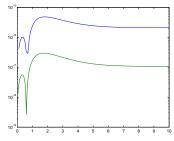


Vhat Happens	Why It Happened	Why PSM
0000000		

PSM

$$u_1' = u_2$$
, $u_1(0) = \pi/2$; $u_2' = u_2 u_3$, $u_2(0) = 1$; $u_3' = -u_2^2$, $u_3(0) = 0$.

Power Series Method: at t = 0, replace variables by power series, explicitly find coefficients using Cauchy products and earlier coefficients (related to AD, Taylor methods). Equal step on [0, 10] with 100, 200 intervals:





What	Happens
0000	

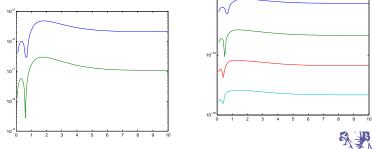
PSM

$$u_1' = u_2, \ u_1(0) = \pi/2; \ u_2' = u_2 u_3, \ u_2(0) = 1; \ u_3' = -u_2^2, \ u_3(0) = 0.$$

Power Series Method: at t = 0, replace variables by power series, explicitly find coefficients using Cauchy products and earlier coefficients (related to AD, Taylor methods). Equal step on [0, 10] with 100, 100 intervals, order 4, 6, 8, 10:

10

200 intervals:



What Happens	Why It Happened	Why PSM
○○○●○○○○○	0000	0000000
Arbitrary Power		

Consider $y' = y^{\alpha}$, $y(0) = y_0$,



What Happens	Why It Happened	Why PSM
○○○●○○○○○	0000	0000000
Arbitrary Power		

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha} \right)^{1/(\alpha-1)} \right)^{-1}$.



What Happens	Why It Happened	Why PSM
0000000		

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha} \right)^{1/(\alpha-1)} \right)^{-1}$.

With $u_1 = y$, $u_2 = y^{\alpha}$, $u_3 = 1/y$,



What Happens	Why It Happened	Why PSM
0000000		

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha} \right)^{1/(\alpha-1)} \right)^{-1}$.

With $u_1 = y$, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,



pened Why PSM
000000
p

W

Consider
$$y' = y^{lpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-lpha} \right)^{1/(lpha - 1)} \right)^{-1}$

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1}y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$,



What Happens	Why It Happened	Why PSM
0000000	0000	0000000

Consider
$$y' = y^{lpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-lpha}\right)^{1/(\alpha-1)} \right)^{-1}$.

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1}y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$, $u'_3 = -y^{-2}y' = -u_3^2 u_2$.



Vhat Happens	Why It Happened	Why PSM
000000		

W

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha} \right)^{1/(\alpha-1)} \right)^{-1}$

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1}y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$, $u'_3 = -y^{-2}y' = -u_3^2 u_2$.

In addition, with $u_4 = u_2 u_3 = y^{\alpha - 1}$,



What	Happens
0000	

Arbitrary Power

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha}\right)^{1/(\alpha-1)} \right)^{-1}$.

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1}y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$, $u'_3 = -y^{-2}y' = -u_3^2 u_2$.

In addition, with
$$u_4 = u_2 u_3 = y^{\alpha - 1}$$
, $u'_4 = (\alpha - 1)y^{\alpha - 2}y' = (\alpha - 1)y^{2\alpha - 2} = (\alpha - 1)u_4^2$,



What Happens	
000000000	

Why PSM

Arbitrary Power

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha}\right)^{1/(\alpha-1)} \right)^{-1}$.

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1} y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$, $u'_3 = -y^{-2} y' = -u_3^2 u_2$.

In addition, with
$$u_4 = u_2 u_3 = y^{\alpha - 1}$$
, $u'_4 = (\alpha - 1)y^{\alpha - 2}y'$
= $(\alpha - 1)y^{2\alpha - 2} = (\alpha - 1)u_4^2$, so we could solve
 $u'_1 = u_2$, $u'_2 = \alpha u_2 u_4$, $u'_3 = -u_3 u_4$, $u'_4 = (\alpha - 1)u_4^2$.



What	Happens
0000	

Why PSM

Arbitrary Power

Consider
$$y' = y^{\alpha}$$
, $y(0) = y_0$, $y = \left(\left(t - \alpha t + y_0^{1-\alpha}\right)^{1/(\alpha-1)} \right)^{-1}$.

With
$$u_1 = y$$
, $u_2 = y^{\alpha}$, $u_3 = 1/y$, we have $u'_1 = y^{\alpha} = u_2$,
 $u'_2 = \alpha y^{\alpha-1} y' = \alpha y^{2\alpha-1} = \alpha u_2^2 u_3$, $u'_3 = -y^{-2} y' = -u_3^2 u_2$.

In addition, with
$$u_4 = u_2 u_3 = y^{\alpha - 1}$$
, $u'_4 = (\alpha - 1)y^{\alpha - 2}y'$
= $(\alpha - 1)y^{2\alpha - 2} = (\alpha - 1)u_4^2$, so we could solve
 $u'_1 = u_2$, $u'_2 = \alpha u_2 u_4$, $u'_3 = -u_3 u_4$, $u'_4 = (\alpha - 1)u_4^2$.

Or more simply $u'_1 = u_1 u_4$, $u'_4 = (\alpha - 1)u_4^2$.



What Happens	
000000000	

Arbitrary Power Errors

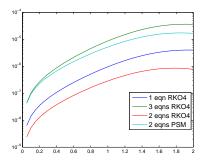
Set $\alpha = e/2 + i/\pi$, y(0) = 1, 40 intervals on [0, 2], RKO4 with one, two, three equation versions, PSM on two equation version.



Arbitrary Power Errors

Set $\alpha = e/2 + i/\pi$, y(0) = 1, 40 intervals on [0, 2], RKO4 with one, two, three equation versions, PSM on two equation version.

Error Magnitude



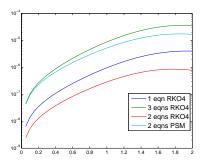


Why PSM 0000000

Arbitrary Power Errors

Set $\alpha = e/2 + i/\pi$, y(0) = 1, 40 intervals on [0, 2], RKO4 with one, two, three equation versions, PSM on two equation version.

Error Magnitude



5th order PSM slightly better than RKO4 with two equations, twelfth order gives machine accuracy (or 100 intervals at eighth order).



What Happens	Why It Happened	Why PSM
○○○○○●○○○	0000	0000000
Simple Pendulum		

The simple pendulum is $\theta'' = -\sin\theta$ with $\theta(0) = \theta_0$, $\theta'(0) = 0$.



The simple pendulum is $\theta'' = -\sin \theta$ with $\theta(0) = \theta_0$, $\theta'(0) = 0$. First order system: $\theta'_1 = \theta_2$, $\theta'_2 = -\sin \theta$ with $\theta_1(0) = \theta_0$, $\theta_2(0) = 0$.



The simple pendulum is $\theta'' = -\sin\theta$ with $\theta(0) = \theta_0$, $\theta'(0) = 0$. First order system: $\theta'_1 = \theta_2$, $\theta'_2 = -\sin\theta$ with $\theta_1(0) = \theta_0$, $\theta_2(0) = 0$. Conservation of energy states that $(\theta')^2/2 - \cos\theta = C$.



The simple pendulum is $\theta'' = -\sin\theta$ with $\theta(0) = \theta_0$, $\theta'(0) = 0$. First order system: $\theta'_1 = \theta_2$, $\theta'_2 = -\sin\theta$ with $\theta_1(0) = \theta_0$, $\theta_2(0) = 0$. Conservation of energy states that $(\theta')^2/2 - \cos\theta = C$.

No closed form solution.



The simple pendulum is $\theta'' = -\sin\theta$ with $\theta(0) = \theta_0$, $\theta'(0) = 0$. First order system: $\theta'_1 = \theta_2$, $\theta'_2 = -\sin\theta$ with $\theta_1(0) = \theta_0$, $\theta_2(0) = 0$. Conservation of energy states that $(\theta')^2/2 - \cos\theta = C$.

No closed form solution.

Letting $u_1 = \theta$, $u_2 = \theta'$, $u_3 = \sin \theta$, $u_4 = \cos \theta$, then $u'_1 = u_2$, $u'_2 = -u_3$, $u'_3 = u_2u_4$, $u'_4 = -u_2u_3$ with $u_1(0) = \theta_0$, $u_2(0) = 0$, $u_3(0) = \sin(\theta_0)$, $u_4(0) = \cos(\theta_0)$.

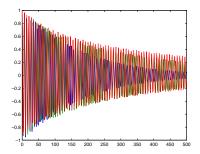


What	Happens
	00000

Why PSM 0000000

Pendulum Errors

500 intervals on [0, 500] angle



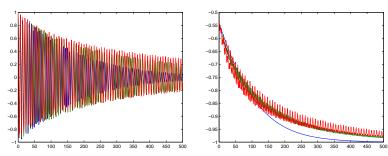


What	Happens
	00000

Pendulum Errors

500 intervals on [0, 500] angle





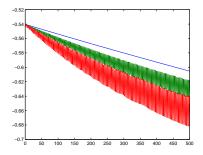


What Happens	
000000000	

Why PSM 0000000

Pendulum Errors 2

1000 intervals on [0, 500] energy

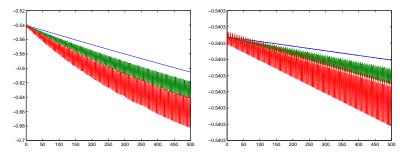




What Happens Why It Happened 000000000 0000

Pendulum Errors 2

1000 intervals on [0, 500] energy 10000 intervals on [0, 500]



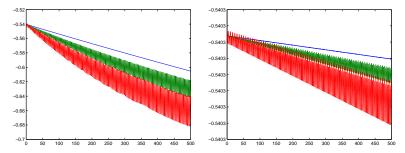


What Happens Why It Happened 000000000 0000

Why PSM

Pendulum Errors 2

1000 intervals on [0, 500] energy 10000 intervals on [0, 500]



10000 intervals on [0, 500] $\Delta e = 2.9 \times 10^{-6}$.

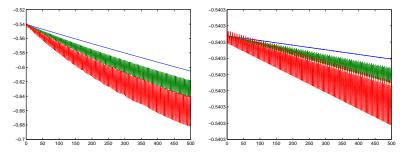


What Happens Why It Happened 000000000 0000

Why PSM

Pendulum Errors 2

1000 intervals on [0, 500] energy 10000 intervals on [0, 500]



10 000 intervals on [0, 500] $\Delta e = 2.9 \times 10^{-6}$. PSM with order 8 has $\Delta e = 2.2 \times 10^{-13}$, and order 12 energy is constant to machine precision.

What Happens	Why It Happened	Why PSM
○○○○○○○●	0000	0000000
Implications		

• Runge-Kutta order 4 solutions to polynomial systems have different error from that of the original system, but function evaluations can be much faster.



What Happens ○○○○○○○●	Why It Happened	Why PSM 0000000
Implications		

• Runge-Kutta order 4 solutions to polynomial systems have different error from that of the original system, but function evaluations can be much faster. Not all differential equations are created equal.



What Happens	Why It Happened	Why F
00000000	0000	0000

Implications

- Runge-Kutta order 4 solutions to polynomial systems have different error from that of the original system, but function evaluations can be much faster. Not all differential equations are created equal.
- Power Series Method order 4 solutions usually have slightly more error than Runge-Kutta order 4 solutions for the same polynomial systems – and usually require more computational work!



SM

Implications

- Runge-Kutta order 4 solutions to polynomial systems have different error from that of the original system, but function evaluations can be much faster. Not all differential equations are created equal.
- Power Series Method order 4 solutions usually have slightly more error than Runge-Kutta order 4 solutions for the same polynomial systems – and usually require more computational work!
- But, the PSM can be made of arbitrary order, and has many other advantages...



pens	Why It Happened
	0000

Euler's method for y' = f(t, y(t)) is $y_{n+1} = y_n + h f(t_n, y_n)$ with local error $O(h^2)$ and global error O(h).



Euler's method for y' = f(t, y(t)) is $y_{n+1} = y_n + h f(t_n, y_n)$ with local error $O(h^2)$ and global error O(h). Typical derivation via Taylor series: $y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{h^2}{2}y''(t_0) + O(h^3)$. Replace $y'(t_0)$ by $f(t_0, y(t_0))$, error is $h^2y''(t_0)/2 + O(h^3)$, or in Lagrange form $h^2y''(\xi)/2$, $\xi \in [t_0, t_0 + h]$.



Euler's method for y' = f(t, y(t)) is $y_{n+1} = y_n + h f(t_n, y_n)$ with local error $O(h^2)$ and global error O(h). Typical derivation via Taylor series: $y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{h^2}{2}y''(t_0) + O(h^3)$. Replace $y'(t_0)$ by $f(t_0, y(t_0))$, error is $h^2y''(t_0)/2 + O(h^3)$, or in Lagrange form $h^2y''(\xi)/2$, $\xi \in [t_0, t_0 + h]$.

Higher order derivations almost always stop here, and leave the impression that error is proportional to h and depends on derivatives of y.



Euler's method for y' = f(t, y(t)) is $y_{n+1} = y_n + h f(t_n, y_n)$ with local error $O(h^2)$ and global error O(h). Typical derivation via Taylor series: $y(t_0 + h) = y(t_0) + hy'(t_0) + \frac{h^2}{2}y''(t_0) + O(h^3)$. Replace $y'(t_0)$ by $f(t_0, y(t_0))$, error is $h^2y''(t_0)/2 + O(h^3)$, or in Lagrange form $h^2y''(\xi)/2$, $\xi \in [t_0, t_0 + h]$.

Higher order derivations almost always stop here, and leave the impression that error is proportional to *h* and depends on derivatives of *y*. But (for Euler), since $y''(\xi) = \frac{\partial f}{\partial t}(\xi, y(\xi)) + \frac{\partial f}{\partial y}(\xi, y(\xi))f(\xi, y(\xi))$, we can relate the error to the RHS.



What Happens	

If
$$y'_i = f_i(t, y_1(t), y_2(t), \dots, y_n(t))$$
 for $i = 1, 2, \dots, n$, errors are $h^2 y''_i(\xi_i)/2$ where $y''_i(\xi_i) = \frac{\partial f_i}{\partial t} + \sum_{j=1}^n \frac{\partial f_i}{\partial y_j} f_j$.



What Happens	

If
$$y'_i = f_i(t, y_1(t), y_2(t), \dots, y_n(t))$$
 for $i = 1, 2, \dots, n$, errors are $h^2 y''_i(\xi_i)/2$ where $y''_i(\xi_i) = \frac{\partial f_i}{\partial t} + \sum_{j=1}^n \frac{\partial f_i}{\partial y_j} f_j$.

$$y' = \sin y$$
, error $\frac{h}{2}y''(\xi) = \frac{h}{2}\cos(\xi)\sin(\xi)$



What Happens

If
$$y'_i = f_i(t, y_1(t), y_2(t), \dots, y_n(t))$$
 for $i = 1, 2, \dots, n$, errors are $h^2 y''_i(\xi_i)/2$ where $y''_i(\xi_i) = \frac{\partial f_i}{\partial t} + \sum_{j=1}^n \frac{\partial f_i}{\partial y_j} f_j$.

$$y' = \sin y$$
, error $\frac{h}{2}y''(\xi) = \frac{h}{2}\cos(\xi)\sin(\xi)$

$$[u_1 = y, u_2 = \sin y, u_3 = \cos y]: u'_1 = u_2, u'_2 = u_2u_3, u'_3 = -u_2^2,$$



If
$$y'_i = f_i(t, y_1(t), y_2(t), \dots, y_n(t))$$
 for $i = 1, 2, \dots, n$, errors are $h^2 y''_i(\xi_i)/2$ where $y''_i(\xi_i) = \frac{\partial f_i}{\partial t} + \sum_{j=1}^n \frac{\partial f_i}{\partial y_j} f_j$.

$$y' = \sin y$$
, error $\frac{h}{2}y''(\xi) = \frac{h}{2}\cos(\xi)\sin(\xi)$

$$\begin{bmatrix} u_1 = y, & u_2 = \sin y, & u_3 = \cos y \end{bmatrix}: u'_1 = u_2, & u'_2 = u_2 u_3, & u'_3 = -u_2^2, \\ u_1 \text{ error } \frac{h}{2}u_2(\xi_1)u_3(\xi_1), & u_2 \text{ error } \frac{h}{2}\left(u_2^2(\xi_2)u_3(\xi_2) - u_2^3(\xi_2)\right), \\ u_3 \text{ error } -hu_2^2(\xi_3)u_3(\xi_3), & t_0 \le \xi_i \le t_0 + h.$$



If
$$y'_i = f_i(t, y_1(t), y_2(t), \dots, y_n(t))$$
 for $i = 1, 2, \dots, n$, errors are $h^2 y''_i(\xi_i)/2$ where $y''_i(\xi_i) = \frac{\partial f_i}{\partial t} + \sum_{j=1}^n \frac{\partial f_i}{\partial y_j} f_j$.

$$y' = \sin y$$
, error $\frac{h}{2}y''(\xi) = \frac{h}{2}\cos(\xi)\sin(\xi)$

$$\begin{bmatrix} u_1 = y, \ u_2 = \sin y, \ u_3 = \cos y \end{bmatrix}: \ u'_1 = u_2, \ u'_2 = u_2 u_3, \ u'_3 = -u_2^2, \\ u_1 \text{ error } \frac{h}{2} u_2(\xi_1) u_3(\xi_1), \ u_2 \text{ error } \frac{h}{2} \left(u_2^2(\xi_2) u_3(\xi_2) - u_2^3(\xi_2) \right), \\ u_3 \text{ error } -h u_2^2(\xi_3) u_3(\xi_3), \ t_0 \le \xi_i \le t_0 + h.$$

Error in
$$u_1$$
 is $\frac{h}{2}(\sin(\xi_1)\cos(\xi_1)) + O(h^2)$.



Happens	Why It Happened	Why PSM
00000	0000	0000000

• Rewriting a system of differential equations in polynomial form introduces additional variables.



lappens			

What

- Rewriting a system of differential equations in polynomial form introduces additional variables.
- Using an *n*th order solver introduces $O(h^n)$ errors in these terms, which contribute to the $O(h^n)$ error in the variables corresponding to those in the original system.



What	Happens
	00000

- Rewriting a system of differential equations in polynomial form introduces additional variables.
- Using an *n*th order solver introduces $O(h^n)$ errors in these terms, which contribute to the $O(h^n)$ error in the variables corresponding to those in the original system.
- The final error is $O(h^n)$, but the proportionality constant will change. It may increase or decrease depending on the magnitude and sign of the introduced errors.



What Ha	ppens

- Rewriting a system of differential equations in polynomial form introduces additional variables.
- Using an *n*th order solver introduces $O(h^n)$ errors in these terms, which contribute to the $O(h^n)$ error in the variables corresponding to those in the original system.
- The final error is $O(h^n)$, but the proportionality constant will change. It may increase or decrease depending on the magnitude and sign of the introduced errors.
- Polynomial form is superior because the rhs is much more efficient to evaluate compare a few of multiplications to evaluating transcendental functions.



What H	appens

- Rewriting a system of differential equations in polynomial form introduces additional variables.
- Using an *n*th order solver introduces $O(h^n)$ errors in these terms, which contribute to the $O(h^n)$ error in the variables corresponding to those in the original system.
- The final error is $O(h^n)$, but the proportionality constant will change. It may increase or decrease depending on the magnitude and sign of the introduced errors.
- Polynomial form is superior because the rhs is much more efficient to evaluate compare a few of multiplications to evaluating transcendental functions.
- Every system of odes can be rewritten in polynomial form in an algorithmic manner.

What Happens	

- Rewriting a system of differential equations in polynomial form introduces additional variables.
- Using an *n*th order solver introduces $O(h^n)$ errors in these terms, which contribute to the $O(h^n)$ error in the variables corresponding to those in the original system.
- The final error is $O(h^n)$, but the proportionality constant will change. It may increase or decrease depending on the magnitude and sign of the introduced errors.
- Polynomial form is superior because the rhs is much more efficient to evaluate compare a few of multiplications to evaluating transcendental functions.
- Every system of odes can be rewritten in polynomial form in an algorithmic manner. Functions like $(e^t 1)/t$ and $(\sin t)/t$ at t = 0 can cause problems.

What Happens	

In all cases so far, PSM order 4 inferior to Runge-Kutta order 4, in terms of error and computational effort per step.



In all cases so far, PSM order 4 inferior to Runge-Kutta order 4, in terms of error and computational effort per step.

PSM generates the exact Taylor series of order n expanding at a given point. Runge-Kutta matches the initial Taylor coefficients, but has some additional contributions.



In all cases so far, PSM order 4 inferior to Runge-Kutta order 4, in terms of error and computational effort per step.

PSM generates the exact Taylor series of order n expanding at a given point. Runge-Kutta matches the initial Taylor coefficients, but has some additional contributions.

Runge-Kutta is equivalent to an infinite power series, and the approximate tail is usually better than none at all.



In all cases so far, PSM order 4 inferior to Runge-Kutta order 4, in terms of error and computational effort per step.

PSM generates the exact Taylor series of order n expanding at a given point. Runge-Kutta matches the initial Taylor coefficients, but has some additional contributions.

Runge-Kutta is equivalent to an infinite power series, and the approximate tail is usually better than none at all.

Computationally, each multiplication in Runge-Kutta requires Cauchy products in PSM:

$$\left(\sum_{i=0}^{\infty}a_{i}x^{i}\right)\left(\sum_{i=0}^{\infty}b_{i}x^{i}\right)=\sum_{i=0}^{\infty}\left(\sum_{j=0}^{i}a_{j}b_{i-j}\right)x^{i}.$$





• Every system of odes can be rewritten in polynomial form algorithmically. Every analytic function can be equivalently replaced by a system of odes. Every system of polynomial odes has an equivalent quadratic system of odes.





- Every system of odes can be rewritten in polynomial form algorithmically. Every analytic function can be equivalently replaced by a system of odes. Every system of polynomial odes has an equivalent quadratic system of odes.
- A wide range of modeling problems are polynomial odes.



Why PSM

- Every system of odes can be rewritten in polynomial form algorithmically. Every analytic function can be equivalently replaced by a system of odes. Every system of polynomial odes has an equivalent quadratic system of odes.
- A wide range of modeling problems are polynomial odes.
- Arbitrary order available automatically or adaptively. Can balance order versus number of intervals to minimize.



Why PSM

- Every system of odes can be rewritten in polynomial form algorithmically. Every analytic function can be equivalently replaced by a system of odes. Every system of polynomial odes has an equivalent quadratic system of odes.
- A wide range of modeling problems are polynomial odes.
- Arbitrary order available automatically or adaptively. Can balance order versus number of intervals to minimize.
- A priori error estimate available.



What Happens	Why It Happened 0000	Why PSM ○●○○○○○
Why PSM (cont'd)		

• Numerical solution (as a power series) is available for all time, not just at data points (compare with extrapolation methods).



What Happens	Why It Happened	Why PSM
00000000	0000	○●○○○○○
Why PSM (cont'd)		

- Numerical solution (as a power series) is available for all time, not just at data points (compare with extrapolation methods).
 - End condition is g(t, y(t)) = 0.



What Happens

Why PSM (cont'd)

- Numerical solution (as a power series) is available for all time, not just at data points (compare with extrapolation methods).
 - End condition is g(t, y(t)) = 0.
 - Even better, PSM can be used to identify crossing times when differential equation has discontinuities, like $x'' + \mu x^+ \nu x^- = 0, \ \mu, \nu \ge 0, \ x^+ = \max\{x, 0\}, \ x^- = \max\{-x, 0\}.$



What Happens

Why PSM (cont'd)

- Numerical solution (as a power series) is available for all time, not just at data points (compare with extrapolation methods).
 - End condition is g(t, y(t)) = 0.
 - Even better, PSM can be used to identify crossing times when differential equation has discontinuities, like $x'' + \mu x^+ \nu x^- = 0$, $\mu, \nu \ge 0$, $x^+ = \max\{x, 0\}$, $x^- = \max\{-x, 0\}$.
 - Makes delay differential equations trivial to solve.



Why It Happened

Why PSM

Why PSM (cont'd)

What Happens

- Numerical solution (as a power series) is available for all time, not just at data points (compare with extrapolation methods).
 - End condition is g(t, v(t)) = 0.
 - Even better, PSM can be used to identify crossing times when differential equation has discontinuities, like $x'' + \mu x^+ - \nu x^- = 0, \ \mu, \nu > 0, \ x^+ = \max\{x, 0\},\$ $x^{-} = \max\{-x, 0\}.$
 - Makes delay differential equations trivial to solve.
- Arbitrary order means we can easily push to machine accuracy solutions, regardless of the required precision. For Hamiltonian systems of odes, we can conserve energy to machine precision – effectively symplectic.



What Happens	

Symplectic Methods

A symplectic method numerically approximates a system of odes in such a way that a first integral, or Hamiltonian, is conserved.



What Happens	

Symplectic Methods

A symplectic method numerically approximates a system of odes in such a way that a first integral, or Hamiltonian, is conserved.

Leapfrog integration (Feynman Lectures): To solve x' = v, v' = f(x), $x_i = x_{i-1} + v_{i-1/2}\Delta t$, $v_{i+1/2} = v_{i-1/2} + f(x_i)\Delta t$,



Symplectic Methods

A symplectic method numerically approximates a system of odes in such a way that a first integral, or Hamiltonian, is conserved.

Leapfrog integration (Feynman Lectures): To solve x' = v, v' = f(x), $x_i = x_{i-1} + v_{i-1/2}\Delta t$, $v_{i+1/2} = v_{i-1/2} + f(x_i)\Delta t$, or $x_{i+1} = x_i + v_i\Delta t + \frac{f(x_i)}{2}\Delta t^2$, $v_{i+1} = v_i + \frac{1}{2}(f(x_i) + f(x_{i+1})\Delta t$.



Symplectic Methods

A symplectic method numerically approximates a system of odes in such a way that a first integral, or Hamiltonian, is conserved.

Leapfrog integration (Feynman Lectures): To solve x' = v, v' = f(x), $x_i = x_{i-1} + v_{i-1/2}\Delta t$, $v_{i+1/2} = v_{i-1/2} + f(x_i)\Delta t$, or $x_{i+1} = x_i + v_i\Delta t + \frac{f(x_i)}{2}\Delta t^2$, $v_{i+1} = v_i + \frac{1}{2}(f(x_i) + f(x_{i+1})\Delta t$. It is invariant under time reversal, and "area preserving" in position/momentum space, and energy is nearly conserved (periodic).



Symplectic Methods

A symplectic method numerically approximates a system of odes in such a way that a first integral, or Hamiltonian, is conserved.

Leapfrog integration (Feynman Lectures): To solve x' = v, v' = f(x), $x_i = x_{i-1} + v_{i-1/2}\Delta t$, $v_{i+1/2} = v_{i-1/2} + f(x_i)\Delta t$, or $x_{i+1} = x_i + v_i\Delta t + \frac{f(x_i)}{2}\Delta t^2$, $v_{i+1} = v_i + \frac{1}{2}(f(x_i) + f(x_{i+1})\Delta t$. It is invariant under time reversal, and "area preserving" in position/momentum space, and energy is nearly conserved (periodic).

Forest-Ruth (1990) is fourth order: Given x_i , v_i : $x_a = x_i + \theta h v_i/2$, $v_a = v_i + \theta h f(x_a)$, $x_b = x_a + (1 - \theta) h v_a/2$, $v_b = v_a + (1 - 2\theta) h f(x_b)$, $x_c = x_b + (1 - \theta) h v_b/2$, $v_{i+1} = v_b + \theta h f(x_c)$, $x_{i+1} = x_c + \theta h v_{i+1}/2$ with $\theta = 1/(2 - \sqrt[3]{2}) \approx 1.35$.

What Happens	

Why It Happened

Why PSM

Symplectic Simple Pendulum

10000 intervals on [0,500]: energy periodic, range 2.6 \times 10^{-4}.



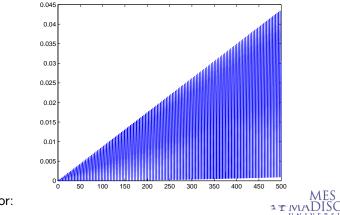
What Happens	

Why It Happened

Why PSM

Symplectic Simple Pendulum

10 000 intervals on [0, 500]: energy periodic, range 2.6×10^{-4} .



But actual error:

• More accurate fourth order require more function evaluations, or are implicit.



- More accurate fourth order require more function evaluations, or are implicit.
- Symplectic solvers for more complicated Hamiltonians can be very complicated.



- More accurate fourth order require more function evaluations, or are implicit.
- Symplectic solvers for more complicated Hamiltonians can be very complicated.
- (Apparently,) all symplectic algorithms require equal step sizes.



- More accurate fourth order require more function evaluations, or are implicit.
- Symplectic solvers for more complicated Hamiltonians can be very complicated.
- (Apparently,) all symplectic algorithms require equal step sizes.
- Symplectic methods still have error. Since it is not in the "energy," it is in the "phase."



What Happer	

We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form.



We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form. Any numerical method that gives the true solution to machine precision will conserve energy to machine precision, and hence be effectively symplectic.



Why It Happened

Why PSM

Effectively Symplectic

We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form. Any numerical method that gives the true solution to machine precision will conserve energy to machine precision, and hence be effectively symplectic. The PSM or any other related method can easily be effectively symplectic, and is adaptive



We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form. Any numerical method that gives the true solution to machine precision will conserve energy to machine precision, and hence be effectively symplectic. The PSM or any other related method can easily be effectively symplectic, and is adaptive

• Simple pendulum example: order twelve, 10 000 intervals on [0, 500].



We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form. Any numerical method that gives the true solution to machine precision will conserve energy to machine precision, and hence be effectively symplectic. The PSM or any other related method can easily be effectively symplectic, and is adaptive

- Simple pendulum example: order twelve, 10 000 intervals on [0, 500].
- Pruett, Ingham & Herman (2011): An adaptive and parallel implementation of the PSM method for the *N*-body problem, currently fastest accurate solver for such problems.



We call a numerical method "effectively symplectic" if the energy is conserved without explicitly using the Hamiltonian form. Any numerical method that gives the true solution to machine precision will conserve energy to machine precision, and hence be effectively symplectic. The PSM or any other related method can easily be effectively symplectic, and is adaptive

- Simple pendulum example: order twelve, 10 000 intervals on [0, 500].
- Pruett, Ingham & Herman (2011): An adaptive and parallel implementation of the PSM method for the *N*-body problem, currently fastest accurate solver for such problems.
- Double pendulum: later today!



00000000	0000	000000
Future Mork		

• Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.



What Happens	

- Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.
- Automatically converting a system to polynomial form, minimizing of number of Cauchy products (quadratic terms on rhs) using "intermediate variables."



- Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.
- Automatically converting a system to polynomial form, minimizing of number of Cauchy products (quadratic terms on rhs) using "intermediate variables."
- Automatically dealing with "difficult" functions like $(\sin u(t))/u(t)$ or $(e^{u(t)} 1)/u(t)$ near u(t) = 0.



- Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.
- Automatically converting a system to polynomial form, minimizing of number of Cauchy products (quadratic terms on rhs) using "intermediate variables."
- Automatically dealing with "difficult" functions like $(\sin u(t))/u(t)$ or $(e^{u(t)} 1)/u(t)$ near u(t) = 0.
- A more careful survey of symplectic methods, and comparison with the PSM.



- Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.
- Automatically converting a system to polynomial form, minimizing of number of Cauchy products (quadratic terms on rhs) using "intermediate variables."
- Automatically dealing with "difficult" functions like $(\sin u(t))/u(t)$ or $(e^{u(t)} 1)/u(t)$ near u(t) = 0.
- A more careful survey of symplectic methods, and comparison with the PSM.
- Implementation for delay differential equations, piecewise functions, ...



- Using a priori error bound and requested error, identify most efficient combination of order and interval width for PSM.
- Automatically converting a system to polynomial form, minimizing of number of Cauchy products (quadratic terms on rhs) using "intermediate variables."
- Automatically dealing with "difficult" functions like $(\sin u(t))/u(t)$ or $(e^{u(t)} 1)/u(t)$ near u(t) = 0.
- A more careful survey of symplectic methods, and comparison with the PSM.
- Implementation for delay differential equations, piecewise functions, ...



