# CS 101

# Numerical Geometric Integration

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## Today's Show

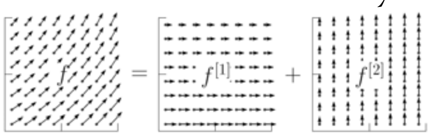
Two related topics
- Splitting
- Composition

Basically, ways to split and splice existing methods



## Splitting

Deal with different terms differently

$\dot{y} = f(y)$ 



- decompose the vector field
- treat each component differently
  - based on known specificities



## Fast/Slow Splitting

Got two vastly different time scales?
- treat fast and slow separately—and sum
  - particularly useful for
    - planetary dynamics
    - inhomogeneous elasticity
    - molecular dynamics
- often, implicit for fast, explicit for slow
  - slow forces often non-linear—but slow



## Let's Jump Right Into It [Stern 08]

Suppose two potentials: $U$ and $W$
- respectively, slow and fast

Define discrete Lagrangian as:

$$L(q_k, q_{k+1}) = \frac{h}{2}\left(\frac{q_{k+1}-q_k}{h}\right)^t M \left(\frac{q_{k+1}-q_k}{h}\right) - h\frac{U(q_k)+U(q_{k+1})}{2} - hW\left(\frac{q_k+q_{k+1}}{2}\right)$$

Then, the "IMEX" DEL is:

$$M\frac{q_{k+1}-2q_k+q_{k-1}}{h^2} = -\left[\nabla U(q_k) + \frac{1}{2}\nabla W\left(\frac{q_{k-1}+q_k}{2}\right) + \frac{1}{2}\nabla W\left(\frac{q_k+q_{k+1}}{2}\right)\right]$$



## Revisiting the Update Rule

Legendre to the rescue

$$p_k = M\left(\frac{q_{k+1}-q_k}{h}\right) + \frac{h}{2}\nabla U(q_k) + \frac{h}{2}\nabla W\left(\frac{q_k+q_{k+1}}{2}\right)$$

$$p_{k+1} = M\left(\frac{q_{k+1}-q_k}{h}\right) - \frac{h}{2}\nabla U(q_{k+1}) - \frac{h}{2}\nabla W\left(\frac{q_k+q_{k+1}}{2}\right)$$

Not very enlightening just yet...

Define: $p_k^+ = p_k - \frac{h}{2}\nabla U(q_k)$

$p_{k+1}^- = p_{k+1} + \frac{h}{2}\nabla U(q_{k+1})$

# Kicking and Integrating

Integrator corresponds to:

From $(p_k, q_k)$,

$$p_k^+ = p_k - \frac{h}{2}\nabla U(q_k)$$ kick

$$\begin{cases} p_{k+1}^- = p_k^+ - h\nabla W\left(\frac{q_k + q_{k+1}}{2}\right) \\ q_{k+1} = q_k + hM^{-1}\left(\frac{p_k^+ + p_{k+1}^-}{2}\right) \end{cases}$$ implicit step

$$p_{k+1} = p_{k+1}^- - \frac{h}{2}\nabla U(q_{k+1})$$ kick



# Fermi–Pasta–Ulam Problem

System made out of *2M* unit masses

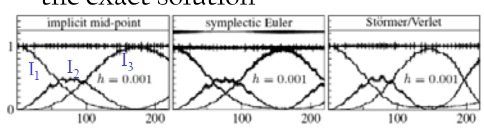
- chained together in series
- with alternating weak nonlinear springs and stiff linear springs
  - the non-linearity is introduced as a perturbation to a primarily linear problem




# Behavior for M=3

Stiff springs slowly exchange energy

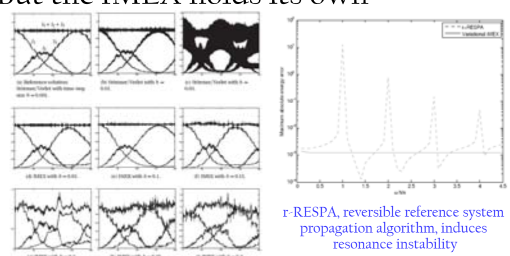
- symplectic methods work if h small
- the slow energy exchange in the numerical solution is consistent with the exact solution






# Not For Larger Time Steps…

But the IMEX holds its own



r-RESPA, reversible reference system propagation algorithm, induces resonance instability



# Another Advantage of Splitting

Volume-preserving Integration

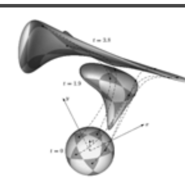
- how to integrate $\dot{y} = f(y)$ with $\nabla \cdot f(y) = 0$ ?
- we could simply add a constraint
  - see next week!
  - but unnecessary here
- splitting methods can help



# Examples of V.P. Flows

ABC Flow

$$\dot{x} = \frac{1}{2}\sin z + \cos y$$
$$\dot{y} = \sin x + \frac{1}{2}\cos z$$
$$\dot{z} = \sin y + \cos x$$



Vortex flow

## Didactic Example

3D flow: $\frac{d}{dt}\begin{pmatrix}x\\y\\z\end{pmatrix} = \mathbf{v}(x,y,z)$

with $\mathbf{v}(x,y,z) = \begin{pmatrix} -\sin x\cos y\cos z + b\sin 2x\cos 2z \\ -\cos x\sin y\cos z + b\sin 2y\cos 2z \\ 2\cos x\cos y\sin z - b(\cos 2x + \cos 2y)\sin 2z \end{pmatrix}$

- well, where do we go from here?
- decompose velocity in 8 terms

$$\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_3 + \mathbf{v}_4 + \mathbf{v}_5 + \mathbf{v}_6 + \mathbf{v}_7 + \mathbf{v}_8$$



## The Eight Terms

$\mathbf{v}_1 = \sin(x+y+z)\begin{pmatrix}-1/4\\-1/4\\1/2\end{pmatrix}$ $\mathbf{v}_2 = \sin(x+y-z)\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix}$

$\mathbf{v}_3 = \sin(x-y+z)\begin{pmatrix}-1/4\\1/4\\1/2\end{pmatrix}$ $\mathbf{v}_4 = \sin(x-y-z)\begin{pmatrix}-1/4\\1/4\\-1/2\end{pmatrix}$

$\mathbf{v}_5 = \sin(2y+2z)\begin{pmatrix}0\\b/2\\-b/2\end{pmatrix}$ $\mathbf{v}_6 = \sin(2y-2z)\begin{pmatrix}0\\b/2\\b/2\end{pmatrix}$

$\mathbf{v}_7 = \sin(2x+2z)\begin{pmatrix}b/2\\0\\-b/2\end{pmatrix}$ $\mathbf{v}_8 = \sin(2x-2z)\begin{pmatrix}b/2\\0\\b/2\end{pmatrix}$



## Magic Happens

Each velocity term is:

- divergence free (check)
- integrable explicitly & exactly (& easily)!

Lets' try: $\frac{d}{dt}\begin{pmatrix}x\\y\\z\end{pmatrix} = \sin(x+y-z)\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix}$

- Notice: $x+y-z$ invariant
- Euler exact! $\begin{pmatrix}x(t)\\y(t)\\z(t)\end{pmatrix} = \begin{pmatrix}x_0\\y_0\\z_0\end{pmatrix} + t\sin(x_0+y_0-z_0)\begin{pmatrix}-1/4\\-1/4\\-1/2\end{pmatrix}$



## Volume-Preserving Integration

Compose all the Euler steps together

- Integrate $\mathbf{v}_1$ by step h,
  Integrate $\mathbf{v}_2$ by step h, ... etc
- iterate

Fully explicit (first-order) volume preserving integrator of the ODE!

- see VI.9 in book for generalization



## Segue

Latest integrator can be written:

$$\Psi_h = \varphi_{1,h}\circ\varphi_{2,h}\circ\varphi_{3,h}\circ\varphi_{4,h}\circ\varphi_{5,h}\circ\varphi_{6,h}\circ\varphi_{7,h}\circ\varphi_{8,h}$$

Previous one was also:

$$\Psi_h = \phi^U_{h/2}\circ\Phi^{K+W}_h\circ\phi^U_{h/2}$$

... two examples of *compositions*



## Composition Methods

Quite common in the literature

- as we've just seen

Interesting even for self-composition

- simple way to increase accuracy order

Suppose we have a single-step method

- $\Phi_h$ of order $p$

## Self-Composition

Take coefficients such as

$$\sum_{i=1}^{i=N} \alpha_i = 1 \qquad \sum_{i=1}^{i=N} \alpha_i^{p+1} = 0$$

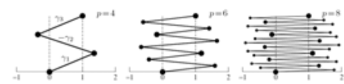
Then $\Psi_h = \Phi_{\alpha_1 h} \circ \ldots \circ \Phi_{\alpha_N h}$ is of order $\geq p+1$

- proof? (Hairer's book, page 44)
- remember that:
  $\Phi_h(y_0) = \phi_h(y_0) + C(y_0)h^{p+1} + \mathcal{O}(h^{p+2})$

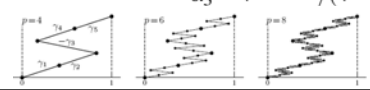


## Examples

Triple jump: $\alpha_1 = \alpha_3 = 1/(2 - 2^{1/(p+1)})$
$\alpha_2 = -2^{1/(p+1)}/(2 - 2^{1/(p+1)})$



Suzuki's fractals: $\alpha_{1|2|4|5} = 1/(4 - 4^{1/(p+1)})$
$\alpha_3 = 4^{1/(p+1)}/(4 - 4^{1/(p+1)})$





## Extensions using Adjoint

One can also use adjoint integrator

- see lecture 5 $\qquad \Phi_h^* = \Phi_{-h}^{-1}$

Compose regular and adjoint

- simplest case:
  $$\Psi_h = \Phi_{h/2} \circ \Phi_{h/2}^*$$
- turn explicit Euler into midpoint
- more generally, makes it symmetric!



## More Composition Methods

Many other compositions!

- composition of Ruge-Kutta methods
  - page 59
- composition of "B-series"
  - page 61