Structure Preserving Numerical Methods

for Ordinary Differential Equations

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Analytical methods often provide qualitative information about a dynamical system even in cases where an explicit solution is not available. For example, it is well known that Hamiltonian systems are symplectic. If the problem is solved numerically, this information may be lost, so it is important to develop and use numerical methods which preserve the qualitative structure of the system. An example of a structure preserving method is the Stormer-Verlet integrator, which preserves the symplecticity of a Hamiltonian system.

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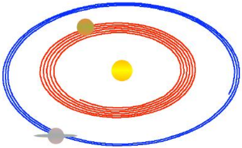
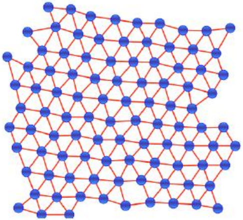
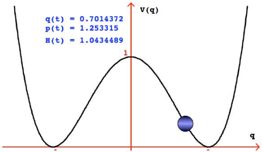
History and Applications

- Nonstiff Differential equations
  Adams (1855), multistep methods, Bashforth (1883),
  Runge (1895) and Kutta (1901), one-step methods
- Stiff differential equations
  Dahlquist (1963), A-stability of multistep methods,
  Gear (1971), backward differentiation
- Geometric numerical integration
  Structure-preserving integration of differential equations
  (time reversible, symplectic, energy), Hamiltonian systems
  Feng (1985), Sanz-Serna (1988), Hairer et. al (1993), Marsden
    - Mathematics: spring-mass, pendulum, n-body, constraints
    - Biology: predator-pray (nonlinear)
    - Astronomy: Kepler (2-bocy), outer solar system
      (very large time scales)
    - Chemistry: molecular dynamics, crystals
      (very small time scales)
    - Physics: double well potential







Ernst Hairer, Geometric Integration, course announcement, winter 2009/10

Review Harmonic Oscillator

- Balance of forces (Newton's second law)

$$m\ddot{u}(t) = -cu(t) \qquad u(0) = 0, \dot{u}(0) = 0$$

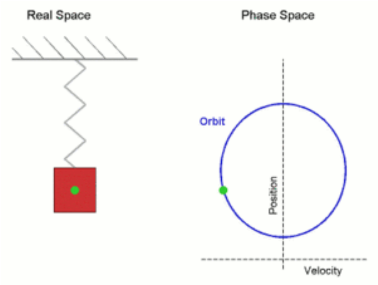
has solution

$$u(t) = \cos(\omega t)$$

mass m, spring constant c, frequency $\omega = \sqrt{c/m}$

- Set $p = m\dot{u}$ and write as two 1^{st} order differential equations

$$\dot{u} = p/m \qquad \begin{bmatrix} \dot{u} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} & 1/m \\ -1c & \end{bmatrix}}_{\text{skew, } A^T = -A} \begin{bmatrix} u \\ p \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ p(0) \end{bmatrix}$$
$$\dot{p} = -cu$$



- Skew symmetric differential equation

$$\dot{\mathbf{y}}(t) = A\mathbf{y}(t), \quad \mathbf{y}(0) = \mathbf{y}_0$$

has solution $(m = c = 1)$

$$\mathbf{y}(t) = \underbrace{\mathrm{e}^{At}}_{\text{rotation, } R^T = R^{-1}} \mathbf{y}_0 \qquad \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix} = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Review Numerical Methods for ODEs

- (Linear system of) ordinary differential equations (ODEs)

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0$$
$$\dot{\mathbf{y}} = A\mathbf{y}$$

- Rewrite difference quotient

$$\dot{\mathbf{y}} = \lim_{h \to 0} \frac{\mathbf{y}(t+h) - \mathbf{y}(t)}{h}$$

$$\mathbf{y}(t+h) = \mathbf{y}(t) + h\mathbf{f}(\mathbf{y})$$

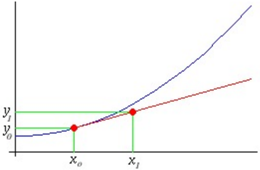
- Euler explicit

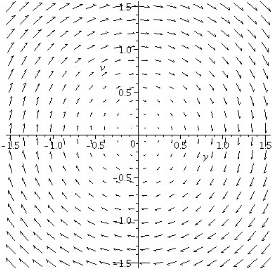
$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_n)$$
$$= \left[I - hA\right] \mathbf{y}_n$$

- Euler implicit

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_{n+1})$$

$$\left[I - hA\right] \mathbf{y}_{n+1} = \mathbf{y}_n$$





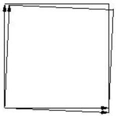
Both are 1^{st} order methods, Euler explicit is only pedagogical
Euler implicit is stable for larger step size, need to solve linear equation system

www.math.buffalo.edu/ apeleg/mth306y_maple.html
calculuslab.deltacollege.edu/ODE/7-C-1/7-C-1-h-a.html

Hamiltonian Systems and Symplecticity

- Hamiltonian = kinetic + potential Energy (scalar fcn of generalized coord.)

$$H(u, p = m\dot{u}) = \frac{1}{2}m\dot{u}^2(t) + \frac{1}{2}cu^2(t)$$
$$= \frac{1}{2m}p^2(t) + \frac{1}{2}cu^2(t)$$

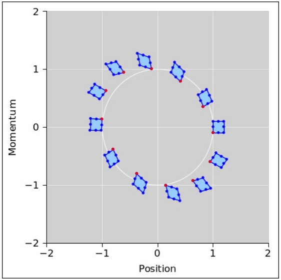


$$\begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ -h \end{bmatrix}$$
$$\begin{bmatrix} 1 & h \\ -h & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} h \\ 1 \end{bmatrix}$$

- Hamiltonian System

$$\dot{u} = \frac{\partial H}{\partial p} = p/m$$
$$\dot{p} = -\frac{\partial H}{\partial u} = cu$$

$$\begin{bmatrix} \dot{u} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} & 1 \\ -1 & \end{bmatrix}}_{J^{-1}=J^T=-J} \begin{bmatrix} \frac{\partial H}{\partial p} \\ \frac{\partial H}{\partial u} \end{bmatrix}$$



- A Hamiltonian system has *symplectic* structure

$$\dot{\mathbf{y}}(t) = J\nabla H, \quad \mathbf{y}(0)$$

- Symplectic Euler method (here explicit 2^{nd} order method)

$$u_{n+1} = u_n + h\frac{\partial H}{\partial p}(u_{n+1}, p_n)$$
$$p_{n+1} = p_n - h\frac{\partial H}{\partial u}(u_{n+1}, p_n)$$

$$\begin{bmatrix} u \\ p \end{bmatrix}_{n+1} = \begin{bmatrix} 1 & h/m \\ -hc & 1 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix}_n$$

- Symplectic integrators preserve area in phase space

www.av8n.com/physics/symplectic-integrator.html

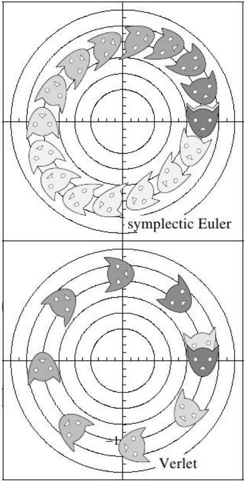
Stormer-Verlet method and the Symplectic Cat

- Stormer Verlet method

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2}\frac{\partial H}{\partial u}\left(p_{n+\frac{1}{2}}, u_n\right)$$

$$u_{n+1} = u_n + \frac{h}{2}\left[\frac{\partial H}{\partial p}\left(p_{n+\frac{1}{2}}, u_n\right) + \frac{\partial H}{\partial p}\left(p_{n+\frac{1}{2}}, u_{n+1}\right)\right]$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2}\frac{\partial H}{\partial u}\left(p_{n+\frac{1}{2}}, u_{n+1}\right)$$



- Rewrite equation 2, add equation 1 and 3 and rewrite

$$\frac{u_{n+1} - u_n}{h} = \frac{1}{2}\left[\frac{\partial H}{\partial p}\left(p_{n+\frac{1}{2}}, u_n\right) + \frac{\partial H}{\partial p}\left(p_{n+\frac{1}{2}}, u_{n+1}\right)\right]$$

$$\frac{p_{n+1} - p_n}{h} = -\frac{1}{2}\left[\frac{\partial H}{\partial u}\left(p_{n+\frac{1}{2}}, u_n\right) + \frac{\partial H}{\partial u}\left(p_{n+\frac{1}{2}}, u_{n+1}\right)\right]$$

- Stormer Verlet is equal to discretizing $m\ddot{u} = -cu$ with 2^{nd} order differences. Start with $\dot{u} = p/m$ and $\dot{p} = -cu$, subtract and divide by h

$$m\frac{u_{n+1} - u_n}{h} = p_{n+\frac{1}{2}} \qquad m\frac{u_n - u_{n-1}}{h} = p_{n-\frac{1}{2}}$$

$$m\frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} = \frac{p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}}}{h} = -cu_n$$

- Stormer Verlet is symmetric, time reversible, symplectic, 2^{nd} order, preserves energy almost (h=const)
  Position and momentum are discretized at staggered points

Geometric Numerical Integration, Ernst Hairer, 1999

Matlab code (only the loop, no graphic commands, etc)

```
j = 1;
for t=0:h:tend

    % unit circle
    plot(x,y,'k');

    % Euler explicit
    ue(:,end+1) = ue(:,end) + h*ve(:,end);
    ve(:,end+1) = ve(:,end) - h*ue(:,end-1);
    plot(ue,ve,'b','LineWidth',2)

    % Euler implicit, solve M y_n+i = y_n
    w(:,end+1) = M\w(:,end);
    ui = w(1,:);
    vi = w(2,:);
    plot(ui,vi,'g','LineWidth',2)

    % Symplectic Euler
    us(:,end+1) = us(:,end) + h*vs(:,end);
    vs(:,end+1) = vs(:,end) - h*us(:,end);
    plot(us,vs,'r','LineWidth',2)

    pause(.01)
    print(strcat("f",num2str(j),".jpg"),"-djpg","-S1600,800");
    j = j+1;
end
```

Harmonic Oscillator Integrated with Symplectic Euler

End

Thank You