A picture book of geometric numerical integration

Mats Vermeeren

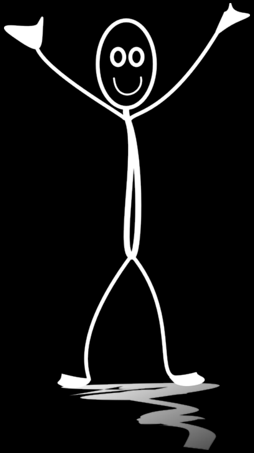
TU Berlin

Discretization in
Geometry and Dynamics
SFB Transregio 109

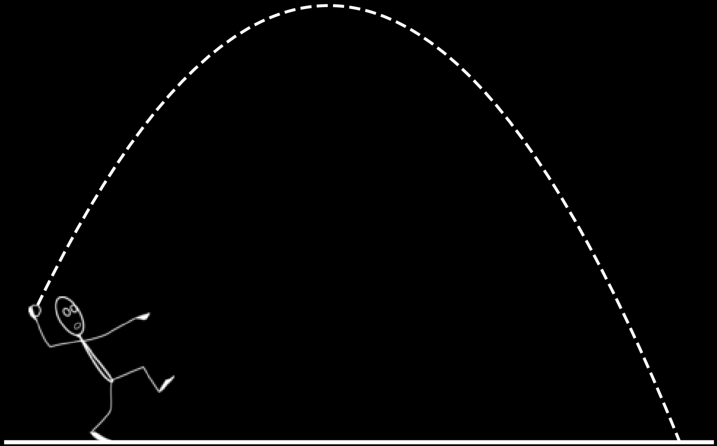
BMS Student Conference

17 February 2016

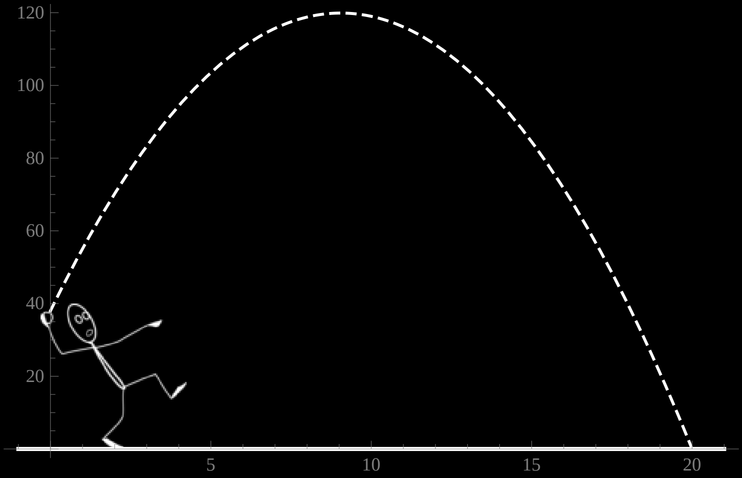
This is Bob



Bob likes to throw things

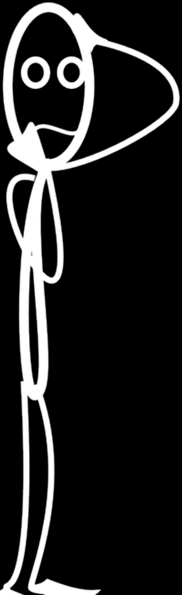


Bob would like to know the curve his projectiles describe



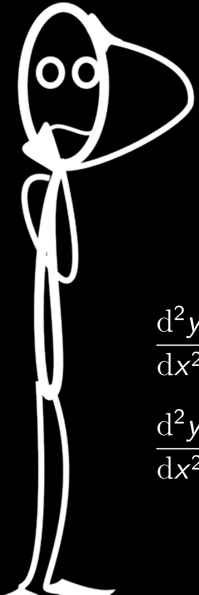
$$\ddot{y} = -g \qquad \Rightarrow \qquad \frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -\frac{g}{v^2}$$

Bob doesn't know how to solve differential equations



$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -G$$

Bob doesn't know how to solve differential equations

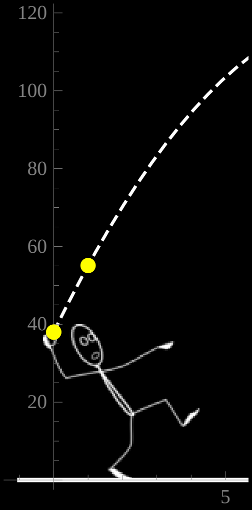


$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -G$$

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} \approx \frac{y(t+\varepsilon) - 2y(t) + y(t-\varepsilon)}{\varepsilon^2}$$

$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -G \quad \rightarrow \quad \frac{y_{k+1} - 2y_k + y_{k-1}}{\varepsilon^2} = -G$$

Now Bob can calculate!

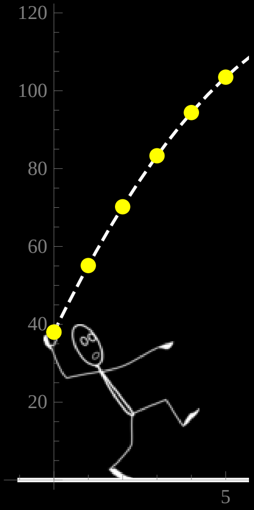


$$y_{k+1} = 2y_k - y_{k-1} - 2$$

Given two initial points, say

$$y_0 = 38 \qquad \text{and} \qquad y_1 = 55.1$$

Now Bob can calculate!



$$y_{k+1} = 2y_k - y_{k-1} - 2$$

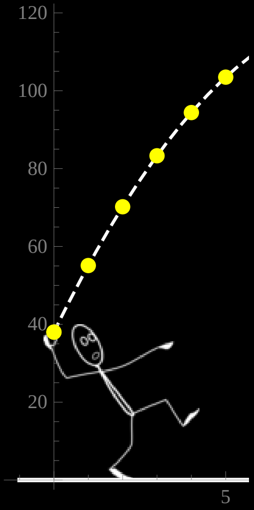
Given two initial points, say

$$y_0 = 38 \qquad \text{and} \qquad y_1 = 55.1$$

All the rest follow by simple calculations

$$y_2 = 2 \cdot 55.1 - 38 - 2 = 70.2$$

Now Bob can calculate!



$$y_{k+1} = 2y_k - y_{k-1} - 2$$

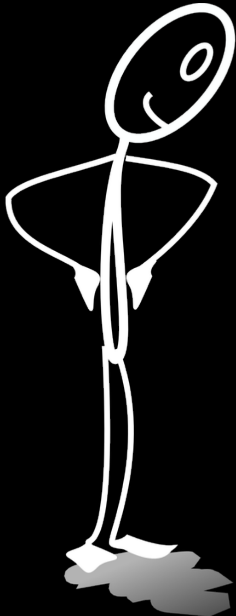
Given two initial points, say

$$y_0 = 38 \qquad \text{and} \qquad y_1 = 55.1$$

All the rest follow by simple calculations

$$y_2 = 2 \cdot 55.1 - 38 - 2 = 70.2$$
$$y_3 = 2 \cdot 70.2 - 55.1 - 2 = 83.3$$

Now Bob can calculate!



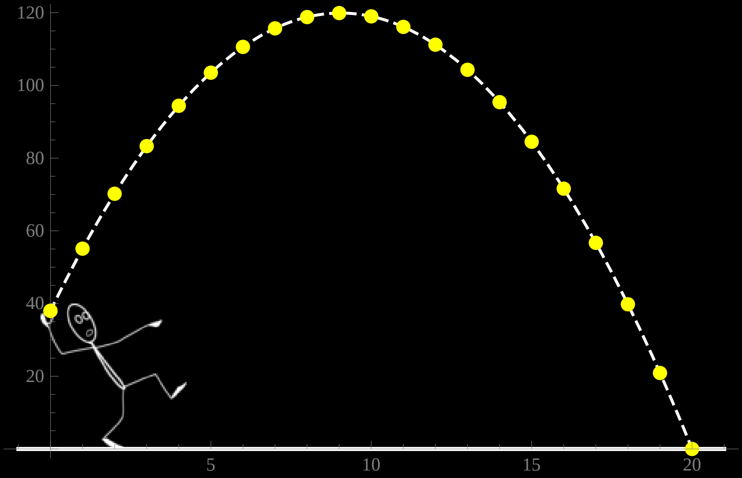
$$y_{k+1} = 2y_k - y_{k-1} - 2$$

Given two initial points, say

$$y_0 = 38 \qquad \text{and} \qquad y_1 = 55.1$$

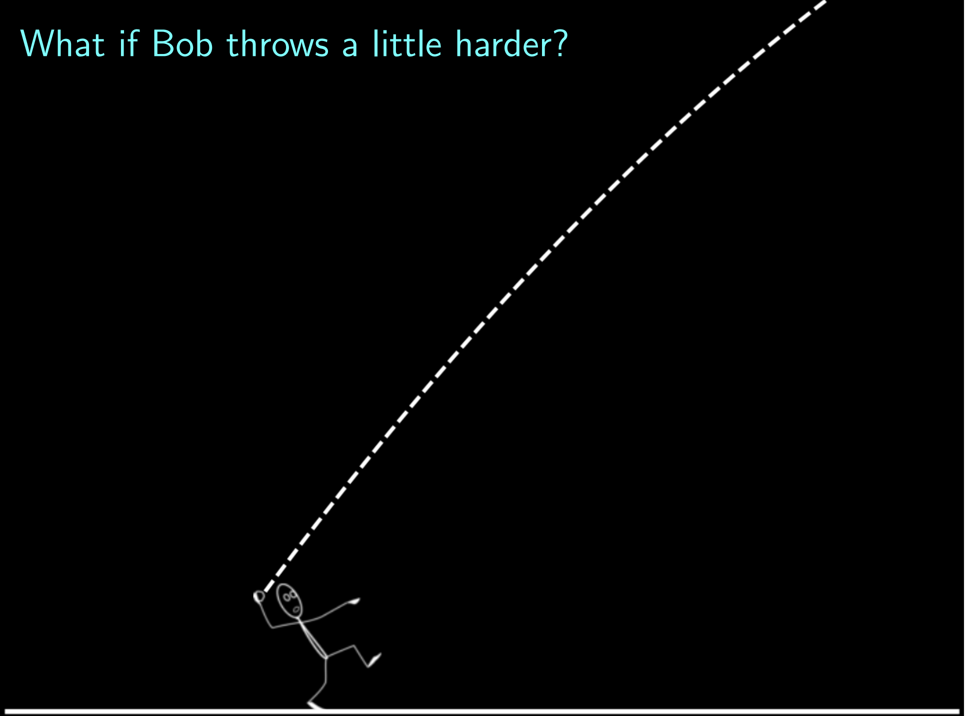
All the rest follow by simple calculations

$$y_2 = 2 \cdot 55.1 - 38 - 2 = 70.2$$
$$y_3 = 2 \cdot 70.2 - 55.1 - 2 = 83.3$$
$$y_4 = 2 \cdot 83.3 - 70.2 - 2 = 94.4$$
$$y_5 = 2 \cdot 94.4 - 83.3 - 2 = 103.5$$
$$y_6 = 2 \cdot 103.5 - 94.4 - 2 = 110.6$$
$$y_7 = 2 \cdot 110.6 - 103.5 - 2 = 115.7$$
$$y_8 = 2 \cdot 115.7 - 110.6 - 2 = 118.8$$
$$y_9 = 2 \cdot 118.8 - 115.7 - 2 = 119.9$$
$$y_{10} = 2 \cdot 119.9 - 118.8 - 2 = 119$$

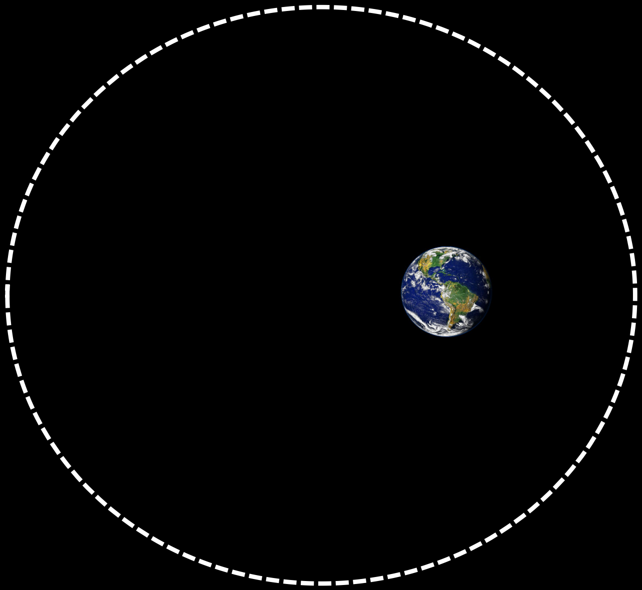


$$\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = -G \qquad \rightarrow \qquad \frac{y_{k+1} - 2y_k + y_{k-1}}{\varepsilon^2} = -G$$

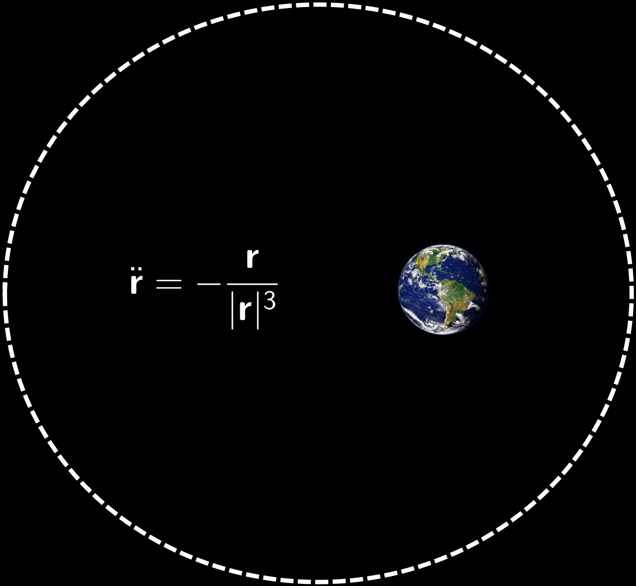
What if Bob throws a little harder?



Great throw, Bob!

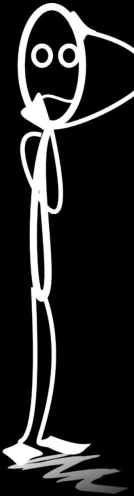


Great throw, Bob!



$$\ddot{\mathbf{r}} = -\frac{\mathbf{r}}{|\mathbf{r}|^3}$$

How to discretize $\ddot{r} = f(r)$?



$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k-1})$$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_k)$$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k+1})$$

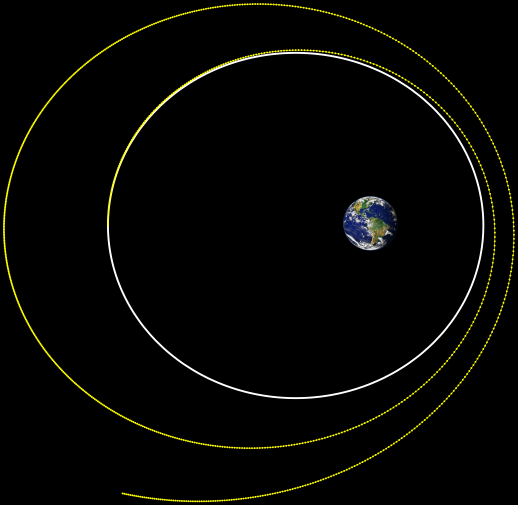
$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{1}{2} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{2} f\left(\frac{\mathbf{r}_k + \mathbf{r}_{k+1}}{2}\right)$$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{2}{3} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{3} f(\mathbf{r}_{k+1})$$

$$\begin{aligned}\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} &= (1-\alpha) f\left(\alpha \mathbf{r}_{k-1} + (1-\alpha)\mathbf{r}_k\right) \\ &\quad + \alpha f\left(\alpha \mathbf{r}_k + (1-\alpha)\mathbf{r}_{k+1}\right)\end{aligned}$$

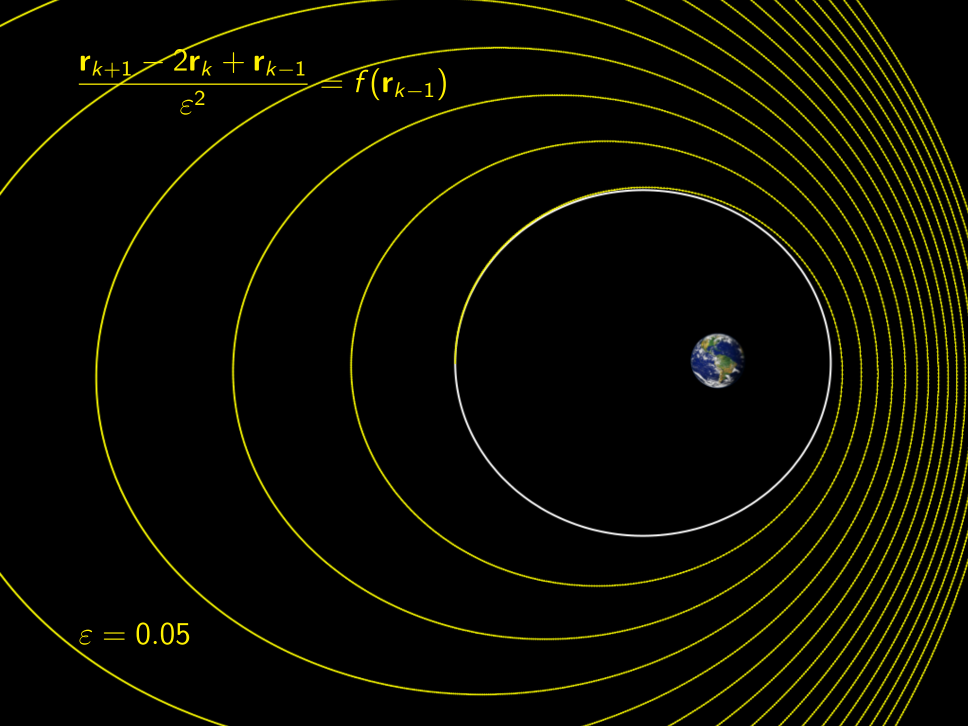
$$\vdots$$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k-1})$$



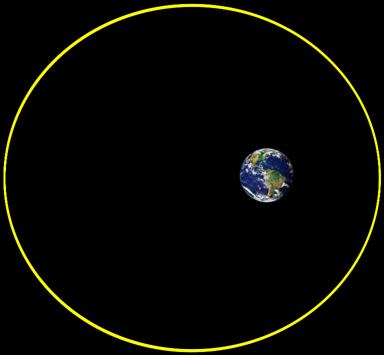
$\varepsilon = 0.05$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k-1})$$



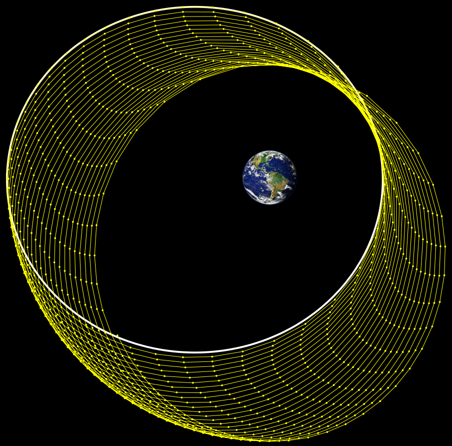
$\varepsilon = 0.05$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_k)$$



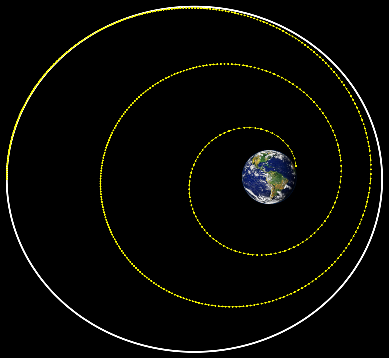
$\varepsilon = 0.05$

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_k)$$



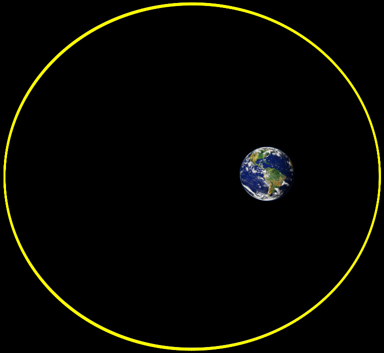
$\varepsilon = 0.5$
(large)

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k+1})$$



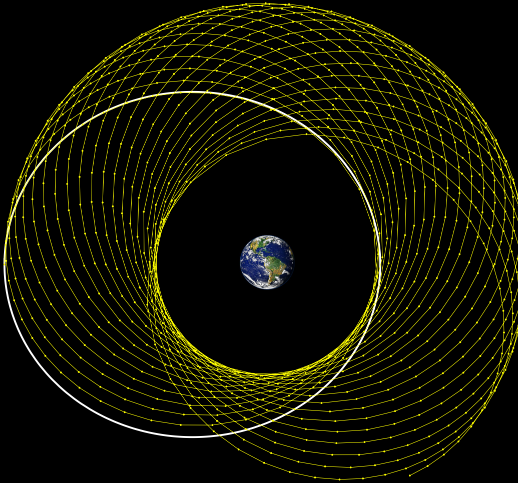
$\varepsilon = 0.05$
(small)

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{1}{2} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{2} f\left(\frac{\mathbf{r}_k + \mathbf{r}_{k+1}}{2}\right)$$



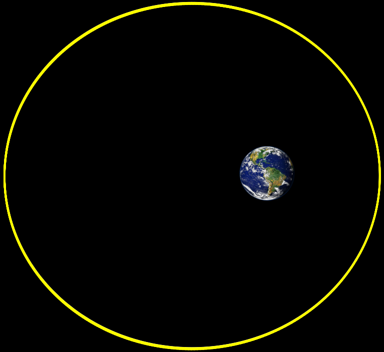
$\varepsilon = 0.05$
(small)

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{1}{2} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{2} f\left(\frac{\mathbf{r}_k + \mathbf{r}_{k+1}}{2}\right)$$



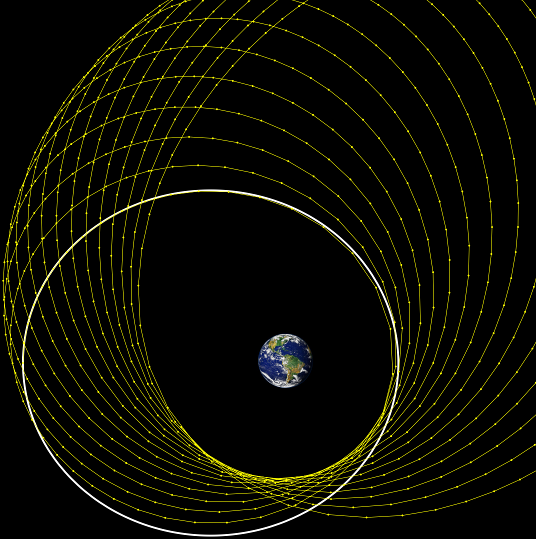
$\varepsilon = 0.5$
(large)

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2}$$
$$= \frac{2}{3} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right)$$
$$+ \frac{1}{3} f(\mathbf{r}_{k+1})$$



$\varepsilon = 0.05$
(small)

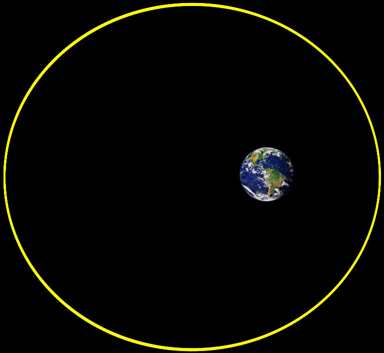
$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{2}{3} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{3} f(\mathbf{r}_{k+1})$$



$\varepsilon = 0.5$
(large)

$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2}$$
$$= (1-\alpha) f(\alpha \mathbf{r}_{k-1} + (1-\alpha)\mathbf{r}_k)$$
$$+ \alpha f(\alpha \mathbf{r}_k + (1-\alpha)\mathbf{r}_{k+1})$$

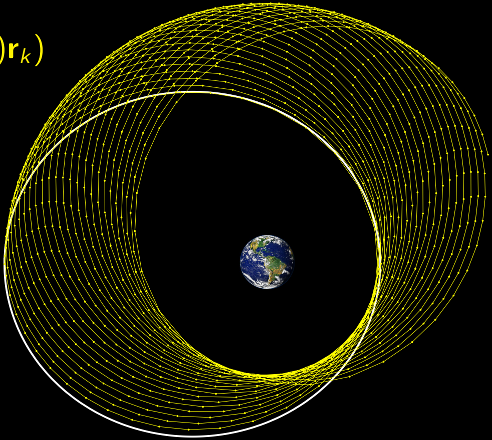
with $\alpha = \frac{1}{4}$



$\varepsilon = 0.05$
(small)

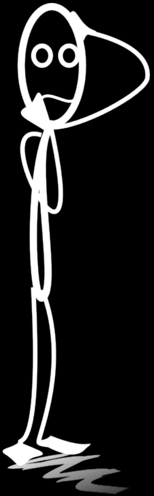
$$\frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2}$$
$$= (1-\alpha) f(\alpha \mathbf{r}_{k-1} + (1-\alpha)\mathbf{r}_k) + \alpha f(\alpha \mathbf{r}_k + (1-\alpha)\mathbf{r}_{k+1})$$

with $\alpha = \frac{1}{4}$



$\varepsilon = 0.5$
(large)

Why are some discretizations so much better than others?



$$\times \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k-1})$$

$$\checkmark \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_k)$$

$$\times \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = f(\mathbf{r}_{k+1})$$

$$\checkmark \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{1}{2} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{2} f\left(\frac{\mathbf{r}_k + \mathbf{r}_{k+1}}{2}\right)$$

$$\times \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = \frac{2}{3} f\left(\frac{\mathbf{r}_{k-1} + \mathbf{r}_k}{2}\right) + \frac{1}{3} f(\mathbf{r}_{k+1})$$

$$\checkmark \quad \frac{\mathbf{r}_{k+1} - 2\mathbf{r}_k + \mathbf{r}_{k-1}}{\varepsilon^2} = (1-\alpha) f\left(\alpha \mathbf{r}_{k-1} + (1-\alpha)\mathbf{r}_k\right) + \alpha f\left(\alpha \mathbf{r}_k + (1-\alpha)\mathbf{r}_{k+1}\right)$$

$$\vdots$$

Geometric numerical integration

Look for a discretization with the correct qualitative behavior:

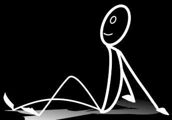
- conserved quantities
- geometry of the orbit
- ...

instead of optimizing the local error.

$\rightarrow$ Leads to better results for long-time simulations.

Tools:

- Hamiltonian/symplectic structure
- Lagrangian structure
- Reversibility
- ...



Geometric numerical integration

Look for a discretization with the correct qualitative behavior:

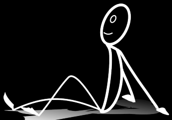
- conserved quantities
- geometry of the orbit
- ...

instead of optimizing the local error.

$\rightarrow$ Leads to better results for long-time simulations.

Tools:

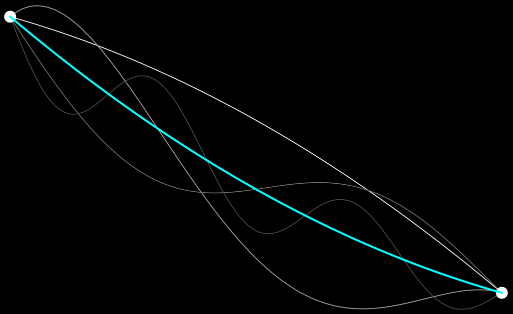
- Hamiltonian/symplectic structure
- Lagrangian structure
- Reversibility
- ...

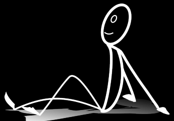


Lagrangian mechanics

Given a *Lagrange function* $\mathcal{L} : T\mathbb{R}^d \to \mathbb{R} : (y, \dot{y}) \to \mathcal{L}(y, \dot{y})$, find the curve $y : [a, b] \to \mathbb{R}^d$, with $y(a) = y_a$ and $y(b) = y_b$, that minimizes the *action*

$$\int_a^b \mathcal{L}(y(t), \dot{y}(t))\,\mathrm{d}t$$

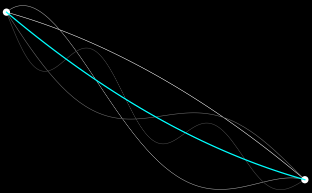




Lagrangian mechanics

A curve y is critical if for any infinitesimal variation δy

$$
\begin{aligned}
0 &= \delta \int_a^b \mathcal{L}(y(t), \dot{y}(t))\,\mathrm{d}t \\
&= \int_a^b \frac{\partial \mathcal{L}}{\partial y}\delta y + \frac{\partial \mathcal{L}}{\partial \dot{y}}\delta \dot{y}\,\mathrm{d}t \\
&= \int_a^b \left(\frac{\partial \mathcal{L}}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{y}}\right)\delta y\,\mathrm{d}t + \frac{\partial \mathcal{L}}{\partial \dot{y}}\delta y\Big|_a^b
\end{aligned}
$$

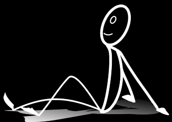


Fixed endpoints $\Rightarrow \delta y(a) = \delta y(b) = 0$, so y is critical if it satisfies the *Euler-Lagrange equations*

$$\frac{\partial \mathcal{L}}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{y}} = 0$$

In the case of mechanics:

$$\mathcal{L} = \text{kinetic energy} - \text{potential energy}$$



Energy and momentum

Lagrangian systems conserve the energy

$$E = \frac{\partial \mathcal{L}}{\partial \dot{y}} \dot{y} - \mathcal{L}.$$

Indeed

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{y}} \right) \dot{y} + \frac{\partial \mathcal{L}}{\partial \dot{y}} \ddot{y} - \frac{\partial \mathcal{L}}{\partial y} \dot{y} - \frac{\partial \mathcal{L}}{\partial \dot{y}} \ddot{y} = \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{y}} - \frac{\partial \mathcal{L}}{\partial y} \right) \dot{y} = 0$$

(In the case of mechanics: $\mathcal{L} =$ kinetic $+$ potential energy)

- If $\mathcal{L}$ is translation invariant, $\frac{\partial \mathcal{L}}{\partial y_i}$, then $\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{y}_i} = 0$ and the linear momentum $p_i = \frac{\partial \mathcal{L}}{\partial \dot{y}_i}$ is conserved.
- If $\mathcal{L}$ is rotation invariant, the angular momentum is conserved.
- ...

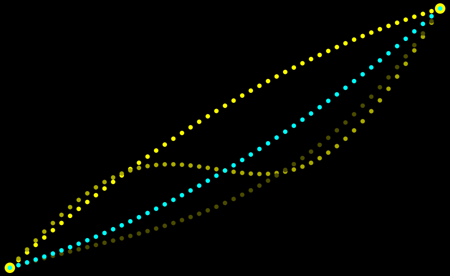
Discrete Lagrangian mechanics

Given a *discrete Lagrange function*

$$L : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} : \quad (y_{k-1}, y_k) \to L(y_{k-1}, y_k),$$

find the discrete curve $y : \{0, 1, \dots, N\} \to \mathbb{R}^d$, with $y(0) = y_0$ and $y(N) = y_N$, that minimizes the *action*

$$\sum_{k=1}^{N} L(y_{k-1}, y_k)$$



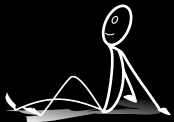
Discrete Lagrangian mechanics

We can vary each y_k individually, so y is critical if for each j

$$0 = \frac{\partial}{\partial y_j} \sum_{k=1}^{N} L(y_{k-1}, y_k) = \frac{\partial}{\partial y_j} L(y_{j-1}, y_j) + \frac{\partial}{\partial y_j} L(y_j, y_{j+1}).$$

Energy and momentum:

- Symmetries still give conserved quantities.
- No conservation of energy.



Variational integrators

Instead of discretizing the differential equation $\ddot{y} = -U'(y)$, discretize the Lagrangian $\mathcal{L} = \frac{1}{2}\dot{y}^2 - U(y)$. For example:

$$L(y_{k-1}, y_k) = \left|\frac{y_k - y_{k-1}}{\varepsilon}\right|^2 - \tfrac{1}{2}U(y_{k-1}) - \tfrac{1}{2}U(y_k)$$

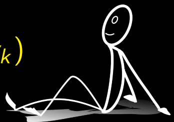
$$\rightarrow \quad \frac{y_{k+1} - 2y_k + y_{k-1}}{\varepsilon^2} = -U'(y_k)$$

$$L(y_{k-1}, y_k) = \left|\frac{y_k - y_{k-1}}{\varepsilon}\right|^2 - U\left(\frac{y_{k-1} + y_k}{2}\right)$$

$$\rightarrow \quad \frac{y_{k+1} - 2y_k + y_{k-1}}{\varepsilon^2} = -\frac{1}{2}U'\left(\frac{y_{k-1} + y_k}{2}\right) - \frac{1}{2}U'\left(\frac{y_k + y_{k+1}}{2}\right)$$

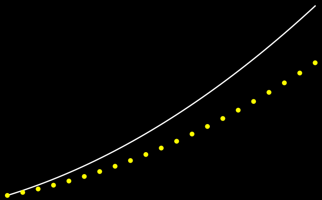
$$L(y_{k-1}, y_k) = \left|\frac{y_k - y_{k-1}}{\varepsilon}\right|^2 - U(\alpha y_{k-1} + (1-\alpha)y_k)$$

$$\rightarrow \quad \frac{y_{k+1} - 2y_k + y_{k-1}}{\varepsilon^2} = -(1-\alpha)U'(\alpha y_{k-1} + (1-\alpha)y_k) - \alpha U'(\alpha y_{k-1} + (1-\alpha)y_k)$$

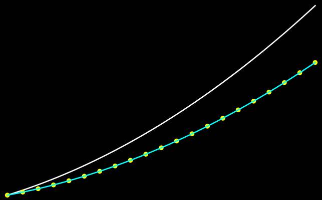


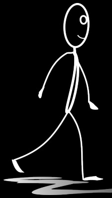
Modified Equations

Given a differential equation and a discretization,

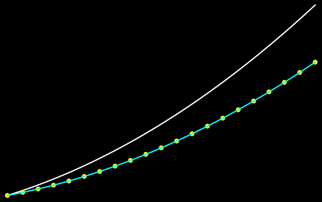


find a modified differential equation that interpolates solutions of the difference equation





Modified Equations



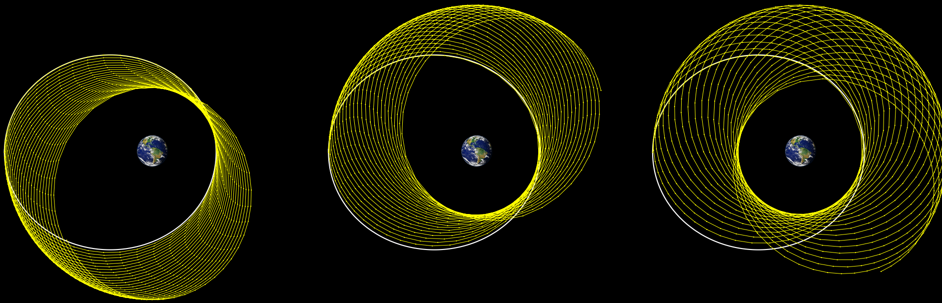
If we start with a Lagrangian system and use a variational integrator, then the modified equation is again Lagrangian:

$$\mathcal{L}_{\mathrm{mod}}(y, \dot{y}) = \mathcal{L}(y, \dot{y}) + \varepsilon \mathcal{L}_1(y, \dot{y}) + \varepsilon^2 \mathcal{L}_2(y, \dot{y}) + \dots$$

- This power series generally does not converge,
- but it explains why the error in energy stays very small over very long time intervals.

Variational integrators

- preserve momentum if the discretization respects the symmetries,
- almost preserve the energy over very long time intervals.

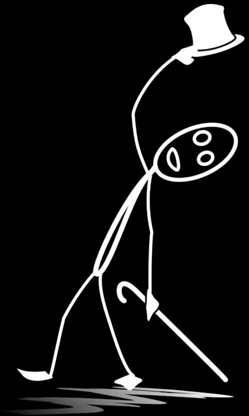


Further reading

[1] Hairer E, Lubich C, Wanner G. Geometric numerical integration: structure-preserving algorithms for ordinary differential equations. Springer, 2006.

[2] Marsden JE, West M. Discrete mechanics and variational integrators. Acta Numerica 10, 357–514, 2001.

Bob wants to thank you for your attention!



Drawings by OpenClipartVectors on `pixabay.com`