Modified Equations for Variational Integrators

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[4] V. Modified equations for variational integrators applied to Lagrangians linear in velocities. arXiv:1709.09567.

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Continuous Lagrangian Mechanics

Lagrange function: $L : \mathbb{R}^{2N} \cong TQ \to \mathbb{R} : (q, \dot{q}) \mapsto L(q, \dot{q})$.

Solutions are curves $q(t)$ that minimize (or are critical points of) the action

$$S = \int_{t_0}^{t_1} L(q(t), \dot{q}(t)) \,\mathrm{d}t$$

where the integration interval $[t_0, t_1]$ and the boundary values $q(t_0)$ and $q(t_1)$ are fixed.

$$\begin{aligned} 0 = \delta S &= \int_{t_0}^{t_1} \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q} \,\mathrm{d}t \\ &= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} \right) \delta q \,\mathrm{d}t + \left(\frac{\partial L}{\partial \dot{q}} \delta q \right) \Bigg|_{t_0}^{t_1} \end{aligned}$$

Euler-Lagrange Equation: $\dfrac{\partial L}{\partial q} - \dfrac{\mathrm{d}}{\mathrm{d}t}\dfrac{\partial L}{\partial \dot{q}} = 0.$

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Legendre transformation

Relates Hamiltonian and Lagrangian formalism:

$$p\dot{q} = H(q,p) + L(q,\dot{q}).$$

Differentiating w.r.t. $\dot{q}$, p and q,

$$\begin{aligned} p &= \frac{\partial L}{\partial \dot{q}} \\ \dot{q} &= \frac{\partial H}{\partial p} \\ 0 &= \frac{\partial H}{\partial q} + \frac{\partial L}{\partial q} \quad = \left(\frac{\partial H}{\partial q} + \dot{p} \right) + \left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}} \right), \end{aligned}$$

establishes equivalence between Lagrangian and Hamiltonian equations of motion.

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establishes equivalence between Lagrangian and Hamiltonian equations of motion.

Only works if the Lagrangian is nondegenerate: $\left| \frac{\partial^2 L}{\partial \dot{q}^2} \right| \neq 0$

Hamiltonian systems preserve the symplectic 2-form $\omega = \sum_i \mathrm{d}p_i \wedge \mathrm{d}q_i$.

Symplectic structure

Let Φ_t be the flow of a Hamiltonian system, i.e.

$$\Phi_0(q,p) = (q,p)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_t(q,p) = \left(\frac{\partial H}{\partial p}(\Phi_t(q,p)), -\frac{\partial H}{\partial q}(\Phi_t(q,p)) \right).$$

Then for each t, Φ_t is a symplectic map,

$$\Phi_t^* \omega = \omega,$$

where ω is the canonical symplectic form

$$\omega = \sum_i \mathrm{d}q_i \wedge \mathrm{d}p_i.$$

Definition

A symplectic integrator is a discretization (in time) of a Hamiltonian systems, such that each discrete time-step is given by a symplectic map.

Discrete Lagrangian mechanics

Lagrange function: $L : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R} : (x, \tilde{x}) \mapsto L(x, \tilde{x})$.

Solutions are discrete curves $x = (x_0, x_1, \ldots, x_n)$ that are critical points of the action

$$S_{\mathrm{disc}} = \sum_{j=1}^{n} h L_{\mathrm{disc}}(x_{j-1}, x_j)$$

Euler-Lagrange equation:

$$\mathrm{D}_2 L_{\mathrm{disc}}(x_{j-1}, x_j) + \mathrm{D}_1 L_{\mathrm{disc}}(x_j, x_{j+1}) = 0,$$

where D_1, D_2 denote the partial derivatives of L_{disc}.

Definition

A variational integrator for a continuous system with Lagrangian $\mathcal{L}$ is a discrete Lagrangian system with

$$L_{\mathrm{disc}}\big(x(t-h), x(t)\big) \approx \mathcal{L}(x(t), \dot{x}(t)),$$

and hence $S_{\mathrm{disc}} \approx S$.

Equivalence

Theorem

If the Lagrangian/Hamiltonian is regular, variational and symplectic integrators are equivalent.

Proof. The discrete Lagrangian is a generation function of the symplectic map describing one time step,

$$\begin{aligned} p_j &= -h\mathrm{D}_1 L_{\mathrm{disc}}(x_j, x_{j+1}) \\ p_{j+1} &= h\mathrm{D}_2 L_{\mathrm{disc}}(x_j, x_{j+1}) \end{aligned}$$

∎

Example: Störmer-Verlet method

Consider a mechanical system $\ddot{x} = -U'(x)$ with Lagrangian

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2} \langle \dot{x} , \dot{x} \rangle - U(x)$$

The Störmer-Verlet discretization is given by the discrete Lagrangian

$$L_{\mathrm{disc}}(x_j, x_{j+1}) = \frac{1}{2} \left\langle \frac{x_{j+1} - x_j}{h} , \frac{x_{j+1} - x_j}{h} \right\rangle - \frac{1}{2} U\left(x_j\right) - \frac{1}{2} U\left(x_{j+1}\right)$$

Its discrete Euler-Lagrange equation is $\dfrac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j)$

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Its discrete Euler-Lagrange equation is $\dfrac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j)$

Abstract notation: $\psi(x_{j-1}, x_j, x_{j+1}; h) = 0$ with

$$\psi(x_{j-1}, x_j, x_{j+1}; h) = \frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} + U'(x_j)$$

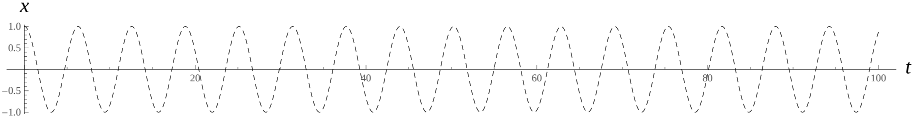
Symplectic equivalent:

$$x_{j+1} = x_j + hp_j - \frac{h^2}{2} U'(x_j)$$

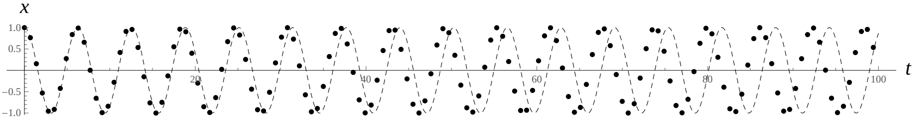
$$p_{j+1} = p_j - \frac{h}{2} U'(x_j) - \frac{h}{2} U'(x_{j+1})$$

Modified Equations

Exact solution of a differential equation:



Numerical solution with a variational integrator:



Notice conservation of Energy:

- Easy to prove for (continuous) Hamiltonian systems
- Follows by Noether's theorem from invariance under time-translation of the Lagrangian
- Symplectic/variational integrators very nearly preserve energy. Why?

Modified Equations

Conservation of Energy:

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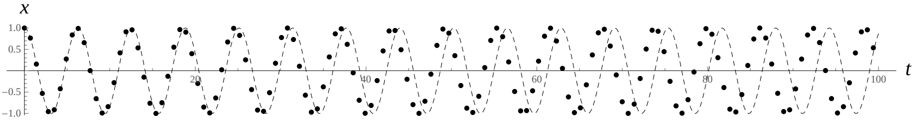
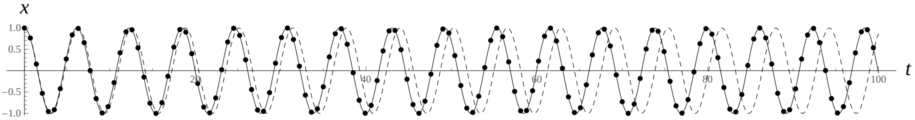


Idea of proof: find a modified equation, a differential equation with solutions that interpolate the numerical solutions:



Modified Equations

Modified equations are usually given by power series.
Often they do not converge.

Definition

The differential equation $\ddot{x} = f(x, \dot{x}; h)$*, where*

$$f(x, \dot{x}; h) \simeq f_0(x, \dot{x}) + hf_1(x, \dot{x}) + h^2 f_2(x, \dot{x}) + \ldots$$

is a modified equation for the second order difference equation $\Psi(x_{j-1}, x_j, x_{j+1}; h) = 0$ *if, for every* k*, every solution of the truncated differential equation*

$$\begin{aligned} \ddot{x} &= \mathcal{T}_k\big(f_h(x, \dot{x})\big) \\ &= f_0(x, \dot{x}) + hf_1(x, \dot{x}) + h^2 f_2(x, \dot{x}) + \ldots + h^k f_k(x, \dot{x}). \end{aligned}$$

satisfies

$$\Psi\big(x(t-h), x(t), x(t+h); h\big) = \mathcal{O}\big(h^{k+1}\big).$$

Modified Equations for symplectic integrators

Symplectic integrators are known the very nearly preserve energy, because

Theorem

The modified equation for a symplectic integrator is a Hamiltonian equation.

Can we arrive at a similar result purely on the Lagrangian side?

Are modified equations for variational integrators Lagrangian?

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General idea

Look for a modified Lagrangian $\mathcal{L}_{\mathrm{mod}}(x, \dot{x})$ such that the discrete Lagrangian L_{disc} is its exact discrete Lagrangian, i.e.

$$\int_{(j-1)h}^{jh} \mathcal{L}_{\mathrm{mod}}(x(t), \dot{x}(t)) \mathrm{d}t = h L_{\mathrm{disc}}\big(x((j-1)h), x(jh)\big).$$

The Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod}}$ will then be the modified equation.

The best we can hope for is to find such a modified Lagrangian up to an error of arbitrarily high order in h.

The discrete Lagrangian evaluated on a continuous curve

We can write the discrete Lagrangian as a function of x and its derivatives, all evaluated at the point $jh - \frac{h}{2}$,

$$\begin{aligned}\mathcal{L}_{\mathrm{disc}}[x] &= L_{\mathrm{disc}}\bigg(x - \frac{h}{2}\dot{x} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \ddot{x} - \ldots, \\ &\qquad\qquad x + \frac{h}{2}\dot{x} + \frac{1}{2}\left(\frac{h}{2}\right)^2 \ddot{x} + \ldots, \quad h \bigg). \\ &= L_{\mathrm{disc}}(x_{j-1}, x_j; h)\end{aligned}$$

Here and in the following:

- $[x]$ denotes dependence on x and any number of its derivatives,
- we evaluate at $t = jh - \frac{h}{2}$ whenever we omit the variable t, i.e. $x = x\left(jh - \frac{h}{2}\right)$,
- $x_j = x(jh)$ and $x_{j-1} = x((j-1)h)$.

A truly continuous Lagrangian

We want to write the discrete action

$$S_{\mathrm{disc}} = \sum_{j=1}^{n} h L_{\mathrm{disc}}(x_{j-1}, x_j) = \sum_{j=1}^{n} h \mathcal{L}_{\mathrm{disc}}\left[x\left(jh - \tfrac{h}{2}\right)\right]$$

as an integral.

Lemma (Euler-MacLaurin formula)

For any smooth function $f : \mathbb{R} \to \mathbb{R}^N$ we have

$$\begin{aligned}\sum_{j=1}^{n} hf\left(jh - \frac{h}{2}\right) &\simeq \int_0^{nh} \sum_{i=0}^{\infty} h^{2i}\left(2^{1-2i} - 1\right)\frac{B_{2i}}{(2i)!} f^{(2i)}(t)\,\mathrm{d}t \\ &= \int_0^{nh}\left(f(t) - \frac{h^2}{24}\ddot{f}(t) + \frac{7h^4}{5760} f^{(4)}(t) + \dots\right)\mathrm{d}t,\end{aligned}$$

where B_i are the Bernoulli numbers.

The symbol $\simeq$ indicates that this is an asymptotic series.

A truly continuous Lagrangian

Definition

We call

$$\mathcal{L}_{\mathrm{mesh}}[x(t)] = \mathcal{L}_{\mathrm{disc}}[x(t)] + \sum_{i=1}^{\infty} \left(2^{1-2i} - 1\right) \frac{h^{2i} B_{2i}}{(2i)!} \frac{\mathrm{d}^{2i}}{\mathrm{d}t^{2i}} \mathcal{L}_{\mathrm{disc}}[x(t)]$$
$$= \mathcal{L}_{\mathrm{disc}}[x(t)] - \frac{h^2}{24} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \mathcal{L}_{\mathrm{disc}}[x(t)] + \frac{7h^4}{5760} \frac{\mathrm{d}^4}{\mathrm{d}t^4} \mathcal{L}_{\mathrm{disc}}[x(t)] + \dots$$

the meshed modified Lagrangian of L_{disc}.

Formally, the meshed modified Lagrangian satisfies

$$\int \mathcal{L}_{\mathrm{mesh}}[x(t)] \,\mathrm{d}t = \sum h L_{\mathrm{disc}}(x_j, x_{j+1})$$

where $x_j = x(jh)$.

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where $x_j = x(jh)$.

Are we finished?

$\mathcal{L}_{\mathrm{mesh}}[x]$ depends on many more derivatives than the original $\mathcal{L}(x, \dot{x})$.

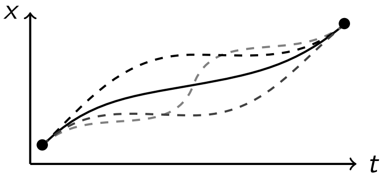
The meshed variational problem

Definition

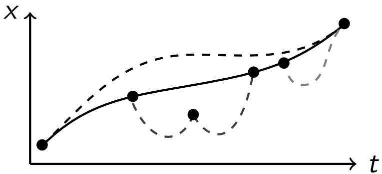
classical variational problem: find critical curves of some action $\int_a^b \mathcal{L}[x(t)]\,\mathrm{d}t$ *in the set of smooth curves* $\mathcal{C}^\infty$.

meshed variational problem: find critical curves of some action $\int_a^b \mathcal{L}[x(t)]\,\mathrm{d}t$ *in the set of piecewise smooth curves that are consistent with a mesh of size* h,

$$\mathcal{C}^{\mathcal{M},h} = \{x \in \mathcal{C}^0([a,b]) \mid \exists t_0 \in [a,b] : \forall t \in [a,b] : \\ x \text{ not smooth at } t \Rightarrow t - t_0 \in h\mathbb{N}\}.$$



Classical variational problem



Meshed variational problem

The meshed variational problem

Criticality conditions of a meshed variational problem:

Euler-Lagrange equations: $\dfrac{\delta \mathcal{L}}{\delta x} = 0,$

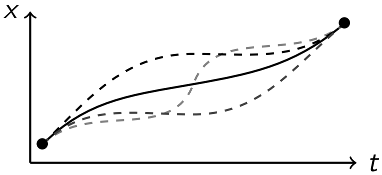
Natural interior conditions: $\forall j \geq 2 : \dfrac{\delta \mathcal{L}}{\delta x^{(j)}} = 0,$

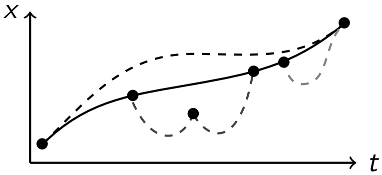
or equivalently: $\forall j \geq 2 : \dfrac{\partial \mathcal{L}}{\partial x^{(j)}} = 0,$

where

$$\frac{\delta \mathcal{L}}{\delta x^{(j)}} = \sum_{k=0}^{\infty} (-1)^k \frac{\mathrm{d}^k}{\mathrm{d}t^k} \frac{\partial \mathcal{L}}{\partial x^{(j+k)}}.$$

If $\mathcal{L}$ is a non-convergent power series, these equations are formal.





Exploiting the natural interior conditions

$$S_{\mathrm{disc}}(x(0), x(h), \ldots) = \int \mathcal{L}_{\mathrm{mesh}}([x], h) \,\mathrm{d}t,$$

hence

$$S_{\mathrm{disc}} \text{ critical } \Leftrightarrow \frac{\delta \mathcal{L}_{\mathrm{mesh}}}{\delta x} = 0.$$

Variations that are supported on a single mesh interval

- do not change the discrete action

  $\Rightarrow$ do not change $\displaystyle\int \mathcal{L}_{\mathrm{mesh}}([x], h) \,\mathrm{d}t.$
- are the variations that produce natural interior conditions

It follows that for $\mathcal{L}_{\mathrm{mesh}}$ the NIC are automatically satisfied:

$$\frac{\delta \mathcal{L}_{\mathrm{mesh}}}{\delta x} = 0 \qquad \Rightarrow \qquad \forall j \geq 2 : \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x^{(j)}} = 0$$

Definition

The modified Lagrangian is the formal power series

$$\mathcal{L}_{\mathrm{mod}}(x, \dot{x}) = \mathcal{L}_{\mathrm{mesh}}[x]\Big|_{\ddot{x}=f_h(x,\dot{x}),\ x^{(3)}=\frac{\mathrm{d}}{\mathrm{d}t}f_h(x,\dot{x}),\ \dots},$$

where $\ddot{x} = f_h(x, \dot{x})$ is the modified equation.

The k-th truncation of the modified Lagrangian is

$$\mathcal{L}_{\mathrm{mod},k} = \mathcal{T}_k\left(\mathcal{L}_{\mathrm{mod}}(x, \dot{x})\right) = \mathcal{T}_k\left(\mathcal{L}_{\mathrm{mesh}}[x]\Big|_{x^{(j)}=F^j_{k-2}(x,\dot{x})}\right),$$

where $\mathcal{T}_k$ denotes truncation after the h^k-term and

$$\ddot{x} = F_k^2(x, \dot{x}; h) + \mathcal{O}(h^{k+1}) = F_k(x, \dot{x}; h) + \mathcal{O}(h^{k+1}),$$
$$x^{(3)} = F_k^3(x, \dot{x}; h) + \mathcal{O}(h^{k+1}), \quad x^{(4)} = F_k^4(x, \dot{x}; h) + \mathcal{O}(h^{k+1}), \ \dots.$$

are the k-th truncation of the modified equation and its derivatives.

Lemma

The meshed modified Lagrangian $\mathcal{L}_{\mathrm{mesh}}[x]$ and the modified Lagrangian $\mathcal{L}_{\mathrm{mod}}(x,\dot{x})$ have the same critical curves.

Proof.

$$\frac{\partial \mathcal{L}_{\mathrm{mod},k}}{\partial x} = \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x} + \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial \ddot{x}} \frac{\partial F_k^2}{\partial x} + \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x^{(3)}} \frac{\partial F_k}{\partial x} + \dots \bigg|_{x^{(j)} = F_{k-1}^j(x,\dot{x})}$$

$$= \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x} + \mathcal{O}(h^{k+1}),$$

Also,

$$\frac{\partial \mathcal{L}_{\mathrm{mod},k}}{\partial \dot{x}} = \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial \dot{x}} + \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial \ddot{x}} \frac{\partial F_k^2}{\partial \dot{x}} + \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x^{(3)}} \frac{\partial F_k^3}{\partial \dot{x}} + \dots \bigg|_{x^{(j)} = F_{k-1}^j(x,\dot{x})}$$

$$= \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial \dot{x}} + \mathcal{O}(h^{k+1}),$$

$$\Rightarrow \frac{\partial \mathcal{L}_{\mathrm{mod},k}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}_{\mathrm{mod},k}}{\partial \dot{x}} = \sum_{j=0}^{\infty} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}t^j} \frac{\partial \mathcal{L}_{\mathrm{mesh}}}{\partial x^{(j)}} + \mathcal{O}(h^{k+1}). \qquad \blacksquare$$

Main result

Theorem

For a discrete Lagrangian L_{disc} that is a consistent discretization of some $\mathcal{L}$, the k-th truncation of the Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod},k}(x,\dot{x})$ is the k-th truncation of the modified equation.

Proof. Let x be a solution of the Euler-Lagrange equation for $\mathcal{L}_{\mathrm{mod}}(x,\dot{x})$. Consider the discrete curve $x_j = x(jh)$.

- x is critical for the action $\int \mathcal{L}_{\mathrm{mod}}(x,\dot{x})\,\mathrm{d}t$.
- By the Lemma, x is critical for the action $\int \mathcal{L}_{\mathrm{mesh}}[x]\,\mathrm{d}t$.
- By construction, the actions $S_{\mathrm{disc}} = \sum_j L_{\mathrm{disc}}(y(jh), y((j+1)h))$ and $S = \int_a^b \mathcal{L}_{\mathrm{mod}}[y(t)]\,\mathrm{d}t$ are equal for any smooth curve y.
- Therefore the discrete curve $(x(jh))_j$ is critical for the discrete action S_{disc}. Hence

$$\mathrm{D}_2 L_{\mathrm{disc}}(x(t-h), x(t)) + \mathrm{D}_1 L_{\mathrm{disc}}(x(t), x(t+h)) = 0. \qquad \blacksquare$$

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Example: Störmer-Verlet discretization

$$\mathcal{L}(x, \dot{x}) = \frac{1}{2}|\dot{x}|^2 - U(x),$$
$$L_{\mathrm{disc}}(x_j, x_{j+1}) = \frac{1}{2}\left|\frac{x_{j+1} - x_j}{h}\right|^2 - \frac{1}{2}U\left(x_j\right) - \frac{1}{2}U\left(x_{j+1}\right).$$

Its Euler-Lagrange equation is

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j).$$

We have

$$\begin{aligned}\mathcal{L}_{\mathrm{disc}}[x] &= \left\langle \dot{x} + \tfrac{h^2}{24}x^{(3)} + \dots, \dot{x} + \tfrac{h^2}{24}x^{(3)} + \dots \right\rangle \\ &\quad - \tfrac{1}{2}U\left(x - \tfrac{h}{2}\dot{x} + \tfrac{1}{2}\left(\tfrac{h}{2}\right)^2\ddot{x} - \dots\right) - \tfrac{1}{2}U\left(x + \tfrac{h}{2}\dot{x} + \tfrac{1}{2}\left(\tfrac{h}{2}\right)^2\ddot{x} + \dots\right) \\ &= \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\Big(\left\langle \dot{x}, x^{(3)}\right\rangle - 3U'\ddot{x} - 3U''(\dot{x},\dot{x})\Big) + \mathcal{O}(h^4)\end{aligned}$$

Example: Störmer-Verlet discretization

$$\mathcal{L}_{\mathrm{disc}}[x] = \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\left(\left\langle \dot{x} \,, x^{(3)} \right\rangle - 3U'\ddot{x} - 3U''(\dot{x},\dot{x}) \right) + \mathcal{O}(h^4),$$

From this we calculate the meshed modified Lagrangian,

$$\begin{aligned}
\mathcal{L}_{\mathrm{mesh}}[x] &= \mathcal{L}_{\mathrm{disc}}[x] - \frac{h^2}{24}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{L}_{\mathrm{disc}}[x] + \mathcal{O}(h^4) \\
&= \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\left(\left\langle \dot{x} \,, x^{(3)} \right\rangle - 3U'\ddot{x} - 3U''(\dot{x},\dot{x}) \right) \\
&\qquad - \frac{h^2}{24}\left(\left\langle \ddot{x} \,, \ddot{x} \right\rangle + \left\langle \dot{x} \,, x^{(3)} \right\rangle - U'\ddot{x} - U''(\dot{x},\dot{x}) \right) + \mathcal{O}(h^4) \\
&= \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\left(- \left\langle \ddot{x} \,, \ddot{x} \right\rangle - 2U'\ddot{x} - 2U''(\dot{x},\dot{x}) \right) + \mathcal{O}(h^4).
\end{aligned}$$

Eliminate second derivatives using $\ddot{x} = -U' + \mathcal{O}(h^2)$,

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\left(|U'|^2 - 2U''(\dot{x},\dot{x}) \right).$$

Example: Störmer-Verlet discretization

The modified Lagrangian is

$$\mathcal{L}_{\mathrm{mod},3}(x,\dot{x}) = \frac{1}{2}\langle \dot{x}\,,\dot{x}\rangle - U + \frac{h^2}{24}\left(|U'|^2 - 2U''(\dot{x},\dot{x})\right).$$

Observe that this Lagrangian is not separable for general U.

The corresponding Euler-Lagrange equation is

$$-\ddot{x} - U' + \frac{h^2}{24}\left(2U''U' - 2U'''(\dot{x},\dot{x}) + 4U'''(\dot{x},\dot{x}) + 4U''\ddot{x}\right) = 0.$$

Solving this for $\ddot{x}$ we find the modified equation

$$\ddot{x} = -U' + \frac{h^2}{12}\left(U'''(\dot{x},\dot{x}) - U''U'\right) + \mathcal{O}(h^4).$$

The Kepler problem

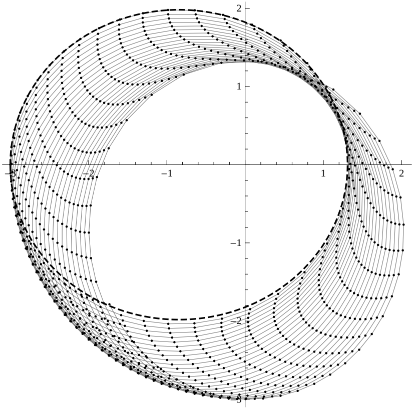
Potential: $U(x) = -\frac{1}{|x|}$.

Lagrangian: $\mathcal{L} = \frac{1}{2}\langle \dot{x}\,,\dot{x}\rangle + \frac{1}{|x|}$.

Equation of motion $\ddot{x} = -\frac{x}{|x|^3}$.

Störmer-Verlet discretization:

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j).$$



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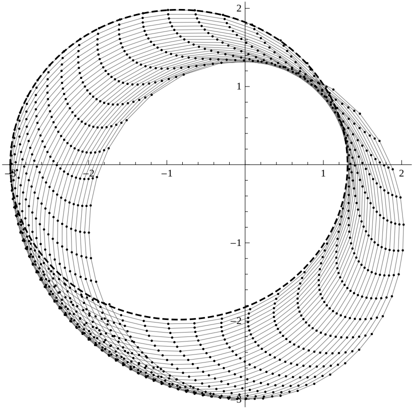


Störmer-Verlet discretization:

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -U'(x_j).$$

Midpoint discretization:

$$\frac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = -\frac{1}{2}U'\left(\frac{x_{j-1} + x_j}{2}\right) - \frac{1}{2}U'\left(\frac{x_j + x_{j+1}}{2}\right).$$

Störmer-Verlet discretization of the Kepler problem

The modified Lagrangian of the Störmer-Verlet discretization is

$$\mathcal{L}_{\mathrm{mod},3}(x, \dot{x}) = \frac{1}{2}|\dot{x}|^2 - U + \frac{h^2}{24}\left(U'U' - 2U''(\dot{x}, \dot{x})\right).$$

For the Kepler problem we have $U(x) = -\frac{1}{|x|}$, hence

$$\mathcal{L}_{\mathrm{mod},3}\big(x, \dot{x}\big) = \frac{1}{2}|\dot{x}|^2 + \frac{1}{|x|} + \frac{h^2}{24}\left(\frac{1}{|x|^4} - 2\frac{\big\langle \dot{x}, \dot{x}\big\rangle}{|x|^3} + 6\frac{\big\langle x, \dot{x}\big\rangle^2}{|x|^5}\right).$$

Laplace-Runge-Lenz vector

The shape and orientation of an orbit for the kepler Problem is determined by the Laplace-Runge-Lenz vector, which is the Noether integral for a generalized variational symmetry.

For the modified Lagrangian this is only an approximate symmetry.

Lemma (From a perturbative version of Noether's theorem)

The precession rate for the perturbed Lagrangian

$$\mathcal{L} = \frac{1}{2}\langle \dot{x}\,, \dot{x} \rangle + \frac{1}{|x|} + \Delta U(x, \dot{x}),$$

is in first order approximation

$$2\pi a^2 \frac{\partial \langle \Delta U(x, \dot{x}) \rangle}{\partial b}$$

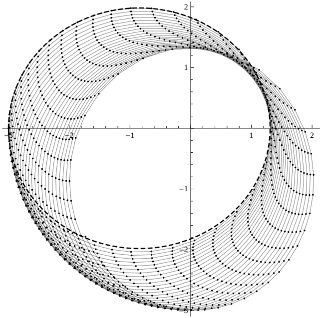
radians per period, where a and b are the semimajor and seminor axes, and $\langle \cdot \rangle$ denotes the time-average along the unperturbed orbit.

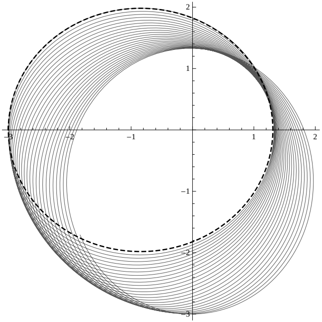
Störmer-Verlet discretization of the Kepler problem

Proposition

The numerical precession rate of the Störmer-Verlet method is

$$\frac{\pi}{24}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right)h^2 + \mathcal{O}(h^4)$$





Predicted: 0.0673 rad per revolution.

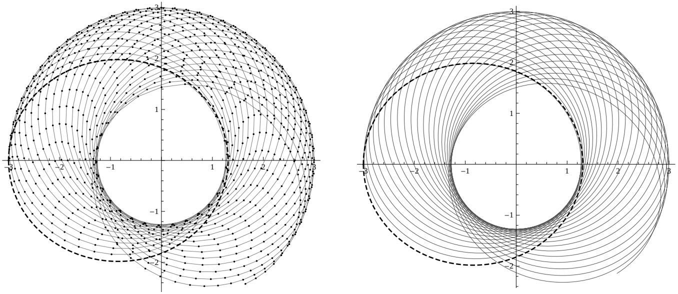
Measured: 0.0659 rad per revolution.

Midpoint discretization of the Kepler problem

Proposition

The numerical precession rate of the midpoint rule is

$$-\frac{\pi}{12}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right)h^2 + \mathcal{O}(h^4)$$



Predicted: -0.134 rad per revolution.

Measured: -0.152 rad per revolution.

New methods

Precession rate Störmer-Verlet: $\frac{\pi}{24}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right)h^2 + \mathcal{O}(h^4)$

Precession rate Midpoint rule: $-\frac{\pi}{12}\left(15\frac{a^3}{b^6} - 3\frac{a}{b^4}\right)h^2 + \mathcal{O}(h^4)$

This allows us to construct new integrators with precession of order h^4.

Mixed Lagrangian $L(x_j, x_{j+1}) = \frac{2}{3}L_{SV}(x_j, x_{j+1}) + \frac{1}{3}L_{MP}(x_j, x_{j+1})$

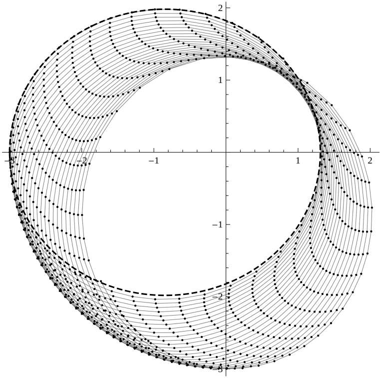
Lagrangian composition $L_j(x_k, x_{k+1}) = \begin{cases} L_{MP}(x_k, x_{k+1}) & \text{if } 3|j, \\ L_{SV}(x_k, x_{k+1}) & \text{otherwise.} \end{cases}$

Composition of difference equations

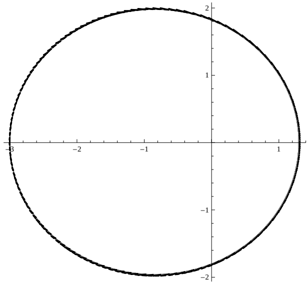
$$\begin{cases} x_{j+1} - 2x_j + x_{j-1} = -\frac{h^2}{2}U'\left(\frac{x_{j-1}+x_j}{2}\right) - \frac{h^2}{2}U'\left(\frac{x_j+x_{j+1}}{2}\right) & \text{if } j \equiv 2 \bmod 3, \\ x_{j+1} - 2x_j + x_{j-1} = -h^2 U'(x_j) & \text{otherwise.} \end{cases}$$

Is this a variational integrator?

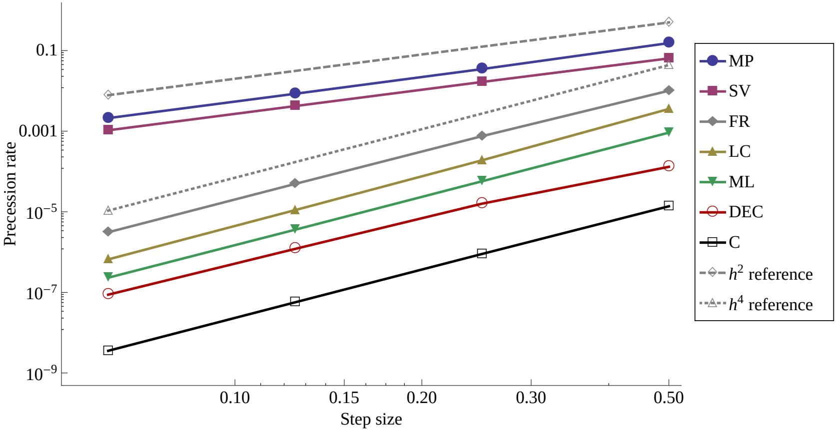
Qualitative analysis of new methods



$\rightarrow$



Precession rates



MP,SV: old methods LC, ML, DEC: new methods

FR: Forest, Ruth. Fourth-order symplectic integration, 1989.

C: Chin. Symplectic integrators from composite operator factorizations, 1997.

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[1] Hairer, Lubich, Wanner. Geometric Numerical Integration. Springer, 2006.

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[4] V. Modified equations for variational integrators applied to Lagrangians linear in velocities. arXiv:1709.09567.

[5] Work in progress with Alessandro Bravetti and Marcello Seri.

[6] V. Continuum limits of Pluri-Lagrangian systems. arXiv:1706.06830

Lagrangians linear in velocities

$\mathcal{L} : T\mathbb{R}^N \cong \mathbb{R}^{2N} \to \mathbb{R}$ of the form

$$\mathcal{L}(q, \dot{q}) = \langle \alpha(q) \, , \dot{q} \rangle - H(q),$$

where $\alpha : \mathbb{R}^N \to \mathbb{R}^N$, $H : \mathbb{R}^N \to \mathbb{R}$, and the brackets $\langle \, , \rangle$ denote the standard scalar product.

Let

$$A(q) = \alpha'(q) = \left(\frac{\partial \alpha_i(q)}{\partial q_j} \right)_{i,j=1,\dots,N} \qquad \text{and} \qquad A_{\mathrm{skew}}(q) = A(q)^T - A(q)$$

We assume that $A_{\mathrm{skew}}(q)$ is invertible, then the Euler-Lagrange equation for $\mathcal{L}$ is given by

$$\dot{q} = A_{\mathrm{skew}}(q)^{-1} H'(q)^T$$

Examples of Lagrangians linear in velocities

- Dynamics of point vortices in the (complex) plane

$$\mathcal{L}(z, \overline{z}, \dot{z}, \dot{\overline{z}}) = \sum_{j=1}^{N} \Gamma_j \operatorname{Im}(\overline{z}_j \dot{z}_j) - \frac{1}{\pi} \sum_{j=1}^{N} \sum_{k=1}^{j-1} \Gamma_j \Gamma_k \log \left| z_j - z_k \right|,$$

$$\hookrightarrow \quad \dot{z}_j = \frac{i}{2\pi} \sum_{k \neq j} \frac{\Gamma_k}{\overline{z}_j - \overline{z}_k} \qquad \text{for } j = 1, \ldots, N.$$

- Variational formulation in phase space

$$\mathcal{L}(p, q, \dot{p}, \dot{q}) = \langle p \,, \dot{q} \rangle - H(p, q).$$

$$\hookrightarrow \quad \dot{q} = \left(\frac{\partial H}{\partial p} \right)^T \quad \text{and} \quad \dot{p} = -\left(\frac{\partial H}{\partial q} \right)^T.$$

- Guiding centre motion (plasma physics)
- Many PDEs, e.g. nonlinear Schrödinger equation.

  (But modified equations are not so useful for PDEs)

Possible discretization of $\mathcal{L}(q, \dot{q}) = q^T A \dot{q} - H(q)$

$$L_{\mathrm{disc}}(q_j, q_{j+1}, h) = \left(\frac{q_j + q_{j+1}}{2} \right)^T A \left(\frac{q_{j+1} - q_j}{h} \right) - \frac{1}{2} H(q_j) - \frac{1}{2} H(q_{j+1})$$

Discrete EL equation $\dfrac{q_{j+1} - q_{j-1}}{2h} = (A^T - A)^{-1} H'(q_j)^T.$

Possible discretization of $\mathcal{L}(q, \dot{q}) = q^T A \dot{q} - H(q)$

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Discrete EL equation $\dfrac{q_{j+1} - q_{j-1}}{2h} = (A^T - A)^{-1} H'(q_j)^T.$

The EL equation involves 3 points $\Rightarrow$ needs 2 points of initial data.

The differential equation is of 1st order $\Rightarrow$ needs only 1 point of initial data.

This means we are dealing with a 2-step method.

- We have a multi-step method, so parasitic oscillations may occur.

  Solution: double the dimension of the system: principal and parasitic part. The enlarged system is still Lagrangian.

- We cannot replace $\dot{q}$ in the Lagrangian.

  Reason: NIC only involve $\ddot{q}, q^{(3)}, \cdots$.

Modified equations for 2-step methods

Principal modified equation

$$\dot{q} = f(q) + hf_1(q) + h^2 f_2(q) + \ldots + h^k f_k(q)$$

satisfies

$$\frac{a_0 q(t) + a_1 q(t+h) + a_2 q(t+2h)}{h}$$
$$= b_0 f(q(t)) + b_1 f(q(t+h)) + b_2 f(q(t+2h)) + \mathcal{O}(h^{k+1}).$$

Full system of modified equations

$$\dot{x} = f_0(x,y) + hf_1(x,y) + \ldots + h^k f_k(x,y)$$
$$\dot{y} = g_0(x,y) + hg_1(x,y) + \ldots + h^k g_k(x,y),$$

such that the discrete curve $q_j = x(t+jh) + (-1)^j y(t+jh)$ satisfies

$$\frac{a_0 q_j + a_1 q_{j+1} + a_2 q_{j+2}}{h} = b_0 f(q_j) + b_1 f(q_{j+1}) + b_2 f(q_{j+2}) + \mathcal{O}(h^{k+1})$$

Doubling the dimension

The discrete curve $(x_j, y_j)_{j\in\mathbb{Z}}$ is critical for

$$\widehat{L}(x_j, y_j, x_{j+1}, y_{j+1}, h) = \frac{1}{2}L(x_j+y_j, x_{j+1}-y_{j+1}, h)+\frac{1}{2}L(x_j-y_j, x_{j+1}+y_{j+1}, h),$$

if and only if the discrete curves $(q_j^+)_{j\in\mathbb{Z}}$ and $(q_j^-)_{j\in\mathbb{Z}}$, defined by

$$q_j^\pm = x_j \pm (-1)^j y_j,$$

are critical for $L(q_j, q_{j+1}, h)$.

Lagrangian for the full system of modified equations
$=$ Lagrangian for the principal modified equation of the extended system.

Hence we can calculate a Lagrangian for the full system of modified equations with the tools we already have.

Example 1

For

$$L_{\mathrm{disc}}(q_j, q_{j+1}, h) = \left\langle \frac{1}{2} A q_j + \frac{1}{2} A q_{j+1} \, , \frac{q_{j+1} - q_j}{h} \right\rangle - \frac{1}{2} H(q_j) - \frac{1}{2} H(q_{j+1})$$

we find

$$\widehat{\mathcal{L}}_{\mathrm{mod},0}(x, y, \dot{x}, \dot{y}, h) = \langle Ax \, , \dot{x} \rangle + \langle A\dot{y} \, , y \rangle - \frac{1}{2} H(x+y) - \frac{1}{2} H(x-y).$$

Its Euler-Lagrange equations are

$$\dot{x} = A_{\mathrm{skew}}^{-1} \left(\frac{1}{2} H'(x+y)^T + \frac{1}{2} H'(x-y)^T \right) + \mathcal{O}(h),$$
$$\dot{y} = A_{\mathrm{skew}}^{-1} \left(-\frac{1}{2} H'(x+y)^T + \frac{1}{2} H'(x-y)^T \right) + \mathcal{O}(h).$$

Linearize the second equation around $y = 0$

$$\dot{y} = -A_{\mathrm{skew}}^{-1} H''(x) y + \mathcal{O}(|y|^2 + h)$$

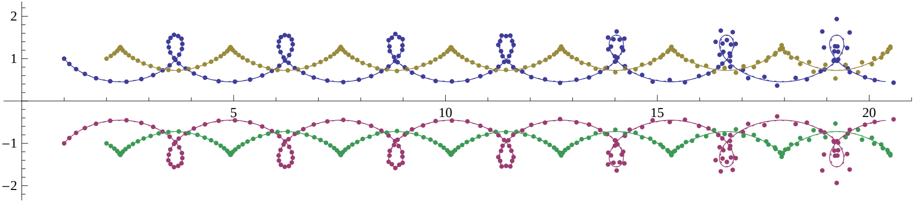
Example 1

Magnitude of oscillations satisfies

$$\dot{y} = -A_{\mathrm{skew}}^{-1} H''(x) y + \mathcal{O}(|y|^2 + h)$$

Unless the matrix $-A_{\mathrm{skew}}^{-1} H''(x)$ is exceptionally friendly, we expect growing parasitic oscillations.

(Note that an eigenvalue analysis does not apply because $-A_{\mathrm{skew}}^{-1} H''(x)$ is not constant)



Example 2

For

$$L_{\text{disc}}(q_j, q_{j+1}, h) = \left\langle A \frac{q_j + q_{j+1}}{2}, \frac{q_{j+1} - q_j}{h} \right\rangle - H\left(\frac{q_j + q_{j+1}}{2} \right)$$

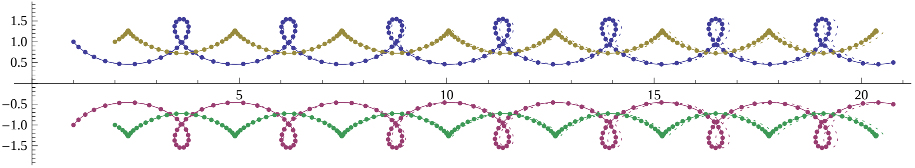
we find

$$\widehat{\mathcal{L}}_{\text{mod},0}(x, y, \dot{x}, \dot{y}, h) = \langle Ax, \dot{x} \rangle + \langle A\dot{y}, y \rangle - H(x).$$

Its Euler-Lagrange equations are

$$\begin{aligned} \dot{x} &= A_{\text{skew}}^{-1} H'(x)^T + \mathcal{O}(h), \\ \dot{y} &= 0 + \mathcal{O}(h). \end{aligned}$$

Even better, $\dot{y} = 0$ to any order $\rightarrow$ no growing oscillations.



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Contact Hamiltonian dynamics

Contact geometry is an odd-dimensional counterpart to symplectic geometry. In mechanics, we typically work on $T^*Q \times \mathbb{R}$, a Hamilton function

$$H : T^*Q \times \mathbb{R} \to \mathbb{R} : (q, p, z) \mapsto H(q, p, z)$$

generates dynamics by

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{z} = p\frac{\partial H}{\partial p} - H$$
$$\dot{p} = -\frac{\partial H}{\partial q} - p\frac{\partial H}{\partial z}$$

Example. $H(q, p, z) = \frac{1}{2}p^2 + V(q) + \alpha z$ describes a damped mechanical system:

$$\dot{q} = p \qquad \dot{z} = p^2 - H$$
$$\dot{p} = -V'(q) - \alpha p$$

Contact variational principle

Given a Lagrange function

$$L : TQ \times \mathbb{R} \to \mathbb{R},$$

consider the ode

$$\dot{z} = L(q, \dot{q}, z)$$

on a fixed interval $[0, T]$, with $z(0)$, $q(0)$ and $q(T)$ prescribed.

Herglotz variational principle:

$z(T)$ critical under variations of the curve q.

Given a discrete Lagrange function

$$L : Q \times Q \times \mathbb{R} \to \mathbb{R},$$

consider the ode

$$\frac{z_{j+1} - z_j}{h} = L(q_j, q_{j+1}, z_j)$$

for $j \in \{0, \dots, N\}$ with z_0, q_0 and q_N prescribed.

Discrete Herglotz variational principle:

z_N critical under variations of the discrete curve q.

In this framework, we can adapt the theory of variational integrators to contact systems.

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Integrable systems

An integrable system is (a system of) nonlinear differential or difference equation(s), that to some extend behaves like a linear system.

Our perspective

An equation is integrable if it is part of a “sufficiently large” system of “compatible” equations.

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In Mechanics: A Hamiltonian system with Hamilton function $H : T^*Q \simeq \mathbb{R}^{2N} \to \mathbb{R}$ is Liouville-Arnold integrable if there exist N functionally independent Hamilton functions $H = H_1, H_2, \ldots H_N$ in involution:

$$\{H_i, H_j\} = 0.$$

(1+1)-dimensional PDEs: Infinite sequence $H = H_1, H_2, \ldots$ of Hamiltonians in involution.

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(1+1)-dimensional PDEs: Infinite sequence $H = H_1, H_2, \ldots$ of Hamiltonians in involution.

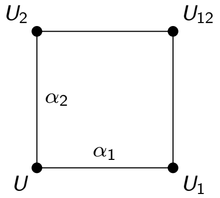
Variational description of an integrable hierarchy:

pluri-Lagrangian or Lagrangian multiform systems.

Quad equations

Quad equation:

$$\mathcal{Q}(U, U_1, U_2, U_{12}, \alpha_1, \alpha_2) = 0$$

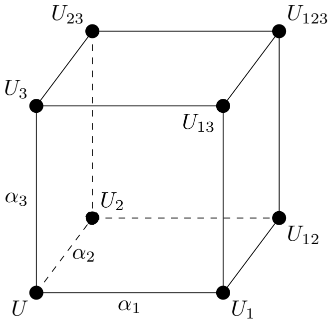


Subscripts of U denote lattice shifts, α_1, α_2 are parameters.
Invariant under symmetries of the square, affine in each of U, U_1, U_2, U_{12}.

Integrability for systems quad equations:
Multi-dimensional consistency of

$$\mathcal{Q}(U, U_i, U_j, U_{ij}, \alpha_i, \alpha_j) = 0,$$

i.e. the three ways of calculating U_{123} give the same result.

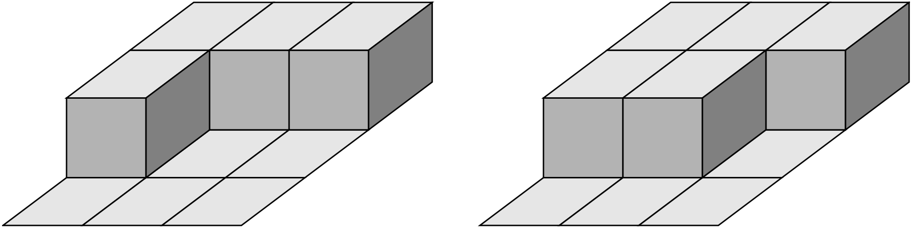


Pluri-Lagrangian structure for quad equations

For some discrete 2-form

$$\mathcal{L}(\square_{ij}) = \mathcal{L}(U, U_i, U_j, U_{ij}, \alpha_i, \alpha_j),$$

the action $\displaystyle\sum_{\square \in \Gamma} \mathcal{L}(\square)$ is critical on all 2-surfaces Γ in $\mathbb{N}^N$ simultaneously.



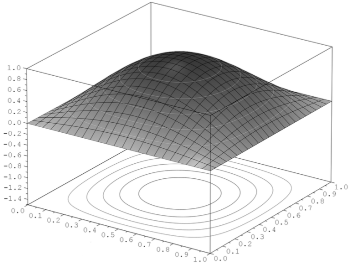
[Lobb, Nijhoff. Lagrangian multiforms and multidimensional consistency. J. Phys. A. 2009]

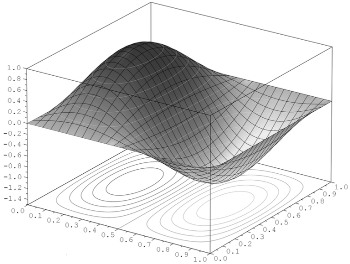
Continuous Pluri-Lagrangian systems

A field $u : \mathbb{R}^N \mapsto Q$ is a solution of the pluri-Lagrangian problem for the Lagrangian 2-form,

$$\mathcal{L} = \sum_{i,j} L_{ij}[u]\, \mathrm{d}t_i \wedge \mathrm{d}t_j.$$

if the action $\int_\Gamma \mathcal{L}$ is critical on all smooth surfaces Γ in $\mathbb{R}^N$.





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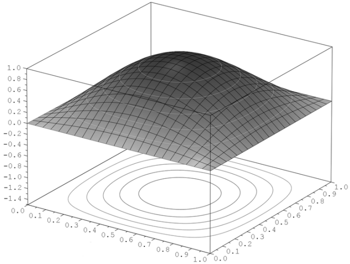

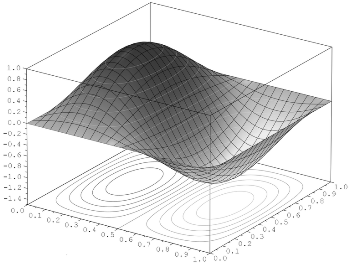

Continuum limits of pluri-Lagrangian systems use many of the ideas presented today.

Summary

1. Basics of Geometric Numerical Integration [1]
2. Modified Lagrangians [2]
3. Variational integration of the Kepler problem [3]
4. A class of degenerate Lagrangians [4]
5. Variational integrators for Contact Hamiltonian systems [5]
6. Related ideas in integrable systems [6]

[1] Hairer, Lubich, Wanner. Geometric Numerical Integration. Springer, 2006.

[2] V. Modified equations for variational integrators. Numer. Math. 137:1001, 2017.

[3] V. Numerical precession in variational discretizations of the Kepler problem. In: Discrete Mechanics, Geometric Integration and Lie–Butcher Series, Springer, 2018.

[4] V. Modified equations for variational integrators applied to Lagrangians linear in velocities. arXiv:1709.09567.

[5] Work in progress with Alessandro Bravetti and Marcello Seri.

[6] V. Continuum limits of Pluri-Lagrangian systems. arXiv:1706.06830

Summary

- Obtaining a high-order modified Lagrangian $\mathcal{L}_{\mathrm{mesh}}[x]$ is relatively straightforward, but its interpretation is not.

  From $\mathcal{L}_{\mathrm{mesh}}[x]$ a first order Lagrangian $\mathcal{L}_{\mathrm{mod},k}(x, \dot{x})$ can be found using the meshed variational principle. (This might be simpler in the contact formulation.)

- If the Lagrangian is nondegenerate, the modified Lagrangian can also be obtained by Legendre transform from the modified Hamiltonian.

  Our approach extends to degenerate Lagrangians that are linear in velocities.

- Similar ideas apply to continuum limits of integrable systems.

- Can we get improved error estimates from the Lagrangian perspective?

  What about nonholonomic constraints?

  What about PDEs?

Thank you for your attention!

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