Generating functions for variational integrators

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GDR-GDM, Lyon, Juin 2026

Newton's second law, 1687

$(F_i)_i \colon \mathbb{R}^k \to \mathbb{R}^k$ a force admitting a potential $V \colon \mathbb{R}^k \to \mathbb{R}$ and $m > 0$ the mass of the particule.

$$
\begin{aligned}
m\ddot{q}_i = F_i(q_1, \ldots, q_d) &\Leftrightarrow \dot{\begin{pmatrix} q \\ v \end{pmatrix}} = \begin{pmatrix} v \\ \frac{1}{m}\nabla V(q) \end{pmatrix} \\
&\Leftrightarrow \dot{\begin{pmatrix} q \\ p \end{pmatrix}} = \begin{pmatrix} \frac{p}{m} \\ \nabla V(q) \end{pmatrix} \\
&\Leftrightarrow \dot{x} = J \cdot \nabla_x H
\end{aligned}
\tag{1}
$$

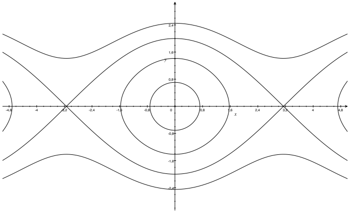
where

- $x = (q, p) \in \mathbb{R}^k \times (\mathbb{R}^k)^*$ a point of the phase space,
- $J = \begin{pmatrix} 0_{d\times d} & Id \\ -Id & 0_{d\times d} \end{pmatrix}$ is the symplectic form,
- $H(q, p) = \frac{1}{2m} \sum_{i=1}^{d} p_i^2 - V(q)$ the Hamiltonian.

Symplecticity

Proposition (Energy conservation)

$$\frac{\partial}{\partial t} H(q(t), p(t)) = 0.$$



Phase plan of $\ddot{q} = -\frac{g}{L} sin(q)$

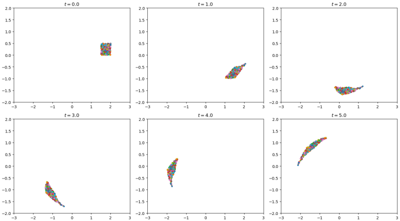
$H(q, p) = \frac{p^2}{2mL^2} + mgL(1 - \cos q)$

$$\phi_t^H : \begin{array}{ccc} \mathbb{R}^k \times (\mathbb{R}^k)^* & \rightarrow & \mathbb{R}^k \times (\mathbb{R}^k)^* \\ q(0), p(0) & \mapsto & q(t), p(t) \end{array}$$

Proposition

Any Hamiltonian flow is symplectic:

$$Jac(\phi_t^H)^T \cdot J \cdot Jac(\phi_t^H) = J$$



$d = 1$: volume preservation

source : furnstahl.github.io

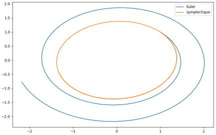
Symplectic integrators

Definition (An integrator)

It is a family $\varphi_{\Delta t} : x_n \mapsto x_{n+1}$ parametrized by the time-step Δt.
$\varphi_{\Delta t}$ is symplectic if $\mathbf{Jac}(\varphi_{\Delta t})^T \cdot J \cdot \mathbf{Jac}(\varphi_{\Delta t}) = J$.

Example (Symplectic Euler method, DeVogelaere, 1956)

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} q_n + \Delta t \frac{\partial H}{\partial p}(q_n, p_{n+1}) \\ p_n - \Delta t \frac{\partial H}{\partial q}(q_n, p_{n+1}) \end{pmatrix}$$



$H(q,p) = \frac{p^2+q^2}{2}$,
$\Delta t = 0.1$, $n = 100$ itérations
Quasi-periodic orbits

Theorem (Quasi-first integral, Benettin et Giorgilli, 1994)

Under some assumptions, $\exists (H_\epsilon)_\epsilon$, $C > 0$, $\epsilon^* > 0$ *s.t.*

$$\forall n \in \mathbb{N}, \forall \epsilon < \epsilon^*, \ |H_\epsilon(\varphi_\epsilon^n(q,p)) - H_\epsilon(q,p)| \leq Cn\epsilon \exp\left(-\frac{\epsilon^*}{\epsilon}\right) \quad (2)$$

Some stability properties of Hamiltonian Poisson integrators, C., 2025

Euler-Lagrange equations, $1750's$

Starting again from Newtonian mechanics (1):

$$\begin{aligned} m\ddot{q}_i = F_i(q_1, \ldots, q_d) &\Leftrightarrow \dot{\begin{pmatrix} q \\ v \end{pmatrix}} = \begin{pmatrix} v \\ \frac{1}{m}\nabla V(q) \end{pmatrix} \\ &\Leftrightarrow \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} = \frac{\partial L}{\partial q} \\ &\Leftrightarrow \delta \int L = 0 \end{aligned}$$

where

- (q, v) position and velocity of the particule,
- $L(q, v) = \frac{1}{2m}\sum_{i=1}^{d} v_i^2 + V(q)$ the Lagrangian.

Generating functions

Definition (The action)

$$S_t : \begin{array}{ccc} \mathbb{R}^k \times \mathbb{R}^k & \to & \mathbb{R} \\ (q_0, q_1) & \mapsto & \int_0^t L(q(s), \dot{q}(s)) \mathrm{d}s \end{array} \tag{3}$$

where $s \in [0, t] \mapsto q(s)$ the extremal path s.t. $\left\{ \begin{array}{cc} q(0) & = q_0, \\ q(t) & = q_1 \end{array} \right.$.

Remark

t is small, q_1 close to q_0.

The graph of the generating function (3) is the graph of the Hamiltonian flow !

$$\begin{array}{ccccc} \mathrm{Graph}(dS_t) & \mapsto & & \mathrm{Graph}(\phi_t^H) & \\ \cap & & & \cap & \\ T^*(\mathbb{R}^k \times \mathbb{R}^k) & \widetilde{\rightarrow} & T^*\mathbb{R}^k & \times & T^*\mathbb{R}^k \\ (q_0, q_1, \frac{\partial S_t}{\partial q_0}(q_0, q_1), \frac{\partial S_t}{\partial q_1}(q_0, q_1)) & \mapsto & (q_0, p_0), & & \phi_t^H(q_0, p_0) \end{array}$$

Variational integrators[1]

Discretize S_t:

$$\int_0^t L(q(s), \dot{q}(s))\mathrm{d}s \approx \int_0^t L(q_0, \frac{q_1 - q_0}{t})\mathrm{d}s$$

and obtain the discrete action

$$\hat{S}_t \colon (q_0, q_1) \mapsto tL(q_0, \frac{q_1 - q_0}{t}).$$

Then, start from, e.g, (q_0, q_1) and iterate:

$$\begin{aligned} p_0 = &\ \partial_1 \hat{S}_t(q_0, q_1) \\ p_1 = &\ \partial_2 \hat{S}_t(q_0, q_1) \quad = -\partial_1 \hat{S}_t(q_1, q_2) \\ &\dots \end{aligned} \tag{4}$$

Remark (Correspondence of Lagrangian spaces)

The numerical method (4) *has the same stability theory than symplectic integrators: long run estimates* (2) *etc...*

[1] Discrete mechanics and variational integrators, Marsden and West, 2001

Composition of Lagrangian spaces and consequences

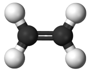
Hamiltonian flows	$\phi^{H_3} = \phi^{H_1} \circ \phi^{H_2}$
Trajectories	Concatenation of paths
Generating functions	$S_3(q_0, q_2) = \underset{q_1}{\mathrm{extr}}\big(S_1(q_0, q_1) + S_2(q_1, q_2)\big)$

Composition of Lagrangian spaces in mechanics

$\Rightarrow$ **This provides a geometric framework towards:**

Symplectic multi-step methods:

- vibration of molecules
- delayed ODEs

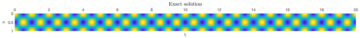


Ethylene

fig.: Wikipedia

Variational integrators for field theories:

- wave equation,
- Poisson equation,
- Geometrically exact beam theory on $SO(3)$



An oscillation mode of the wave equation

fig.: R. Sato

Multisymplectic Hamiltonian variational integrators, Tran, Leok, 2021
Special Symplectic Spaces, Tulczyjew, Lawruk, 1975

Jets and boundary Lagrangian with S. Leyendecker, R. Sato, T. Wang, D. M. de Diego

Given $L\colon (\phi, \phi_t, \phi_s) \mapsto L(\phi, \phi_t, \phi_s)$, Euler-Lagrange equations are:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v_t^i}\right) + \frac{d}{ds}\left(\frac{\partial L}{\partial v_s^i}\right) - \frac{\partial L}{\partial q^i} = 0,\ 1 \leq i \leq k. \tag{5}$$

Define the boundary Lagrangian[2]

$$L_{\partial U}(\psi) = \int_U L(j^1\phi) d^k x \ \text{ where } \phi \text{ solves (5) with } \phi_{|\partial\Omega} = \psi.$$

Remark (The boundary Lagrangian is a generating function)

Compare with $S_t(q_0, q_1) = \int_0^t L(q(s), \dot{q}(s)) ds.$

Remark

In general, to find the definition domain of $L_{\partial U}$ *is intricate.*

[2] Symplectic Framework for Field Theories, Kijowski, Tulczyjew, 1979

An example: the 1d wave equation on the square[3]

$$\phi_{tt} - \phi_{ss} = 0$$

- $U = [0,1] \times [0,1]$
- $L(\phi, \phi_t, \phi_s) = \frac{1}{2}(\phi_t^2 - \phi_s^2)$
- The boundary data ψ needs to satisfy $\psi(\alpha,0) + \psi(1-\alpha,1) - \psi(0,\alpha) - \psi(1,1-\alpha) = 0$
- explicit boundary Lagrangian

$$L_{\partial U}(\psi) = \frac{1}{2}\int_0^1 \psi(0,\alpha)\psi_s(\alpha,0) - \psi(\alpha,0)\psi_t(0,\alpha) + \psi(\alpha,1)\psi_t(1,\alpha) - \psi(1,\alpha)\psi_s(\alpha,1)\, d\alpha$$

[3] Generating functionals and Lagrangian partial differential equations, Vankerschaver, Liao, Leok, 2013

How to discretise the boundary Lagrangian ?

The hyperbolic case, e.g., the wave equation

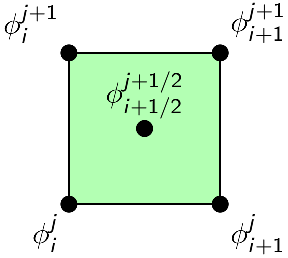
Example (Midpoint-midpoint discretization using corner nodes[4])

$$\phi^j_{i+1/2} := \frac{\phi^j_i + \phi^j_{i+1}}{2}, \qquad \phi^{j+1/2}_i := \frac{\phi^j_i + \phi^{j+1}_i}{2},$$

$\phi^j_i, \phi^j_{i+1}, \phi^{j+1}_i, \phi^{j+1}_{i+1}$ corner nodes

$$\phi^{j+1/2}_{i+1/2} := \frac{\phi^j_i + \phi^j_{i+1} + \phi^{j+1}_i + \phi^{j+1}_{i+1}}{4}.$$

$\approx$ Preissmann Box Scheme[a]



[a] Propagation des intumescences dans les canaux et rivières, Preissmann, 1961

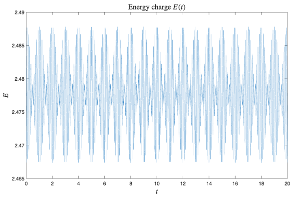
Remark (Interest of a toy model)

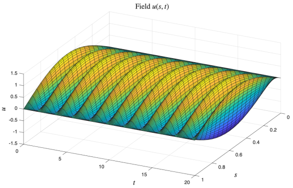
Compare with the analytical solution $\phi(s,t) = \sin(\pi s)\cos(\frac{\pi}{20} t)$

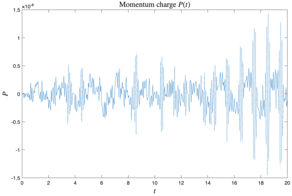
[4] Integrateurs geometriques: applications a la mecanique des fluides, Chhay, 2008

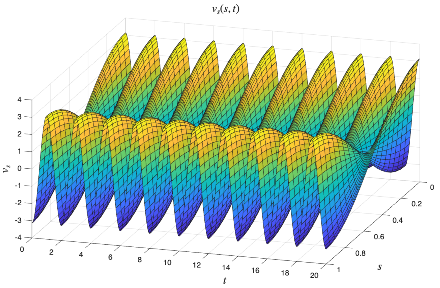
Numerical example: the wave equation on $[0,1] \times [0,20]$

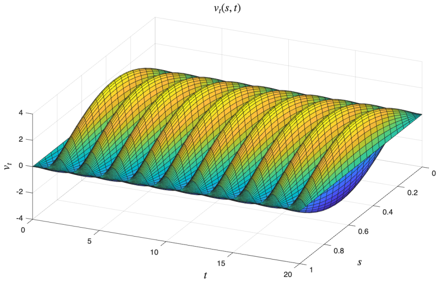
with T. Wang











To be continued

Apply the Method of Virtual Power:

- Wave propagation in generalized media[a]
- Invariant theory for the acoustic tensor[b]

Numerical study:

- Energy exchanges between vibration modes[c]

[a] La méthode des puissances virtuelles en mécanique des milieux continus, Germain, 1973

[b] Characterization of the symmetry class of an elasticity tensor using polynomial covariants, Olive, Kolev, Desmorat, Desmorat, 2022

[c] Ongoing with A. Patel, V. Carlier, L. Le Marrec

Un mécathicien

Develop a backward error analysis for variational integrators in field theory:

- Goal-oriented error estimation[5]
- How about adaptative time-steps? cf Anthony Gravouil's lecture

[5] A pedagogical review on a posteriori error estimation in Finite Element computations, Chamoin, Legoll, 2021