Introduction to geometric numerical methods

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MATHEMATICAL
CENTER IN AKADEMGORODOK

Introduction to geometric numerical methods

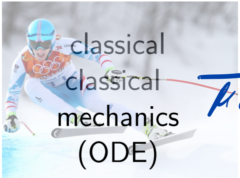
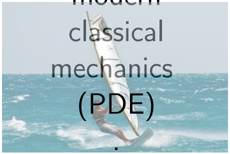
Lecture 1. (today)
Motivation, geometric preliminaries.

Lecture 2. (tomorrow)
Numerical methods for ODEs.

Lecture 3. (Friday)
Structure preserving numerical methods AKA geometric integrators.

Philosophy:

Geometry encodes the physics of the system

	Mechanical property	Geometric description
 classical classical mechanics (ODE)	conservation of energy	Poisson / symplectic
	symmetries Noether G / μ	Lie groups/algebras, Cartan moving frames
	dissipation / interaction power balance; constraints	(almost) Dirac
	control	(singular) foliations
 modern classical mechanics (PDE)	conservation of energy	multisymplectic
	symmetries	Cartan moving frames
	dissipation / interaction	Stokes–Dirac
	$rot(grad) = 0$, $div(rot) = 0$	$d^2 = 0$ – DEC
	control	foliations

Num

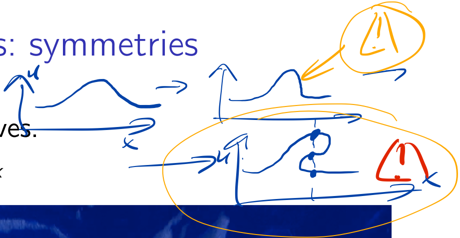
Preserving this geometry in computations is fruitful

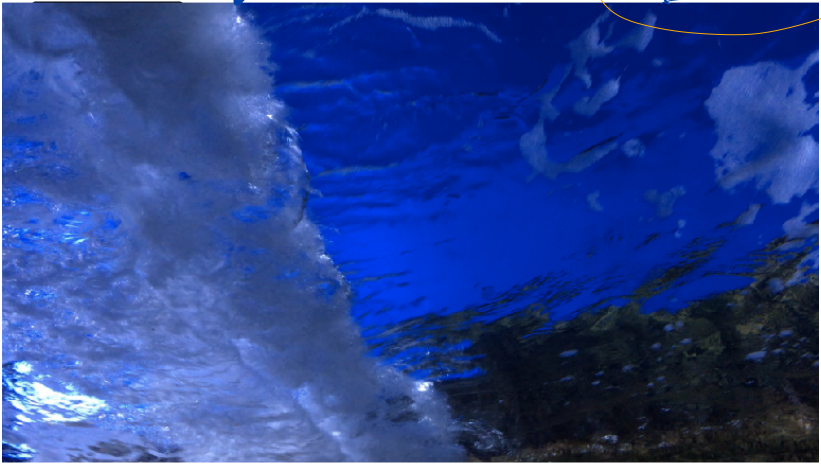
Advanced but well-studied tools: symmetries

Lie symmetries (Noether theorem).

Example: Shallow water shock waves.

Burgers' equation: $u_t + uu_x = \nu u_{xx}$





Advanced and less-studied tools: integrability

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Kadomtsev–Petviashvili equation

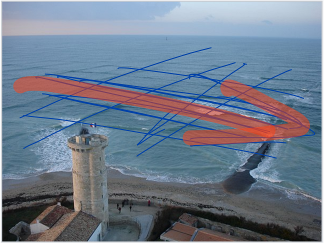
From Wikipedia, the free encyclopedia

In mathematics and physics, the **Kadomtsev–Petviashvili equation** (often abbreviated as **KP equation**) is a partial differential equation to describe nonlinear wave motion. Named after Boris Borisovich Kadomtsev and Vladimir Iosifovich Petviashvili, the KP equation is usually written as:

$$\partial_x(\partial_t u + u\partial_x u + \epsilon^2 \partial_{xxx} u) + \lambda \partial_{yy} u = 0$$

where $\lambda = \pm 1$. The above form shows that the KP equation is a generalization to two spatial dimensions, *x* and *y*, of the one-dimensional Korteweg–de Vries (KdV) equation. To be physically meaningful, the wave propagation direction has to be not-too-far from the *x* direction, i.e. with only slow variations of solutions in the *y* direction.

Like the KdV equation, the KP equation is completely integrable.[1][2][3][4][5] It can also be solved using the inverse scattering transform much like the nonlinear Schrödinger equation.[6]



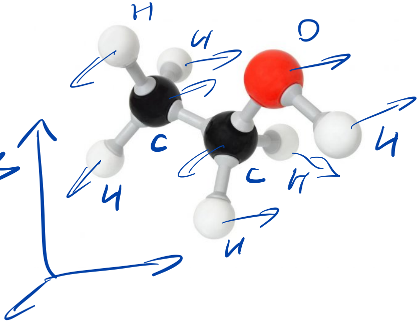
Crossing swells, consisting of near-cnoidal wave trains. Photo taken from Phares des Baleines (Whale Lighthouse) at the western point of Île de Ré (Isle of Rhé), France, in the Atlantic Ocean. The interaction of such near-solitons in shallow water may be modeled through the Kadomtsev–Petviashvili equation.

Contents [hide]

Example: molecular dynamics

$\vec{F}_i$

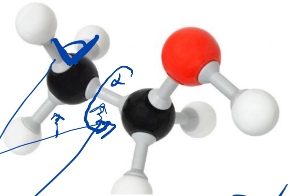
acting on the i-th particle



$$\vec{F}_i = m\vec{a}_i$$

$$\boxed{\ddot{\vec{r}}_i = \frac{\vec{F}_i}{m}}$$

Example: molecular dynamics



$r_i(0) = r_{i0}, \quad v_i(0) = v_{i0}$

$$\boxed{m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i = -\frac{\partial U(\mathbf{r}_1, \ldots, \mathbf{r}_n)}{\partial \mathbf{r}_i}} + \cancel{\mathbf{F}_i^{ext}}, \quad i = 1, \ldots, n \gg 1.$$

$$\frac{\partial U}{\partial r_i}$$

$$r = \begin{pmatrix} r_x \\ r_y \\ r_z \end{pmatrix}$$

$$U = U_b + U_v + U_\varphi + \cancel{U_f} + U_{qq} + U_{VW} + U_{Hb}$$

$$U_b = \sum_i^{N_b} k_{b,i}(r_i - r_{0,i})^2, \qquad U_v = \sum_i^{N_v} k_{v,i}(\alpha_i - \alpha_{0,i})^2$$

$$U_\varphi = \sum_\varphi^{\Phi} \sum_l^{L} k_{\varphi,l}(1 + g_{\varphi,l}\cos(n_{\varphi,l}\alpha_\varphi)) \qquad U_{qq} = \sum_{i,j} \frac{q_i q_j}{\varepsilon r_{ij}}$$

$$U_{VW} = \sum_{i,j} \left(\frac{A}{r_{ij}^{12}} - \frac{A}{r_{ij}^{6}} \right) \qquad U_{Hb} = \sum_{i,j} \left(\frac{C}{r_{ij}^{12}} - \frac{D}{r_{ij}^{10}} \right)$$

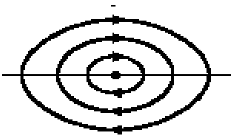
Q: is the energy conserved?

$$E_{tot} = \sum_{i=1}^{n} \frac{m_i v_i^2}{2} + U(r_1 \dots r_n)$$

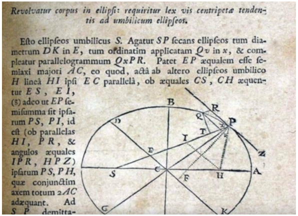
$$\frac{d}{dt} E_{tot} =$$

Exercise on the blackboard.

Very classical story

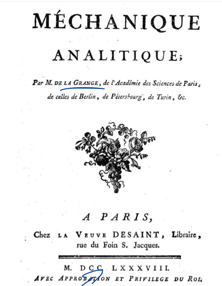
Canonical case: given $H\colon\ T^*Q \to \mathbb{R}$ $\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}$	Symplectic geometry $\omega = \sum_i dp_i \wedge dq^i$ $\iota_{X_H}\omega = \mathrm{d}H$	
More general case: given $H\colon\ M \to \mathbb{R}$ and an antisymmetric $J(\mathbf{x})$ $\dot{\mathbf{x}} = J(\mathbf{x})\frac{\partial H}{\partial \mathbf{x}}$	Poisson geometry $\{\cdot,\cdot\}$ on : $C^\infty(M)$ $X_H = \{H,\cdot\}$ $\dot{\mathbf{x}} = \{H,\mathbf{x}\}$	

History


Revolvatur corpus in ellipsi: requiritur lex vis centripetæ tendentis ad umbilicum ellipseos.

Esto ellipseos umbilicus S. Agatur SP secans ellipseos tum diametrum DK in E, tum ordinatim applicatam Qv in x, & compleatur parallelogrammum QxPR. Patet EP æqualem esse semiaxi majori AC, eo quod, acta ab altero ellipseos umbilico H linea HI ipsi EC parallela, ob æquales CS, CH æquentur ES, EI, (5) adeo ut EP semisumma sit ipsarum PS, PI, id est (ob parallelas HI, PR, & angulos æquales IPR, HPZ) ipsarum PS, PH, quæ conjunctim axem totum 2AC adæquant. Ad SP demitta-

Newton
~1666


MÉCHANIQUE

ANALITIQUE;

Par M. DE LA GRANGE, de l'Académie des Sciences de Paris, de celles de Berlin, de Pétersbourg, de Turin, &c.

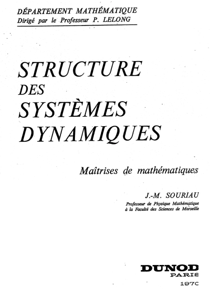
A PARIS,

Chez LA VEUVE DESAINT, Libraire, rue du Foin S. Jacques.

M. DCC. LXXXVIII.

AVEC APPROBATION ET PRIVILEGE DU ROI.

Lagrange

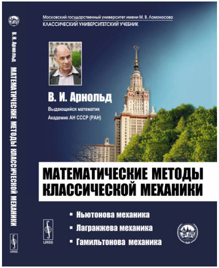

DÉPARTEMENT MATHÉMATIQUE
Dirigé par le Professeur P. LELONG

STRUCTURE DES SYSTÈMES DYNAMIQUES

Maîtrises de mathématiques

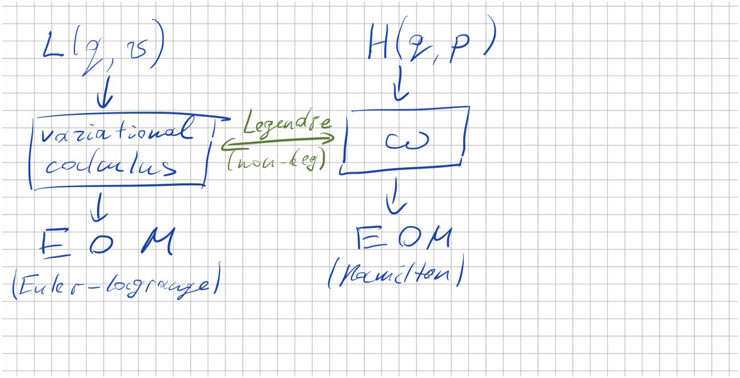
J.-M. SOURIAU
Professeur de Physique Mathématique à la Faculté des Sciences de Marseille

DUNOD
PARIS
1970



Lecture by Jean-Pierre Bourguignon (google: Souriau symplectic)
https://www.youtube.com/watch?v=93hFolIBo0Q

Classical story in modern language



Classical story in modern language