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Geometric Numerical Integration

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Abstract. The subject of this workshop was numerical methods that preserve geometric properties of the flow of an ordinary or partial differential equation. This was complemented by the question as to how preserving the geometry affects the dynamical behaviour.

Mathematics Subject Classification (2000): 65xx.

Introduction by the Organisers

The subject of this workshop was numerical methods that preserve geometric properties of the flow of an ordinary or partial differential equation: symplectic and multisymplectic integrators for Hamiltonian systems, symmetric integrators for reversible systems, methods preserving first integrals and numerical methods on manifolds, inclusive of Lie group methods and integrators for constrained mechanical systems, and methods for problems with highly oscillatory solutions. The unifying theme was structure preservation: not just the "how?" but also "why?", "where?" and "what for?".

The motivation for developing structure-preserving algorithms for special classes of problems originates independently in such diverse areas of research as astronomy, molecular dynamics, mechanics, control theory, theoretical physics and numerical analysis, with important contributions from other areas of both applied and pure mathematics. Moreover, it turns out that preservation of geometric properties of the flow not only produces an improved qualitative behaviour, but also allows for a significantly more accurate long-time integration than with general-purpose methods.

In addition to the construction of geometric integrators, an important aspect of geometric integration is the light it sheds on the relationship between geometric

properties of a numerical method and favourable error propagation in long-time integration. A very successful organising principle is backward error analysis, whereby the numerical one-step map is interpreted as (almost) the flow of a modified differential equation. In this way, geometric properties of the numerical integrator translate seamlessly into structure preservation on the level of the modified equation. Much insight and rigourous error estimates over long time intervals can then be obtained by combining backward error analysis with the KAM theory and related perturbation theories for Hamiltonian and reversible systems. While this approach has been very successful for ordinary differential equations, much less is currently known about highly oscillatory systems and geometric integrators for partial differential equations.

Geometric numerical integration has been an active interdisciplinary research area since the last decade. Although the subject is in a lively phase of intensive development, the results so far are substantive and they impact on a wide range of application areas and on our understanding of core issues in computational mathematics. This is evidenced by the monographs [1, 2].

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Workshop: Geometric Numerical Integration

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Abstracts

Geometric Integrators for Thermostatted Molecular Dynamics

Benedict Leimkuhler

Nosé dynamics is a popular and effective device for simulating molecular systems in the canonical ensemble. Let a closed Hamiltonian system be given with energy function

$$H(q,p) = \frac{1}{2}p^T M^{-1} p + V(q),$$

with q and p positions and momenta, respectively, M a positive definite symmetric mass matrix, and V the potential energy function. Nosé dynamics is derived from the extended phase space Hamiltonian,

$$H_N = H(q, \tilde{p}/\sigma) + \frac{\pi^2}{2\mu} + g k_B T \ln \sigma,$$

where g is the number of degrees of freedom, k_B the Boltzmann constant, and T is the target temperature at which sampling is desired. μ is a parameter that effectively allows the strength of dynamic coupling to be adjusted. The momentum appearing in H_N should be treated as canonical to q, whereas the physical momentum is related to $\tilde{p}$ by the change of variables

$$p = \frac{\tilde{p}}{\sigma}.$$

It was shown by Nosé that canonical sampling can be obtained along (assumed ergodic) trajectories of H_N via the relation

$$\int\int \ldots \int \delta\left[H_N - H_N^0\right] d\tilde{p} d\sigma d\pi = \exp(-\beta H(q,p)) dp,$$

where the integration is performed over the physically accessible phase space of the thermostatting variables, $(\sigma, \pi) \in (0, \infty) \times \mathbf{R}$.

While useful for understanding the concept of Nosé dynamics, H_N is not usually recommended for simulation because, on the one hand, computation of certain types of averages (e.g. autocorrelation functions) requires data at equally spaced points in time, and, more importantly, the equations of motion corresponding to H_N are poorly scaled for $\sigma \to 0$. This is the motivation for the well known Nosé-Hoover reformulation of Nosé dynamics which forms the basis for most numerical treatments (see Section 2). An alternative formulation incorporating time-transformation in the Hamiltonian setting can be used as the basis for symplectic numerical methods ([1]), based on an alternative time-transformation technique (Poincaré transformation). Simulation with the Nosé-Poincaré method is based on the Hamiltonian

$$H_{NP} = \sigma(H_N - H_N^0) \tag{1}$$

where the constant H_N^0 must be chosen so that H_N vanishes at the initial value, and hence for all time along Hamiltonian dynamics in the extended phase space.

The primary advantage anticipated from the Nosé-Poincaré approach is improved stability in long-term simulations and/or at large timestep size, and some evidence for this (in certain situations) was presented in [1] and in a subsequent paper on constant temperature/pressure dynamics [2].

A more subtle problem with the Nosé/Nosé-Hoover/Nosé-Poincaré formulation is that poor ergodicity may be observed, particularly for systems at low temperature (i.e. near-crystalline) or systems with strong harmonic components such as arise in modelling chemical bonds in organic molecules. A number of devices, e.g. Nosé-Hoover chains have been introduced to facilitate more effective sampling of phase space. It is natural to attempt to extend the Hamiltonian framework to allow symplectic treatment with chains of thermostats. Recent papers have introduced Nosé-Poincaré chains [3], in direct analogy to Nosé-Hoover chains, and Recursive Multiple Thermostats [4]. In the most general form, these thermostats can be described by a Hamiltonian of the form

$$H_{GN} = H(q, \tilde{p}/\Pi_\alpha\{\sigma_\alpha\}) + H_G(\sigma_1, \sigma_2, \ldots, \sigma_m, \pi_1, \pi_2, \ldots, \pi_m)$$

where the "bath" H_G is chosen so that the canonical density can be obtained through integration over the thermostatting variables:

$$\int\int\ldots\int(\delta\left[H_{GN} - H^0_{GN}\right]d\tilde{p})d\sigma_1 d\sigma_2 \ldots d\sigma_m d\pi_1 d\pi_2 \ldots d\pi_m = \exp(-\beta H(q,p))dp$$

Examples of this type of thermostatting bath are discussed below. While these methods can enable thermostatting which is quite rapid in relation to the simulation time interval, the numerical methods appear in some cases to require small timesteps compared to unthermostatted molecular dynamics and even compared to alternatives such as Nosé-Hoover chains [5]. Until now, the cause of this has not been explained. The numerical difficulties may actually become worse as the numerical method achieves a better sampling, further complicating the issue. As we show below, the instability is in part due to the fact that the Nosé-Poincaré form enables propagation of the momenta and thermostat variables separately, in such a way that the simple relationship between the physical and scaled Nosé momenta ($\tilde{p}$) may be violated within a timestep. This numerical difficulty can render inconsequential any advantage that might be obtained from the conservation of symplectic structure. Moreover, the way in which typical symplectic methods are constructed is based on a succession of stages. It is observed that within these stages, the thermostatting variables may be driven into strong oscillations which can have detrimental effects both for accuracy and stability of methods.

In this article we show that we can greatly enhance the stability of integrators for Nosé chains (and also for Nosé dynamics proper) by using a simple general principle to construct the *balanced* numerical method wherein, even at each substage of a numerical timestep, *the thermal variables are retained near mechanical equilibrium, provided the physical variables are in thermal equilibrium.* We demonstrate the concept by constructing several integration methods and applying them to model problems including both a harmonic oscillator and a 3-body molecular model problem. We show that the balanced symplectic Nosé-Poincaré based

method and its chain counterpart have very strong advantages over both Nosé-Hoover as well as other symplectic but not balanced integrators.

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Calculating Multidimensional Discrete Variable Representations From Cubature Formulae

Ilan Degani

(joint work with David J. Tannor)

Discrete Variable Representations (DVRs) are heavily used in "real life" high dimensional problems in computational quantum mechanics. First, to semi-discretize the Hamiltonian operator a finite dimensional function space $\mathcal{S}$ is chosen. The basic idea of DVR is to then find a basis of δ-like functions (DVR basis functions), each localized above its DVR point, which have several convenient properties for computation:

(1) The projection of any $f \in \mathcal{S}$ onto a DVR basis function is done simply by evaluating f at the corresponding DVR point.

(2) In the DVR basis the quantum mechanical potential operator is approximated simply by a diagonal matrix obtained by evaluating the potential function on the DVR points.

(3) Orthogonal projection of functions to subspaces spanned by a subset of DVR basis functions is easy to compute using item 1. This is needed if we know that the wavefunctions of interest are localized in a subset of configuration space (view this as the subset of $\mathbf{R}^d$ over which our wavefunctions live).

In this talk I describe the basics of DVR through the familiar example of $\mathcal{S} = \text{span}\{e^{-iqx}, \ldots, e^{iqx}\}$ and the discrete Fourier transform. Then I quote the general definition of a DVR set given by Littlejohn *et. al.* in [1] as a general framework for multidimensional DVRs - not necesarily with cartesian product grids, and not necesarily with Fourier function spaces. However, until very recently almost all known multidimensional DVRs were of the product type, where the dimension of $\mathcal{S}$ grows rapidly with increasing dimension of configuration space. Because

of this problem the search for non product DVRs is one of the major themes in computational quantum mechanics. The talk ends by stating the following problem whose solution gives DVR sets:

Problem. Denote the configuration space by Ω, and the space of multivariable degree q polynomials over Ω by $\mathcal{P}_q^\Omega$. Suppose we are given: (a) A degree $2q$ or $2q+1$ cubature formula for the region Ω and weight function $w(x)$, with nodes $\lambda_1, \ldots, \lambda_N \in \Omega$ and positive weights $\omega_1, \ldots, \omega_N$. (b) An n_1 dimensional function space $\mathcal{B}$ with the inner product $\langle g|h\rangle_w = \int_{Omega} w(x) g^*(x) h(x) dx$, and such that $\mathcal{P}_q^\Omega \subseteq \mathcal{B}$. Find, or prove that there do not exist, N functions $u_1, \ldots, u_N \in mathcalB$ such that

(1) $u_\alpha(\lambda_\beta) = \delta_{\alpha\beta} \frac{1}{\sqrt{\omega_\alpha}}$, $\alpha, \beta = 1, \ldots, N$.
(2) $\langle u_\alpha | u_\beta \rangle_w = \delta_{\alpha\beta}$, $\alpha, \beta = 1, \ldots, N$.
(3) $\mathcal{P}_q^\Omega \subseteq \mathrm{span}\{u_1, \ldots, u_N\}$.

This problem is solved in [2], thus associating families of non product DVRs, whose function space is $\mathrm{span}\{u_1, \ldots, u_N\}$, with any member in the menagerie of existing (positive weight) cubature formulae.

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Sobolev estimates for splitting schemes applied to the linear Schrödinger equation

Erwan Faou
(joint work with Guillaume Dujardin)

The aim of this work is to try to understand the long time behavior of splitting methods applied to the linear Schrödinger equation. Let us consider the equation

$$i\frac{\partial \psi}{\partial t} = H\psi, \quad \psi(0,x) = \psi_0(x), \tag{1}$$

where $H = -\Delta + V$ is the Hamiltonian of the problem. The function $\psi = \psi(t,x)$ is a function depending on the time t and the space variable x in the one-dimensional torus $\mathbb{T}$. The potential $V(x)$ is a real function. We consider the approximation method:

$$\psi_1 = \exp(i(\delta t)\Delta)\exp(-i(\delta t)V)\psi_0, \tag{2}$$

where δt is the stepsize, and where no space approximation is made. What is the long time behavior of the corresponding "numerical" solution?

The eigenvalues of the Laplace operator being the n^2, $n \in \mathbb{Z}$, we expect that the splitting method (2) exhibits resonances (at least this is the case after a spectral discretization). Moreover, even if these resonances are avoided, backward error

analysis cannot be used as in the finite dimensional case. Formally, the modified energy in the case of the scheme (2) can be written

$$\tilde{H} = -\Delta + V + \frac{i\delta t}{2}[-\Delta, V] + \cdots + \delta t^n H_{n+1} + \cdots \tag{3}$$

where H_{n+1} is a symmetric operator of order n. We arrive at the conclusion that Sobolev estimates are the key to analyze the long time behavior of (2) and the possible conservation of the modified energy (3) (see for instance [1]).

We make the following assumption for the potential function:

$$\forall\, n \geq 0, \quad \|D^n V\|_\infty \leq \lambda n!\, \varepsilon^n, \tag{4}$$

where $D = -i\partial_x$. The numbers λ and ε measure the "analytic size" of V: If these parameters are small, V is close to 0 in analytical norm. In the following, we denote by $\|\cdot\|$ the L^2-norm on $\mathbb{T}$.

Before showing anything concerning the solution of the splitting method (2), we first show the following result for the exact solution:

Theorem 1. *Let $\psi(t,x)$ be the solution of* (1) *and assume that ψ_0 satisfies*

$$\forall\, n \geq 0, \quad \|D^n \psi_0\| \leq M_0 n!\, r_0^{-n} \tag{5}$$

for constants M_0 and r_0. Assume moreover that the potential V satisfies (4) *for sufficiently small λ and ε. Then ψ is uniformly L^2-analytic, in the sense that there exist constants M and R such that*

$$\forall\, t \geq 0, \quad \forall\, n \in \mathbb{N}, \quad \|D^n \psi(t,\cdot)\| \leq M n! R^{-n}.$$

The proof of this theorem relies on the fact that for all s, H^s commutes with H and hence the quantities $\|H^{n/2}\psi(t,\cdot)\|$ are constants along the solution of (1). The key is to estimate the difference between the operator $H^{n/2}$ and the derivative D^n for all n. More precisely, we define the formal series:

$$S_\rho(\psi) = \sum_{n\geq 0} \frac{\rho^n}{n!} \|D^n \psi\| \quad \text{and} \quad Z_\rho(\psi) = \sum_{n\geq 0} \frac{\rho^n}{n!} \|H^{n/2}\psi\|\,. \tag{6}$$

Assume that V satisfies (4) with $\lambda \leq \varepsilon^2 \leq \varepsilon_0$. Then there exist positive constants c_1, C_1 depending on ε_0 such that for all analytic function ψ, we have

$$\forall\, \sigma, \quad 0 \leq \sigma \leq r_0, \qquad c_1 S_\sigma(\psi) \leq Z_\sigma(\psi) \leq C_1 S_\sigma(\psi). \tag{7}$$

This relation implies the result.

We consider now the splitting method (2). In the following, δt is considered as a fixed parameter and we introduce the familly of schemes:

$$L_\lambda := \exp(i(\delta t)\Delta)\exp(-i\lambda(\delta t)V).$$

For $\lambda = 0$, we have $L_0 := \exp(i(\delta t)\Delta)$. In particular, we have for all δt, $[D^s, L_0] = 0$ for all $s \in \boldsymbol{R}$. Let H_0 be an operator such that $[H_0, L_0] = 0$. We seek a modified operator $H(\lambda)$ such that

$$[H(\lambda), L_\lambda] = 0. \tag{8}$$

Setting the formal series $H(\lambda) = H_0 + \lambda H_1 + \sum_{n\geq 2} \lambda^n H_n$, the equation (8) is equivalent to the formal series equations

$$\forall\, n \geq 0, \quad [H_n, e^{i\delta t\Delta}] = -\sum_{p=0}^{n-1} \frac{(-i\delta t)^{n-p}}{(n-p)!}[H_p, e^{i\delta t\Delta} V^{n-p}]. \tag{9}$$

Let us write the equation (9) for $n = 1$. We get

$$[H_1, e^{i\delta t\Delta}] = i\delta t e^{i\delta t\Delta}[H_0, V].$$

After a Fourier transormation in $\mathbb{T}$, we denote by $(H_1)_{k\ell}$ the coefficients of the operator H_1 acting on $\mathbb{C}^{\mathbb{Z}}$. To solve this equation, we use the following non-resonance condition (see also [1, 2]): There exist positive numbers $\gamma > 0$ and $\nu > 1$ such that

$$\forall\, k \in \mathbb{Z}, \quad \left|\frac{1 - e^{ik\delta t}}{\delta t}\right| \geq \gamma |k|^{-\nu}. \tag{10}$$

We thus get the bounds on the coefficients, $\forall\, k, \ell \in \mathbb{Z}, \quad |k| \neq |\ell|$,

$$|(H_1)_{k\ell}| \leq \frac{\delta t}{1 - e^{i\delta t(\ell^2 - k^2)}}([H_0, V])_{k\ell} \leq \frac{1}{\gamma}|k^2 - \ell^2|^{\nu}([H_0, V])_{k\ell}.$$

Under smoothness assumptions on V, this shows that H_1 is an analytic operator. Note that we can add to H_1 a diagonal operator without affecting the equation (8), so that we can assume that H_1 is positive. By considering the operator $\tilde{H}(\lambda) := H_0 + \lambda H_1$, we obtain $[\tilde{H}(\lambda), L_\lambda] = \mathcal{O}(\lambda^2)$. Continuing the process, our aim is to obtain a modified operator commuting with L_λ up to a high order in λ and to obtain analytic estimates for it. This work is still in progress.

To conclude, we show a numerical experiment with

$$V(x) = \frac{3}{5 - 4\cos(x)} \quad \text{and} \quad \psi_0(x) = \sin(x)$$

and the stepsizes $h = \dfrac{2\pi}{6^2 - 2^2} = 0.196$ and $h = 0.2$. We plot the corresponding numerical solutions after 10^5 iterations, and the relative energy errors. We observe a drift in the resonant case, while the solution remains quasiperiodic in the case of a non-resonant stepsize.

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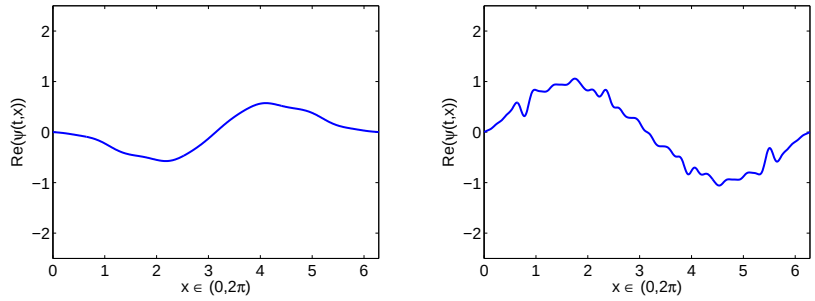

FIGURE 1. Plot the numerical solution after 10^5 time steps for a non-resonnant stepsize (left) and a resonnant stepsize (right).

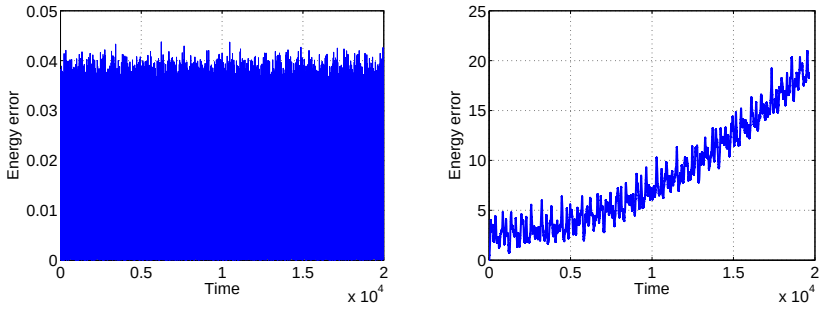

FIGURE 2. Relative energy error for a non-resonnant stepsize (left) and a resonnant stepsize (right).

Parabolic Monge-Ampère Methods for Blow-up problems in several spatial dimensions

CHRIS BUDD
(joint work with John F Williams)

One of the key geometric features associated with the solution of partial differential equations is the evolution of structures on several different length scales. Indeed, the analysis of *multi-scale* phenomenon is now a major source of research activity. In certain problems, for example porous media flows, the length scales are widely separated and these problems can be studied using, for example, multi-scale finite element methods. However, there are many other problems in which length scales are not widely separated and indeed we see a *continuum* of length scales. These are generally driven by some nonlinearity in the problem and are tightly coupled in an essentially geometric manner. Scaling laws are almost universal in many partial differential equations and often describe asymptotic features of a solution such as the formation of singularities and interfaces, when the effects of boundary and initial conditions are less important. Examples arise in fluid mechanics, magneto hydrodynamics, solid mechanics, nonlinear optics and electrostatics. It

is clear that numerical methods which can exploit the scaling structures in a partial differential equation are likely to perform well. To construct such methods we need to understand the *scaling symmetries* that lie behind the various scaling structures. Such symmetries are generally described by Abelian, diagonalizable Lie groups, and thus have a simpler structure than many other problems studied by geometric methods. However, the universality of scaling laws makes it appropriate to develop methods just for them. The sort of problems that we are interested in studying have length scales $L(t)$ driven by nonlinear effects, which are vanishingly small in some limit. Typically there is some time T for which $L \to 0$ as $t \to T$. Such problems pose a challenge for any numerical method, and cannot be studied by using a method with a fixed grid of size h when $L(t) \ll h$. In such cases it is appropriate to use an *adaptive* method, in which the spatial mesh can adapt itself to the natural scale of the solution.

In this talk we will examine a class of r-adaptive moving mesh methods for approximating solutions of the parabolic equation

$$u_t = \Delta u + f(u), \quad \mathbf{x} \in \Omega \subset R^d, \quad u|_{\partial\Omega} = 0. \tag{1}$$

We will consider geometrically based adaptive methods for both slowly evolving solutions of (1) and also solutions be which become singular (blow-up) in a finite time T. We will concentrate in our calculations on the case of $d = 2$, although the methods can in principle work in higher dimensions. Whilst the solution of (1) in one-dimension by using (scale invariant) r-adaptive methods is now fairly well understood, less progress has been made in extending these methods to higher dimensions where there are significant new difficulties. In this talk we describe a new method for solving (1) in spatial dimensions greater than one which is well adapted to exploiting *emergent scaling structures*. These methods will be based on the Parabolic Monge-Ampère method. In this method a fixed mesh in *computational coordinates* ξ is mapped to a moving mesh $\mathbf{x}$ in the physical coordinates. The map from computational to physical coordinates is determined in terms of the gradient of a *mesh potential* Q which satisfies a fully nonlinear parabolic partial differential equation of the form

$$(I - \gamma\Delta)Q_t = M(u)H(Q)^{1/d} \tag{2}$$

where $H(Q)$ is the determinant of the Hessian of Q, d is the spatial dimension and $M(u)$ is a *monitor function* which depends upon the solution. In two dimensions

$$H(Q) = Q_{\xi\xi}Q_{\eta\eta} - Q_{\xi\eta}^2.$$

The equation (2) is solved in parallel with (1) and is constructed (through a careful choice of the function M to have the same scaling symmetries. We show that any scaling structure present in the solution u is inherited by the mesh potential function and derive from this a series of properties of the resulting mesh. We demonstrate through examples, that (when careful attention is paid to mesh

regularity and smoothing) the Parabolic Monge-Ampère method is effective for computing the singular solutions of (1) in two spatial dimensions.

Semidirect Products and Their Relation to Integrable Systems

Tudor S. Ratiu

This talk is a progress report on several topics that are interrelated: semidirect product reduction and the discretization of integrable systems.

The classical theory of reduction for semidirect products of Lie groups with vector spaces goes back to the late seventies ([1], [4], [5], [6]) and took its definitive form in [2] and [3]. Due to lack of space the semidirect product theory will not be reviewed here and we refer to the quoted papers. So only the discretization part of the talk will be summarized below.

Next we shall give an interesting example of an integrable system on the semidirect product SE(3), namely the Kowalevski top, and will discretize it according to the Hirota method. This is joint work with my student Murat Turhan.

The Kowalevski top is the third integrable case of rigid body dynamics:

$$\begin{cases} \dot{\mathbf{\Pi}} = \mathbf{\Pi} \times \mathbf{\Omega} + Mgl\mathbf{\Gamma} \times \boldsymbol{\chi} \\ \dot{\mathbf{\Gamma}} = \mathbf{\Gamma} \times \mathbf{\Omega} \end{cases}$$

where the principal moments of inertia are $I_1 = I_2 = 2I_3$ and the unit vector on the line connecting the fixed point with the center of mass is $\boldsymbol{\chi} = (1, 0, 0)$; M is the total mass of the body, and l is the length of the segment that connects the fixed point to the center of mass. Explicitly, this is

$$2\frac{d\Omega_1}{dt} = \Omega_2\Omega_3, \quad 2\frac{d\Omega_2}{dt} = -\Omega_1\Omega_3 + x_0\Gamma_3, \quad \frac{d\Omega_3}{dt} = -x_0\Gamma_2,$$
$$\frac{d\Gamma_1}{dt} = \Omega_3\Gamma_2 - \Omega_2\Gamma_3, \quad \frac{d\Gamma_2}{dt} = \Omega_1\Gamma_3 - \Omega_3\Gamma_1, \quad \frac{d\Gamma_3}{dt} = \Omega_2\Gamma_1 - \Omega_1\Gamma_2,$$

where $x_0 := \frac{2Mgl}{I_1}$. The Kowalevski equations have four conserved quantities. The first three are standard for any heavy top:

(1) Hamiltonian: $H_1 = \frac{I_1}{2}(2\Omega_1^2 + 2\Omega_2^2 + \Omega_3^2) - x_0\Gamma_1$
(2) Angular momentum (Casimir): $H_2 = I_1(2\Omega_1\Gamma_1 + 2\Omega_2\Gamma_2 + \Omega_3\Gamma_3)$
(3) Spatial gravity vector (Casimir): $H_3 = \Gamma_1^2 + \Gamma_2^2 + \Gamma_3^2$

To prove integrability, one more conserved quantity is needed. Here is how Kowalevski found it. Let $z = \Omega_1 + i\Omega_2$ and $\xi = \Gamma_1 + i\Gamma_2$. Then the equations of motion imply :

$$2\dot{z} = -i\Omega_3 z + ix_0\Gamma_3 \qquad \text{and} \qquad \dot{\xi} = i\Gamma_3 z - i\Omega_3\xi.$$

We can eliminate Γ_3 by considering the combination $z^2 - x_0\xi$:

$$\begin{aligned} \frac{d}{dt}(z^2 - x_0\xi) &= 2z\dot{z} - x_0\dot{\xi} \\ &= z(-i\Omega_3 z + ix_0\Gamma_3) - x_0(i\Gamma_3 z - i\Omega_3\xi) \\ &= -i\Omega_3(z^2 - x_0\xi). \end{aligned}$$

By complex conjugation we get

$$\frac{d}{dt}(\bar{z}^2 - x_0\bar{\xi}) = i\Omega_3(\bar{z}^2 - x_0\bar{\xi}).$$

This implies that $|z^2 - x_0\xi|^2$ is conserved. In terms of the original variables, we obtain the **Kowalevski integral**

$$\begin{aligned} H_4 &= |z^2 - x_0\xi|^2 = |(\Omega_1 + i\Omega_2)^2 - x_0(\Gamma_1 + i\Gamma_2)|^2 \\ &= (\Omega_1^2 - \Omega_2^2 - x_0\Gamma_1)^2 + (2\Omega_1\Omega_2 - x_0\Gamma_2)^2. \end{aligned}$$

It is still a mystery where this comes from. If one writes in matrices what Kowalevski did, one passes from $\mathbb{R}^3$ to $\mathfrak{so}(3)$ to $\mathfrak{su}(2)$ using the Pauli spin matrices. But why this isomorphism of Lie algebras should give one more integrable case is not known.

The discretization of the Kowalevski top according to the Hirota formulation proceeds in the following way. Impose the dependent variable transformation:

$$\Omega_1 = \frac{g_1}{f}, \qquad \Omega_2 = \frac{g_2}{f}, \qquad \Omega_3 = \frac{g_3}{f},$$
$$\Gamma_1 = \frac{g_4}{f}, \qquad \Gamma_2 = \frac{g_5}{f}, \qquad \Gamma_3 = \frac{g_6}{f}$$

and introduce the Hirota operator

$$D_t g_j \cdot f = \frac{dg_j}{dt} f - g_j \frac{df}{dt}, \qquad j = 1, \ldots, 6.$$

The equations of motion become

$$\begin{cases} 2D_t g_1 \cdot f = g_2 g_3 \\ 2D_t g_2 \cdot f = -g_1 g_3 + x_0 g_6 f \\ D_t g_3 \cdot f = -x_0 g_5 f \\ D_t g_4 \cdot f = g_3 g_5 - g_2 g_6 \\ D_t g_5 \cdot f = g_1 g_6 - g_3 g_4 \\ D_t g_6 \cdot f = g_2 g_4 - g_1 g_5 \end{cases}$$

This is invariant under the gauge transformation

$$f(t) \longmapsto f(t)h(t), \qquad g_j(t) \longmapsto g_j(t)h(t)$$

where $h(t)$ is an arbitrary function of t.

Replace the bilinear differential operator $D_t g_j \cdot f$ by the corresponding bilinear difference operator

$$D_t g_j \cdot f \longrightarrow [g_j(t+\delta)f(t) - g_j(t)f(t+\delta)]/(2\delta)$$

where δ is a time interval. Using gauge invariance and time reversibility, we obtain the following bilinear equations :

$$\begin{cases} 2(g_1^{t+1}f^t - g_1^t f^{t+1})/(2\delta) = (g_2^{t+1}g_3^t + g_2^t g_3^{t+1})/2 \\ 2(g_2^{t+1}f^t - g_2^t f^{t+1})/(2\delta) = -(g_1^{t+1}g_3^t + g_1^t g_3^{t+1})/2 \\ \qquad\qquad + x_0(g_6^{t+1}g_3^t + g_6^t g_3^{t+1})/2 \\ I_1(g_3^{t+1}f^t - g_3^t f^{t+1})/(2\delta) = -x_0(g_5^{t+1}f^t + g_5^t f^{t+1})/2 \\ (g_4^{t+1}f^t - g_4^t f^{t+1})/(2\delta) = (g_3^{t+1}g_5^t + g_3^t g_5^{t+1})/2 \\ \qquad\qquad - (g_2^{t+1}g_6^t + g_2^t g_6^{t+1})/2 \\ (g_5^{t+1}f^t - g_5^t f^{t+1})/(2\delta) = (g_1^{t+1}g_6^t + g_1^t g_6^{t+1})/2 \\ \qquad\qquad - (g_3^{t+1}g_4^t + g_3^t g_4^{t+1})/2 \\ (g_6^{t+1}f^t - g_6^t f^{t+1})/(2\delta) = (g_2^{t+1}g_4^t + g_2^t g_4^{t+1})/2 \\ \qquad\qquad - (g_1^{t+1}g_5^t + g_1^t g_5^{t+1})/2 \end{cases}$$

where $f^{t+1} := f(t+\delta)$.

The product $f^t f^{t+1}$ cancels so we get the algorithm:

$$\begin{cases} 2(\Omega_1^{t+1} - \Omega_1^t)/\delta &= (\Omega_2^{t+1}\Omega_3^t + \Omega_2^t\Omega_3^{t+1}) \\ 2(\Omega_2^{t+1} - \Omega_2^t)/\delta &= -(\Omega_1^{t+1}\Omega_3^t + \Omega_1^t\Omega_3^{t+1}) + x_0(\Gamma_3^{t+1} + \Gamma_3^t) \\ (\Omega_3^{t+1} - \Omega_3^t)/\delta &= -x_0(\Gamma_2^{t+1} + \Gamma_2^t) \\ (\Gamma_1^{t+1} - \Gamma_1^t)/\delta &= (\Omega_3^{t+1}\Gamma_2^t + \Omega_3^t\Gamma_2^{t+1}) - (\Omega_2^{t+1}\Gamma_3^t + \Omega_2^t\Gamma_3^{t+1}) \\ (\Gamma_2^{t+1} - \Gamma_2^t)/\delta &= (\Omega_1^{t+1}\Gamma_3^t + \Omega_1^t\Gamma_3^{t+1}) - (\Omega_3^{t+1}\Gamma_1^t + \Omega_3^t\Gamma_1^{t+1}) \\ (\Gamma_3^{t+1} - \Gamma_3^t)/\delta &= (\Omega_2^{t+1}\Gamma_1^t + \Omega_2^t\Gamma_1^{t+1}) - (\Omega_1^{t+1}\Gamma_2^t + \Omega_1^t\Gamma_2^{t+1}) \end{cases}$$

where $\Omega_1^t = \frac{g_1^t}{f^t}$, $\Omega_2^t = \frac{g_2^t}{f^t}$, $\Omega_3^t = \frac{g_3^t}{f^t}$, $\Gamma_1^t = \frac{g_4^t}{f^t}$, $\Gamma_2^t = \frac{g_5^t}{f^t}$, $\Gamma_3^t = \frac{g_6^t}{f^t}$. These are the "Discrete Kowalevski Equations (DKEs)". One can explicitly solve for the variables at time $t+1$, so these equations are "explicit" and "time-reversible" equations.

Discrete Conserved Quantities.

1. Hamiltonian: $H_1^0 = (\Omega_3^t)^2 - H_1^1\big((\Omega_1^t)^2 + (\Omega_2^t)^2\big) - H_1^2(\Gamma_1^t)^2$
2. Angular momentum: $H_2^0 = \Omega_1^t\Gamma_1^t + \Omega_3^t\Gamma_3^t - H_2^1(\Omega_2^t\Gamma_2^t) - H_2^2(\Gamma_1^t)^2$
3. Spatial gravity vector: $H_3^0 = (\Gamma_3^t)^2 - H_3^1(\Gamma_1^t)^2 - H_3^2(\Gamma_2^t)^2$
4. Kowalevski integral: $H_4^0 = \big((\Omega_1^t)^2 + (\Omega_2^t)^2\big)^2 + (\Gamma_1^t)^2 + (\Gamma_2^t)^2 - H_4^1(\Omega_2^t\Gamma_2^t) - H_4^2(\Gamma_1^t)^2$.

H_i^k $(i = 1, 2, 3, 4; k = 1, 2)$ are quantities to be determined by the requirement that the integrals are indeed invariant. For example, let's find H_3^2. Since we want H_3^0, H_3^1 and H_3^2 to be invariant, we must have:

$$\begin{aligned} H_3^0 &= (\Gamma_3^{t+1})^2 - H_3^1(\Gamma_1^{t+1})^2 - H_3^2(\Gamma_2^{t+1})^2, \\ H_3^0 &= (\Gamma_3^t)^2 - H_3^1(\Gamma_1^t)^2 - H_3^2(\Gamma_2^t)^2, \\ H_3^0 &= (\Gamma_3^{t-1})^2 - H_3^1(\Gamma_1^{t-1})^2 - H_3^2(\Gamma_1^{t-1})^2. \end{aligned}$$

Under the condition $\Gamma_k^{t+m} \neq 0 \quad (k = 1,2,3; m = -1,0,1)$, these equations uniquely determine H_3^0, H_3^1 and H_3^2.

H_3^2 can be written of the form N_3^2/D_3^2 in terms of $\Gamma_j^{t+1}, \Gamma_j^t, \Gamma_j^{t-1}$:

$$\begin{aligned} N_3^2 &= \big((\Gamma_1^t)^2 - (\Gamma_1^{t-1})^2\big)\big((\Gamma_3^t)^2 - (\Gamma_3^{t+1})^2\big) \\ &\quad - \big((\Gamma_3^t)^2 - (\Gamma_3^{t-1})^2\big)\big((\Gamma_1^{t+1})^2 - (\Gamma_1^t)^2\big) \\ D_3^2 &= \big((\Gamma_1^t)^2 - (\Gamma_1^{t-1})^2\big)\big((\Gamma_2^{t+1})^2 - (\Gamma_2^t)^2\big) \\ &\quad - \big((\Gamma_2^t)^2 - (\Gamma_2^{t-1})^2\big)\big((\Gamma_1^{t+1})^2 - (\Gamma_1^t)^2\big). \end{aligned}$$

Use DKEs to eliminate Γ_i^{t+1} and Γ_i^{t-1} $(i = 1,2,3)$ and express H_3^2 in terms of Ω_i^t, Γ_i^t $(i = 1,2,3)$ using only information at time t. This is possible and one gets

$$H_3^2 = h_{32}(\Omega_1^t, \Omega_2^t, \Omega_3^t, \Gamma_1^t, \Gamma_2^t, \Gamma_3^t, x_0, \delta)$$

In this way we can express $H_1^0, H_1^1, H_1^2, H_2^0, H_2^1, H_2^2, H_3^0, H_3^1, H_4^0, H_4^1$ and H_4^2.
It is shown that H_3^2 in the expression above is a conserved quantity of the DKEs.

This is done finding a Gröbner basis on the formula manipulation software Risa/ASIR. This shows that $H_3^2(t+1) - H_3^2(t) = 0$.

Now we found many discrete integrals. Actually, after obtaining the generators of the ideal I, we solve those polynomials with using software Maple and we get four independent conserved quantities H_1^0, H_2^2, H_3^1 and H_4^1, the rest of H_i^k's are dependent.

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Doing what comes naturally (learning optimal control from the experts)

Debra Lewis

(joint work with Peter Olver)

Optimal control problems involve minimization of a cost function C subject to constraints: if state variables $x \in \boldsymbol{R}^n$ satisfy the control law $\dot{x} = v(x,u,t)$ for

some function $v : \boldsymbol{R}^n \times \boldsymbol{R}^k \times \boldsymbol{R} \to \boldsymbol{R}^n$ and controls $u \in \boldsymbol{R}^k$, then we can seek a control curve $u : I \to \boldsymbol{R}^k$ minimizing

$$\mathcal{L}(\gamma) = \int_I \big(C(x(t), u(t), t) + p(t)^T(\dot{x}(t) - v(x(t), u(t), t)\big)\, dt.$$

(Appropriate boundary conditions must be imposed.) The Lagrange multiplier $p \in \boldsymbol{R}^n$ serves to enforce the evolution equation $\dot{x} = v$. This variational formulation extends naturally to nonlinear manifolds, with the vector-valued Lagrange multiplier p being replaced by a one-form on the nonlinear state space. However, practical methods for determination of the extremals of such problems typically make use of some additional structure on the manifold. We focus on the case in which the state space is a Lie group G.

The global trivialization of the tangent and cotangent bundles of Lie groups significantly simplifies the analysis of optimal control problems. If we right or left trivialize the vector field for the evolution of the state variables, then the Lagrange multipliers used in the formulation of the variational problem naturally lie in the dual of the Lie algebra. We consider the case in which the state space G and control space H are both Lie groups (both G and H may be vector spaces, products of groups, etc), with evolution equation $\operatorname{triv} \dot{g} = \omega(g, h, t)$ for some map $\omega : G \times H \times \boldsymbol{R} \to \mathfrak{g}$; here $\operatorname{triv} : TG \to \mathfrak{g}$ denotes the algebra component of the right (left) trivialization of the tangent vector $\dot{g}$. Given a cost function $C : G \times H \times \boldsymbol{R} \to \boldsymbol{R}$ we define

$$\mathcal{L}(\gamma) = \int_I (C(g, h, t) + p(t) \cdot (\operatorname{triv} \dot{g}(t) - \omega(g, h, t)))\, dt,$$

where $\gamma = (g, h, p) : I \to G \times H \times \mathfrak{g}^*$. If we define the 'functional derivatives' $\frac{\delta C}{\delta g} : G \to \mathfrak{g}^*$ and $\frac{\delta C}{\delta h} : H \to \mathfrak{h}^*$ by

$$dC(g, h, t) \cdot (\delta g, \delta h, \delta t) = \tfrac{\delta C}{\delta g}(g, h, t) \cdot \delta g + \tfrac{\delta C}{\delta h}(g, h, t) \cdot \delta h + \tfrac{\partial C}{\partial t}(g, h, t)\delta t$$

for all $\delta g \in T_g G$, $g \in G$, $\delta h \in T_h H$, $h \in H$, $\delta t \in \boldsymbol{R}$, $t \in I$, then

$$\begin{aligned} d\mathcal{L}(\gamma) \cdot \delta\gamma \quad = \quad & \int_I \Big(\delta p \cdot (\operatorname{triv} \dot{g} - \omega) + \Big(\tfrac{\delta C}{\delta g} \pm \operatorname{ad}^*_\omega p - \dot{p}\Big) \cdot \xi \\ & + \Big(\tfrac{\delta C}{\delta h} - \tfrac{\delta \omega}{\delta h}^* p\Big) \cdot \eta + \tfrac{\partial C}{\partial t}\delta t\Big)\, dt. \end{aligned}$$

Here $\xi : I \to \mathfrak{g}$ and $\eta : I \to \mathfrak{h}$ denote the trivialized variations of g and h; the sign of the infinitesimal coadjoint action term is determined by the choice of right or left trivialization. If the functional derivative $\frac{\delta C}{\delta h}$ is nondegenerate with respect to h, then the control h for a critical curve γ is determined by the equation $\frac{\delta C}{\delta h} = \frac{\delta \omega}{\delta h}^* p$. If $\frac{\delta C}{\delta h}$ is degenerate, e.g. if C does not depend on the control, then optimal control curves must be sought by other methods.

Our motivating application is the 'falling cat': it is well known that many animals have the ability to right themselves in free-fall, following a trajectory with trivial angular momentum. Etienne-Jules Marey, a physiologist and innovator in high-speed photography, studied the maneuvers used by cats and other quadrupeds to right themselves while falling. Marey (1894) published a brief and apparently

controversial article describing a zero angular momentum cat flip achieved using internal torques and changes of the moments of inertia of the front and back portions of the body. Kane and Scher (1969) constructed a simple, elegant mathematical model of the falling cat, modeling the front and back halves of the cat as rigid bodies coupled by a joint satisfying a 'no-twist' condition and undergoing relatively little backward bending. Montgomery (1993) translated their model into modern geometric language, formulating the evolution equations in terms of connections on an appropriate principal bundle and showing that the Kane-Scher motions are the solutions of an optimal control problem closely related to geodesic flow.

The Kane-Scher model captures some features of the flip, but the twisting and changes of the relative moments described by Marey and others are explicitly ruled out in their model. As a starting point for a more realistic model, we have constructed an alternative simple flip: the cat is modeled as two axisymmetric bodies coupled by a universal joint; the bodies are rigid during each phase of the maneuver, but the moments of inertia differ from phase to phase. The associated equations have solutions consisting of a series of spins about the axes of symmetry (with corresponding counter-rotation of the other half of the body), followed in some cases by a folding motion about the perpendicular axis; the axis of symmetry of the front half remains in the initial vertical plane throughout the flip, and the axes of symmetry of the front and back half are at right angles until the final phase of the flip. Specifically:

- Start with the two halves 'belly up', at right angles and centered about the vertical
- Spin the front half, counter-rotating the back half until its axis of symmetry is perpendicular to the vertical plane
- Spin the back, counter-rotating the front downward
- Spin the front, counter-rotating the back until it returns to the vertical plane
- If necessary, rotate both halves about the perpendicular to achieve an overall rotation through π about the horizontal axis in the initial vertical plane.

The relative speeds of the spins and counter-rotations are determined by the current relative moments of inertia of the two halves.

These motions form two families, which we label odd and even (this labeling is derived from the integers parameter determining each family):

'Odd' flips: The head twist overshoots in first phase and swings back in the third phase. At the end of the first three phases, the axes of symmetry have returned to their original positions, forming a 'V', with backward spinal bend and the belly facing downward; the two halves of the body now fold inward—each half rotates through $\frac{\pi}{2}$ in the vertical plane. The maximum relative rotation is through $\frac{3\pi}{2}$.

'Even' flips: The head twist undershoots in first phase and rotates in the same direction in the third phase. At the end of the three spin/counter-rotation phases

the 'cat' has completed the flip—no folding is necessary. The maximum relative rotation is through 2π.

The Kane-Scher model seems too rigid—it shows just how simple a zero momentum flip can be, but it doesn't look much like what cats actually do—while the alternative model seems too acrobatic—the transitions are unrealistically abrupt and the maximum relative rotations are severe. We intend to construct relatively simple motions between these extremes, using an optimal control formulation with several contributing costs. We soften the Kane-Scher constraints and blend the stages of the alternative method using time-minimization augmented by penalties for implausible behavior:

- *Time:* Elapsed time for flip is weighted heavily.
- *Relative motion of front and back halves:* Severe spinal bending and twisting are penalized, but small-to-moderate relative motions are low-cost.
- *Change of shape of body components:* Variations of the moments of inertia are relatively low-cost for moderate changes, expensive for large changes.
- *Working blind:* Inability to see the ground is penalized, but the penalty for being moderately off the final head position is low.

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Lie Group Variational Integrators and its Applications to Geometric Control Theory

Melvin Leok

(joint work with Anthony M. Bloch, Islam I. Hussein, Taeyoung Lee, N. Harris McClamroch, Amit K. Sanyal)

The geometric approach to mechanics serves as the theoretical underpinning of innovative control methodologies in geometric control theory. These techniques allow the attitude of satellites to be controlled using changes in its shape, as opposed to chemical propulsion, and are the basis for understanding the ability of a falling cat to always land on its feet, even when released in an inverted orientation.

Curiously, while the geometric structure of mechanical systems plays a critical role in the construction of geometric control algorithms, these algorithms have typically been implemented using numerical schemes that ignore the underlying geometry. We introduce new geometric integration techniques that are applicable to the construction of efficient implementations of optimal control algorithms arising from geometric control theory.

Generalized Galerkin Variational Integrators [7]**.** The most common criticism leveled against the geometric integration community is that the preservation of geometric structure alone is not a sufficient criterion for a good numerical method. Variational integrators are obtained by discretizing the action integral in two stages, by choosing a finite-dimensional function space to discretize sections of the configuration bundle over space-time, and by approximating the integral using numerical quadrature. Important considerations in numerical analysis, such as adaptivity, approximability, and accuracy can be incorporated into the context of discrete mechanics through an appropriate choice of function space and numerical quadrature, as discussed in, *Generalized Galerkin Variational Integrators* [7].

Lie Group Variational Integrators [4, 5]**.** Lie group variational integrators preserve the Lie group structure of the configuration space without the use of local charts, reprojection, or constraints. Instead, the discrete solution is updated using the exponential of a Lie algebra element which satisfies a discrete variational principle. These yield highly efficient geometric integration schemes for rigid body dynamics that automatically remain on the rotation group. By representing the attitude as a rotation matrix, we avoid coordinate singularities associated with local charts such as Euler angles, and obtain a global representation of the configuration that is particularly important in efficiently simulating chaotic orbital motion.

These ideas were introduced in the paper, *A Lie Group Variational Integrator for the Attitude Dynamics of a Rigid Body with Applications to the 3D Pendulum* [4]. This is applied to a system of extended rigid bodies interacting under their mutual gravitational potential in the paper, *Lie Group Variational Integrators for the Full Body Problem* [5], wherein symmetry reduction to a relative frame is also addressed.

Discrete Optimal Control on Lie Groups [1, 6, 3]**.** Our approach to discretizing the optimal control problem is in contrast to traditional techniques such as collocation, wherein the continuous equations of motion are imposed as constraints at a set of collocation points. In our approach, modeled after [2], the discrete equations of motion are derived from a discrete variational principle, and this induces constraints on the configuration at each discrete timestep. The discrete dynamics are more faithful to the continuous equations of motion, and consequently more accurate solutions to the optimal control problem are obtained.

For the purpose of numerical simulation, the corresponding discrete optimal control problem is posed on the discrete state space as a two stage discrete variational problem. In the first step, the discrete dynamics for the the rigid body is derived from the discrete Lagrange-d'Alembert principle, as well as methods introduced in the work on Lie group variational integrators [4]. These discrete equations are then imposed as constraints to be satisfied by the extremal solutions to the discrete optimal control problem, and necessary conditions for the discrete

extremal solution are obtained in terms of the given terminal states. This approach is described in the paper, *A Discrete Variational Integrator for Optimal Control Problems on $SO(3)$* [1].

The paper, *Attitude Maneuvers of a Rigid Spacecraft in a Circular Orbit* [6], discusses optimal control problems whereby the forces are only applied at the start and end of the maneuver, but where the relative frame is prescribed by a nominal trajectory, like a circular orbit. The problem is posed as a discrete optimal control problem with constraints, which is solved directly using a sequential quadratic programming method.

An adjoint formulation can also be adopted, wherein the forward computation computes the trajectories, and the backward computation yields the sensitivity of the cost functional in terms of the design parameters. This yields an efficient and robust optimal control algorithm based on multiple shooting, as documented in *Optimal Attitude Control of a Rigid Body using Geometrically Exact Computations on $SO(3)$* [3].

The typical reason for numerical instability in shooting based optimization algorithms is due to the difficulty in computing the sensitivities of the terminal boundary conditions on the initial controls in a stable fashion. We exploit the structure preserving properties of variational integrators to compute the sensitivities in a robust manner.

These ideas are applicable to the efficient construction of quantum gates, since a quantum gate is realized by generating a trajectory in the space of unitary operators from the identity to the desired operator through the use of external controls, and can therefore be formulated in terms of optimal control on Lie groups.

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Semi-implicit semi-Lagrangian time-stepping methods and regularized fluid equations in numerical weather prediction

Sebastian Reich

(joint work with Jason Frank, Nigel Wood, Andrew Staniforth)

The fundamental components of a numerical weather prediction (NWP) code are provided by (i) data assimilation, (ii) dynamic core, and (iii) parameterization of unresolved phenomena such as precipitation. The talk was primarily concerned with numerical aspects of the dynamic core, which is provided by the inviscid Euler equations of stratified and rotating ideal fluid dynamics. I first discussed geometric and conservation aspects of the equations of motion and their potential preservation under numerical discretizations in space and time. I also briefly summarized the multi-scale nature of atmospheric fluid dynamics.

In the second part of my talk, I reviewed the widely used semi-implicit semi-Lagrangian (SISL) time-stepping method. The SISL method is, for example, used by the UK Met Office to overcome the severe step-size restrictions due to unresolved waves as well as strong advection in their non-hydrostatic Unified Model. The idea of the Unified Model is to only use unapproximated Euler equations for the dynamic core and to have the spatial and temporal approximations select the desired spatial and temporal resolution. The practical implementation of the Unified Model methodology poses challenging questions to the practitioners and theoreticians alike. Our own current work focuses on an interpretation of the semi-implicit method as a regularization of the unapproximated Euler equations and the implementation of such a regularization within an explicit time-stepping method.

In the final part of my talk I reported about first results on an explicit time-staggered semi-Lagrangian method. The time-staggered formulation is based on the regularized Störmer-Verlet time-stepping method for the Hamiltonian particle-mesh (HPM) method as proposed in [1, 2]. It has been demonstrated that the explicit Sörmer-Verlet time-stepping of the regularized equations is, on a linear equation level, equivalent to the effect of semi-implicit time-stepping of the unregularized shallow-water equations [3, 4]. Numerical results were presented for the rotating shallow water equations and a non-hydrostatic vertical slice model.

The ultimate goal is to implement the regularized time-staggered semi-Lagrangian method for the three-dimensional Euler equations and to test the methods within the Unified Model framework.

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Parcel Eulerian–Lagrangian fluid dynamics

Marcel Oliver
(joint work with Onno Bokhove)

1. Introduction

Conservation laws play an important role in geophysical fluid mechanics. In the absence of forcing and dissipation, conservations laws can be derived systematically from the variational or Hamiltonian structure of the equations of fluid motion. Conservation or near-conservation of mass, energy, and vorticity in the underlying idealized model and its numerical treatment is considered desirable to enhance stability and accurate ensemble forecasting, even though the dynamics of the atmosphere and oceans are ultimately driven by forcing on the large scales and subject to viscosity on the small scales.

Particle methods for fluids [6] have favorable conservation properties, as can be shown by interpreting the dynamics of particles as a non-autonomous Hamiltonian system with particle position and particle velocity as variables; parcels interact via the transport of mass or vorticity [4]. Generally, the Hamiltonian associated with a particle representation consists of a type of Bernoulli function, that is, the sum of the Lagrangian kinetic energy plus an Eulerian potential function depending on space, evaluated at the position of the particle, and time. It turns out that in continuum fluid dynamics a single fluid parcel satisfies the same non-autonomous Hamiltonian formulation, which is finite dimensional for the one distinguished fluid parcel. The Eulerian potential is now transported by the flow generated by the parcel velocities, thereby coupling the parcels to a continuum. We call this the parcel Eulerian–Lagrangian formulation.

The question we ask is how such parcel Eulerian–Lagrangian formulations relate to the well-known Lagrangian or Eulerian continuum Hamiltonian mechanics. The answer turns out to be natural, but is not immediately obvious: The restriction from continuum to parcel variational principle is done by choosing special variations which are concentrated on points in label space, and which are constrained by the natural local conservation laws of the continuum formulation. Vice versa, the continuum formulation can be recovered from the parcel formulation by a procedure which essentially amounts to integration over label space.

We can therefore, on the one hand, derive parcel formulations, and thus natural particle schemes, for equations of continuum mechanics by a general procedure. On the other hand, we can translate results from one formulation to the other. In particular, the continuum Poisson bracket inherits the Jacobi identity by construction from the parcel formulation, where it is more easily verified.

2. Continuum vs. parcel formulation for shallow water

The rotating shallow water equation are known to be Hamiltonian with

$$\mathcal{H} = \tfrac{1}{2} \int \big(h\,|\boldsymbol{u}|^2 + g\,(h+b)^2 \big)\,\mathrm{d}\boldsymbol{x} \tag{1}$$

and possesses the Poisson formulation $\mathrm{d}\mathcal{F}/\mathrm{d}t = \{\mathcal{F}, \mathcal{H}\}$ with bracket

$$\int \{F, G\}\, h\,\mathrm{d}\boldsymbol{x} = \int \left(q\, \frac{\delta \mathcal{F}}{\delta \boldsymbol{u}}^{\perp} \cdot \frac{\delta \mathcal{G}}{\delta \boldsymbol{u}} - \frac{\delta \mathcal{F}}{\delta \boldsymbol{u}} \cdot \boldsymbol{\nabla} \frac{\delta \mathcal{G}}{\delta h} + \frac{\delta \mathcal{G}}{\delta \boldsymbol{u}} \cdot \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta h} \right) \mathrm{d}\boldsymbol{x} \equiv \{\mathcal{F}, \mathcal{G}\}\,, \tag{2}$$

where $q = (f + \boldsymbol{\nabla}^{\perp} \cdot \boldsymbol{u})/h$ denotes the potential vorticity. Inserting appropriate test functionals, it is easy to derive the Eulerian equations of motion,

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} + f\, \boldsymbol{u}^{\perp} + g\, \boldsymbol{\nabla}(h+b) = 0\,, \tag{3a}$$

$$\partial_t h + \boldsymbol{\nabla} \cdot (h\, \boldsymbol{u}) = 0\,. \tag{3b}$$

In the parcel formulation, on the other hand, each "fluid parcel" is treated as an independent, two degree of freedom nonautonomous Hamiltonian system, where

$$H(\boldsymbol{X}, \boldsymbol{U}, t) = \frac{1}{2}\,|\boldsymbol{U}|^2 + g\,\big(h(\boldsymbol{X}, t) + b(\boldsymbol{X})\big)\,. \tag{4}$$

and Poisson formulation $\mathrm{d}F/\mathrm{d}t = \{F, H\}$ with bracket

$$\{F, G\} = f\, \boldsymbol{\nabla}_{\boldsymbol{U}}^{\perp} F \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} G + \boldsymbol{\nabla}_{\boldsymbol{X}} F \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} G - \boldsymbol{\nabla}_{\boldsymbol{X}} G \cdot \boldsymbol{\nabla}_{\boldsymbol{U}} F\,. \tag{5}$$

The resulting parcel equations of motion are

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{\nabla}_{\boldsymbol{U}} H = \boldsymbol{U}\,, \tag{6a}$$

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -f\, \boldsymbol{\nabla}_{\boldsymbol{U}}^{\perp} H - \boldsymbol{\nabla}_{\boldsymbol{X}} H = -f\, \boldsymbol{U}^{\perp} - g\, \boldsymbol{\nabla}(h+b)\,, \tag{6b}$$

where the dynamics of the parcels is linked through the mass transport equation

$$h(\boldsymbol{X}, t) = \int_D h_0(\boldsymbol{a})\, \delta\big(\boldsymbol{X} - \boldsymbol{\chi}(\boldsymbol{a}, t)\big)\,\mathrm{d}\boldsymbol{a}\,, \tag{6c}$$

which is *not* part of the parcel variational structure, but rather plays the role of an external potential. This parcel formulation readily yields the equations of smoothed particle hydrodynamics [6] upon replacing h_0 by a finite sum of point masses and the δ-distribution in (6c) by a mollifier or blob function. Note that the continuum Hamiltonian $\mathcal{H}$ is not the parcel Hamiltonian H integrated over label space—there is no factor $\frac{1}{2}$ in front of the parcel potential energy.

To pass to the parcel formulation, we start with the continuum Hamilton principle and note that the continuity equation acts as a constraint. (The formalism could be cast into the abstract framework of Euler–Poincaré reduction for semidirect products [5].) Letting η denote the flow map, so that $\dot{\boldsymbol{\chi}} = \boldsymbol{u} \circ \boldsymbol{\chi}$, we must take variations of the shallow water action with respect to the flow map. This corresponds to an Eulerian variation $\boldsymbol{w}$ via $\delta\boldsymbol{\chi} = \boldsymbol{w} \circ \boldsymbol{\chi}$, and the continuity equation implies that $\delta h + \boldsymbol{\nabla} \cdot (\boldsymbol{w} h) = 0$.

The key idea is to restrict, under the above constraint, the class of variations to

$$\delta\boldsymbol{\chi}(\boldsymbol{a},t) = \delta(\boldsymbol{a}-\boldsymbol{A})\,\delta\boldsymbol{X}\,, \tag{7}$$

where $\delta(\,\cdot\,)$ denotes the Dirac mass. In a second step, we identify the restricted variation of the full action integral as the total variation of a per-parcel action integral, which then yields the parcel Hamiltonian structure. We can also reverse this process by integrating the parcel Poisson formulation over label space, which allows us, for example, to prove the Jacobi identity for the continuum Poisson bracket by merely verifying the parcel Poisson bracket; for details, see [1].

3. Continuum vs. parcel formulation for ideal fluids

The procedure applies to any fluid equation with an advected scalar, such as the compressible Euler equations in any dimension [1]. Of particular interest are the incompressible Euler equations in two dimensions, where vorticity plays the role of the advected scalar. The continuum Hamiltonian is the well known kinetic energy Hamiltonian,

$$\mathcal{H} = \frac{1}{2}\int |\boldsymbol{u}|^2 \,\mathrm{d}\boldsymbol{x}\,, \tag{8}$$

the vorticity Poisson bracket reads

$$\{\mathcal{F},\mathcal{G}\} = \int \omega\, \boldsymbol{\nabla}^\perp\!\left(\frac{\delta\mathcal{F}}{\delta\omega}\right)\cdot\boldsymbol{\nabla}\!\left(\frac{\delta\mathcal{G}}{\delta\omega}\right)\mathrm{d}\boldsymbol{x}\,, \tag{9}$$

and the vorticity equations of motion are

$$\partial_t\omega + \boldsymbol{u}\cdot\boldsymbol{\nabla}\omega = 0\,, \tag{10a}$$

$$\omega = \boldsymbol{\nabla}^\perp\cdot\boldsymbol{u}\,, \tag{10b}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0\,. \tag{10c}$$

The parcel formulation, on the other hand, has the nonautonomous Hamiltonian

$$H(\boldsymbol{X},t) = -\psi(\boldsymbol{X},t)\,, \tag{11}$$

Poisson bracket

$$\{F,G\} = \boldsymbol{\nabla}^\perp F\cdot\boldsymbol{\nabla}G\,, \tag{12}$$

and corresponding parcel equations of motion

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = -\boldsymbol{\nabla}^\perp H = \boldsymbol{\nabla}^\perp\psi\,, \tag{13a}$$

$$\Delta\psi = \omega\,, \tag{13b}$$

$$\omega(\boldsymbol{X},t) = \int_D \omega_0(\boldsymbol{a},t)\,\delta\big(\boldsymbol{X}-\boldsymbol{\chi}(\boldsymbol{a},t)\big)\,\mathrm{d}\boldsymbol{a}\,. \tag{13c}$$

Replacing ω_0 by a finite sum of delta distributions yields the familiar point vortex dynamics, and additional smoothing of the Dirac delta in the transport integral will lead to a numerical vortex method [2].

In this case, naively restricting the Hamilton principle to the vorticity transport law results in a tautology. The key observation which allows us to restrict the continuum variational principle in a nontrivial way is that, when starting from an extended Lagrangian formulation, the particle relabeling symmetry yields a vorticity-like conservation law *without* assuming a bijection between momenta and velocities. This conservation law is then used to restrict the extended Lagrangian and the construction can proceed as for the shallow water equations; for details see [1].

Our procedure provides, in particular, a correspondence between the Hamiltonian formulation for ideal fluids, and the Hamiltonian formulation of 2D point vortex dynamics.

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Properties of exponential integrators for nonlinear wave equations

Brynjulf Owren

(joint work with Håvard Berland, Bård Skaflestad)

Semilinear PDEs have the form

$$u_t = Lu + N(u) \tag{1}$$

where L is a linear unbounded operator and N is a nonlinear map. We consider exponential integrators of the form

$$\begin{aligned} U_{n,r} &= \mathrm{e}^{c_r hL} u_n + h \sum_{j=1}^{r-1} a_r^j(hL) N(U_{n,j}),\ r = 1, \ldots, s \\ u_{n+1} &= \mathrm{e}^{hL} u_n + h \sum_{r=1}^{s} b^r(hL) N(U_{n,r}) \end{aligned}$$

The *coefficient functions* $a_{rj}(z)$ and $b_r(z)$ are assumed to be

(1) entire functions in the complex plane
(2) bounded on the imaginary axis

Sometimes we also required that $\phi(\mathrm{i}y) \leq C|y|^{-q}$ for $y \in \mathbf{R}$. Rigorous conditions for order of convergence of exponential integrators applied to semilinear PDEs have been derived by Hochbruck and Ostermann [4]

The cubic Schrödinger equation in 1D on a periodic domain is

$$\mathrm{i}u_t + u_{xx} = (\lambda|u|^2 + V(x))u \tag{2}$$

We treat separately the case when $V(x) \equiv 0$. We consider the Sobolev space H^s as the functions $f(x)$ such that

$$\sum_{k\in\mathbf{Z}} (1+k^2)^s |\hat{f}(k)|^2 < \infty \quad \text{where} \quad \hat{f}(k) = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\,\mathrm{e}^{-\mathrm{i}kx}\,dx$$

It follows from the a paper by Bourgain [2] that the problem (2) with $V(x) \equiv 0$ is well-posed for every $s \geq 0$. Moreover, as pointed out by Christ et al. [3], for non-negative integers k, one has that $\sup_t \|u(t)\|_{H^k}$ is bounded by a constant which depends only on k and the H^k-norm of the initial datum.

One easily sees that for $s > \frac{1}{2}$, $u \in H^s$ implies that $|u|^2 u \in H^s$. From this fact, we observe that any exponential integrator as defined above will map $u_n \in H^s$ to $u_{n+1} \in H^s$ whenever $s > \frac{1}{2}$. For a nonvanishing $V(x)$ one may have the situation that the corresponding $N(u)$ in (1) maps $H^s \to H^\sigma$ for $\sigma < s$. It then follows that the exponential integrators maps H^s to H^s if $s - \sigma < \min\{1, 2q\}$ if all the coefficient functions have decay rate q.

Finally, one may consider nonlinear wave equations of the form

$$w_{tt} = Lw + f(w)$$

which may be transformed into a system of the form (1) by using the vector variable $u = (w, w_t)$. One then finds that if $f : H^s \to H^s$, then the exponential integrator maps elements of $H^s \times H^{s-1}$ to $H^s \times H^{s-1}$.

In general it may be hard to prove that the numerical approximation obtained by an exponential integrator is bounded in H^s independently of the stepsize, even for finite time intervals. However, such bounds have been proved for linearised versions of the equations, and numerical evidence seems to indicate that this may also be valid for the 1D nonlinear Schrödinger equation. Given that such a bound exists, one may combine the above mentioned smoothness properties with the nonstiff order conditions derived in [1] to prove order of convergence results for the exponential integrators expressed in terms if smoothness of the data.

A MATLAB toolbox which implements a wide range of exponential integrators for many examples of PDEs is available for free at

`http://www/math.ntnu.no/num/expint/`

This package also facilitates easy addition of new problems and integrators.

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Numerical Methods for Multiscale Problems

Assyr Abdulle

Consider u^ε, the solution of a (partial) differential equation

$$L^\varepsilon u^\varepsilon = f^\varepsilon, \tag{1}$$

where L^ε is a linear differential operator for which ε indicates the small scales in the coefficients. Due to the oscillations in these coefficients, u^ε will typically exhibit small scale oscillations. The scale gap between the length of the oscillation and the phenomena of interest (large scale behavior) makes direct simulation of (1) with a standard numerical method often impossible. A common approach is to compute an effective or homogenized operator $\bar{L}$, in which the small scales have been averaged out and to solve the corresponding homogenized equation (see [9] and references therein)

$$\bar{L}\bar{u} = \bar{f}. \tag{2}$$

The problem (2) can be solved with standard methods. However, this procedure has several drawbacks. First, restrictive assumptions on the data (periodicity, homogeneity) are needed to derive explicit equations for the homogenized problem 2 . Second, the coefficients of the homogenized equation have usually to be computed numerically so that a *control* of the overall procedure (i.e. the numerical discretization of the homogenized equations with numerically computed coefficients) is difficult. Third, the fine scale behavior, i.e. the oscillations of the solution, is lost in the homogenization process.

In this report we discuss several numerical methods for multiscale problems constructed within the framework of the Heterogeneous Multiscale Methods (HMM) [1], [2], [3], [4], [5], [6], [7], [8]. These methods discretize the physical problem directly by a "macroscopic numerical model" with a macroscopic discretization. The input coefficients of the macroscopic numerical model are unknown, since the macroscopic model is not supposed to be known (we do not precompute an averaged equation as (2)). These coefficients are recovered on the fly by solving a "microscopic numerical model" on sampling domains within the macro discretization. A variety of micro-macro approaches based on iterative schemes, have been proposed in the literature, mainly for elasticity problems, including nonlinear problems (see [5] for a discussion and references). The iterative procedure in these approaches increases the cost of the methods and makes a full error control of these micro-macro schemes difficult even for linear problems.

Heterogeneous multiscale methods for variational problems. We consider the following elliptic model problem in the domain $\Omega \subset \mathbb{R}^d$

$$-\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial\Omega, \tag{3}$$

where we assume that the tensor $a^\varepsilon(x) = a(x, \frac{x}{\varepsilon}) = a(x, y)$ is symmetric, coercive and periodic with respect to each component of y in the unit cube $Y = (0,1)^d$. We further assume that $f \in L^2(\Omega)$, $a_{ij}(x,\cdot) \in L^\infty(\mathbb{R}^d)$, that $x \to a_{ij}(x,\cdot)$ is smooth from $\bar{\Omega} \to L^\infty(\mathbb{R}^d)$ and that Ω is a convex polygon. The FE-HMM for the elliptic homogenization problem, based on the macro finite element (FE) space $S_0^1(\Omega, \mathcal{T}_H)$ ($\mathcal{T}_H$ is the macro triangulation) is defined by a *modified macro bilinear form* [3],[8],

$$B(u^H, v^H) = \sum_{K \in \mathcal{T}_H} \frac{|K|}{|K_\varepsilon|} \int_{K_\varepsilon} \nabla u^h \; a(x_k, x/\varepsilon)(\nabla v^h)^T dx, \tag{4}$$

where $K_\varepsilon = x_k + \varepsilon[-1/2, 1/2]^d$ is a sampling sub-domain centered at the barycenter x_k of the triangle K, where $|K|, |K_\varepsilon|$ denote the measure of K and K_ε, respectively, and where u^h is the solution of the following *micro problem*: find u^h such that $(u^h - u^H) \in W^1_{per}(K_\varepsilon)$ and

$$\int_{K_\varepsilon} \nabla u^h \; a(x_k, x/\varepsilon)(\nabla z^h)^T dx = 0 \quad \forall z^h \in S^1_{per}(K_\varepsilon, \mathcal{T}_h). \tag{5}$$

For $K_\varepsilon \subset K \in \mathcal{T}_H$, we consider the micro FE space $S^1_{per}(K_\varepsilon, \mathcal{T}_h) \subset H^1_{per}(K_\varepsilon)/\mathbb{R}$ of piecewise linear polynomials on the micro triangulation $\mathcal{T}_h$, periodic on the boundary ∂K_ε. The meshsizes of the macro and micro spaces are denoted by H and h, respectively. The following convergence estimates have been obtained in [3] for the *fully discrete* FE-HMM

$$\|u^0 - u^H\|_{H^1(\Omega)} \le C\Big(H + \big(\frac{h}{\varepsilon}\big)^2\Big), \quad \|u^0 - u^H\|_{L^2(\Omega)} \le C\Big(H^2 + \big(\frac{h}{\varepsilon}\big)^2\Big), \tag{6}$$

$$\|u^\varepsilon - u_p^\varepsilon\|_{\bar{H}^1(\Omega)} \le C\Big(H + \varepsilon + \frac{h}{\varepsilon}\Big), \tag{7}$$

where u^ε is the solution of problem (3), u^0 is the solution of the homogenized problem corresponding to (3) and u_p^ε is a reconstructed solution obtained from u^H with fine scale solution $(u - u^H)$ periodically extended on each element K (see [8],[1]). For the estimate (7), the norm $\bar{H}$ is mesh dependent since u_p^ε can be discontinuous across the macro elements K. Similar fully discrete estimates have also be derived for the effective velocity in transport problems [4] and for elasticity problems [5].

Heterogeneous multiscale methods for dynamic problems. Consider the parabolic homogenization problem

$$\frac{\partial u^\varepsilon}{\partial t} = \nabla \cdot (a^\varepsilon \nabla u^\varepsilon) \text{ in } (0,T) \times \Omega \tag{8}$$

$$u^\varepsilon = 0 \quad \text{on } (0,T) \times \partial\Omega, \qquad u^\varepsilon(0,x) = g(x) \quad \text{on } \Omega, \tag{9}$$

where $u^\varepsilon = u^\varepsilon(t,x)$, $\Omega \subset \mathbb{R}^d$ is a bounded domain, and $a^\varepsilon(x)$ is symmetric, uniformly coercive and bounded. We further assume that $a^\varepsilon(x)$ and $g(x)$ are regular

enough in order to have a smooth solution of the above problem. In the sequel we describe the algorithm in one dimension for simplicity (see [1] for generalizations). A coarse model for (8) is given by $\frac{\partial U}{\partial t} = \nabla \cdot (a^0 \nabla U)$, where a^0 (the homogenized tensor) reflects the large scale impact of a^ε. As for the previous problem, we do not assume that a^0 is known. The finite difference heterogeneous multiscale method (FD-HMM) [1] is defined by a macroscopic scheme on a coarse grid $\{x_i\}_{i=0}^N$ of Ω

$$U_i^{k+1} = U_i^k + \Delta t \frac{J_{i+1/2}^k + J_{i-1/2}^k}{\Delta x} \tag{10}$$

with meshsize Δx and evolved with a coarse time step Δt. The unknown fluxes $J_{i\pm 1/2} = \frac{\pm 1}{|K^\varepsilon_{x_{i\pm 1/2}}|} \int_{K^\varepsilon_{x_{i\pm 1/2}}} a^\varepsilon \nabla \hat{u}^\varepsilon dx$ are given by the average of micro solutions $\hat{u}^\varepsilon$ obtained by solving small scale problems on sampling domains $K^\varepsilon_{x_{i\pm 1/2}}$ of size ε centered around $x_{i\pm 1/2}$ for a small time $[t^k, t^k + \delta]$

$$\frac{\partial \hat{u}^\varepsilon}{\partial t} = \nabla \cdot (a^\varepsilon \nabla \hat{u}^\varepsilon)\,(t,x) \in (t^k, t^k + \delta) \times K^\varepsilon_{x_{i\pm 1/2}}, \tag{11}$$

$$\hat{u}^\varepsilon - U^k(x) \quad \varepsilon-\text{periodic on } (t^k, t^k + \delta) \times \partial K^\varepsilon_{x_{i\pm 1/2}}, \quad \hat{u}(t^k, x) = U^k(x), \tag{12}$$

where δ is a relaxation time (see [1]). The initial values at the cells $K^\varepsilon_{x_{i\pm 1/2}}$ are obtained by linear reconstruction of the known solution $\{U_i^k\}_{i=0}^N$ at time t^k.

For the convergence analysis [1] we have to introduce an intermediate problem. Let $\{U_i^k\}_{i=0}^N$ be the solution of the FD-HMM at time $t^k = t_0 + k\Delta t$ and let $\{\bar{U}_i^k\}_{i=0}^N$ be the solution of a finite difference method similar to (10) but with fluxes $\bar{J}_{i\pm 1/2} = (a^0(\bar{U}_{i\pm 1/2} - \bar{U}_i))/\Delta x$. Then it can be shown [1]

$$\max_{0\le i\le N} |U_i^k - \bar{U}_i^k| \le CT\frac{\varepsilon}{\Delta x} \quad \forall t_k \in [0,T].$$

$\{\bar{U}_i^k\}_{i=0}^N$ can be seen as a standard FD method for the homogenized problem, for which standard convergence results, provided enough smoothness of the solution, give $\max_i |U(t^k, x_i) - \bar{U}_i^k| \le CT(\Delta t + (\Delta x)^2) \quad \forall t_k \in [0,T]$. Combining both results, we obtain the following error estimate for the FD-HMM when compared to the homogenized solution of problem (8)

$$\max_{0\le i\le N} |U(t^k, x_i) - U_i^k| \le CT\Big(\Delta t + (\Delta x)^2 + \frac{\varepsilon}{\Delta x}\Big) \quad \forall t_k \in [0,T].$$

Here, the exact solution for the micro problem (11) has been assumed. For a fully discrete analysis, the discretization of this problem with a micro spatial mesh with meshsize $\delta\xi$ has to be considered. The term $\frac{\delta\xi}{\varepsilon}$ is expected to appear [6].

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Structural Preserving Isospectral Flows for Quadratic Pencils

Moody T. Chu
(joint work with Nicoletta Del Buono)

The eigeninformation $(\lambda, \mathbf{u})$ of the quadratic pencil,

$$Q(\lambda) := Q(\lambda; M_0, C_0, K_0) = \lambda^2 M_0 + \lambda C_0 + K_0, \tag{1}$$

is critical to the understanding of the dynamical system

$$M_0\ddot{\mathbf{x}} + C_0\dot{\mathbf{x}} + K_0\mathbf{x} = f(t), \tag{2}$$

which arises frequently in many important applications, including applied mechanics, electrical oscillations, vibro-acoustics, fluid mechanics, and signal processing. It is easy to see that the linear pencil,

$$L(\lambda) := L(\lambda; M_0, C_0, K_0) = \begin{bmatrix} C_0 & M_0 \\ M_0 & 0 \end{bmatrix} \lambda + \begin{bmatrix} K_0 & 0 \\ 0 & -M_0 \end{bmatrix}, \tag{3}$$

in the so called Lancaster structure, is equivalent to $Q(\lambda)$. Recently, it has been shown that for almost all quadratic pencils there exists real-valued $2n \times 2n$ real matrices Π_ℓ and Π_r such that

$$\Pi_\ell^\top L(\lambda)\Pi_r = L(\lambda; M_D, C_D, K_D) = \begin{bmatrix} C_D & M_D \\ M_D & 0 \end{bmatrix} \lambda + \begin{bmatrix} K_D & 0 \\ 0 & -M_D \end{bmatrix}, \tag{4}$$

where M_D, C_D, K_D are all real-valued $n \times n$ diagonal matrices [2, 3, 4]. Such a transformation is significant in that it links the dynamical behavior of a multiple-degree-of-freedom system directly to that of a system consisting of n independent single-degree-of-freedom subsystems. It breaks down the interlocking connectivity in the original system into totally disconnected subsystems while preserving the entire spectral properties. Thus it will be of great value in practice if the transformations Π_ℓ and Π_r can be found from any given pencil. The theory of existence of Π_ℓ and Π_r in [2, 3] was established on the basis of the complete spectral information of $L(\lambda)$. To construct Π_ℓ and Π_r from the availability of spectral information certainly is impractical. The emphasis of this talk is to construct Π_ℓ and Π_r numerically by structure preserving isospectral flows without knowing the spectral information.

Denote

$$\Pi_\ell = \begin{bmatrix} \ell_{11} & \ell_{12} \\ \ell_{21} & \ell_{22} \end{bmatrix}, \quad \Pi_r = \begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix}, \tag{5}$$

where each ℓ_{ij} or r_{ij} is an $n \times n$ matrices. In order to maintain the Lancaster structure in the transformation $\Pi_\ell^\top L(\lambda)\Pi_r$, it is necessary that the following five equations hold:

$$\begin{aligned} -\ell_{11}^\top K_0 r_{12} + \ell_{21}^\top M_0 r_{22} &= 0, \\ -\ell_{12}^\top K_0 r_{11} + \ell_{22}^\top M_0 r_{21} &= 0, \\ \ell_{12}^\top C_0 r_{12} + \ell_{22}^\top M_0 r_{12} + \ell_{12}^\top M_0 r_{22} &= 0, \\ \ell_{11}^\top C_0 r_{12} + \ell_{21}^\top M_0 r_{12} + \ell_{11}^\top M_0 r_{22} &= \ell_{12}^\top C_0 r_{11} + \ell_{22}^\top M_0 r_{11} + \ell_{12}^\top M_0 r_{21} \\ &= -\ell_{12}^\top K_0 r_{12} + \ell_{22}^\top M_0 r_{22}. \end{aligned} \tag{6}$$

Additionally, the matrices Π_ℓ and Π_r must be such that the left-hand sides of the following three expressions,

$$\begin{aligned} -\ell_{12}^\top K_0 r_{12} + \ell_{22}^\top M_0 r_{22} &= M_D, \\ \ell_{11}^\top C_0 r_{11} + \ell_{21}^\top M_0 r_{11} + \ell_{11}^\top M_0 r_{21} &= C_D, \\ \ell_{11}^\top K_0 r_{11} - \ell_{21}^\top M_0 r_{21} &= K_D, \end{aligned} \tag{7}$$

are diagonal matrices. The conditions (6) and (7) together constitute a homogeneous second-degree polynomial system of $8n^2 - 3n$ equations in $8n^2$ unknowns. It is not obvious how the system could be solved analytically. The underdetermined system does suggest, however, that there is plenty of leeway to choose the transformation matrices Π_ℓ and Π_r. In particular, the "orbit" of $L(\lambda)$ under (Lancaster) structure preserving equivalence transformations is a nontrivial manifold on which perhaps a smooth path connecting (M_0, C_0, K_0) to (M_D, C_D, K_D) can be defined.

To characterize the orbit, denote the Lancaster pair in (3) by (A_0, B_0) where

$$A_0 = \begin{bmatrix} K_0 & 0 \\ 0 & -M_0 \end{bmatrix}, \qquad B_0 = \begin{bmatrix} C_0 & M_0 \\ M_0 & 0 \end{bmatrix}. \tag{8}$$

We are interested in developing two one-parameter families of structured preserving transformations $T_L(t), T_R(t) \in \mathbb{R}^{2n\times 2n}$, with $T_L(0) = T_R(0) = I_{2n}$. Consider the actions of these families of transformations on (A_0, B_0) by

$$A(t) = T_L^\top(t) A_0 T_R(t), \qquad B(t) = T_L^\top(t) B_0 T_R(t), \tag{9}$$

respectively. Clearly, regardless how $T_L(t)$ and $T_R(t)$ are defined, $(A(t), B(t))$ is isospectral to (A_0, B_0) for any t. It appears sufficient to limit ourselves to a special class of transformations where matrices $T_L(t)$ and $T_R(t)$ satisfy, respectively,

$$\frac{dT_L(t)}{dt} = T_L(t)\mathcal{L}(t) = T_L(t) \begin{bmatrix} L_{11}(t) & L_{12}(t) \\ L_{21}(t) & L_{22}(t) \end{bmatrix}, \tag{10}$$

$$\frac{dT_R(t)}{dt} = T_R(t)\mathcal{R}(t) = T_R(t) \begin{bmatrix} R_{11}(t) & R_{12}(t) \\ R_{21}(t) & R_{22}(t) \end{bmatrix}, \tag{11}$$

where each $L_{ij}(t)$ or $R_{ij}(t)$, $i,j=1,2$, is a $n\times n$ real one-parameter matrix yet to be defined. Upon substitution, we observe from (9) that

$$\begin{aligned}\frac{dA}{dt} &= \dot{T}_L^\top A_0 T_R + T_L A_0 \dot{T}_R &= \mathcal{L}^\top A + A\mathcal{R},\\ \frac{dB}{dt} &= \dot{T}_L^\top B_0 T_R + T_L B_0 \dot{T}_R &= \mathcal{L}^\top B + B\mathcal{R}.\end{aligned}$$

It is interesting to note that these differential equations are similar to those discussed in [1] which leads to a Lie-Poisson system. By insisting that $(A(t),B(t))$ maintains the Lancaster structure, that is,

$$A(t)=\begin{bmatrix} K(t) & 0\\ 0 & -M(t)\end{bmatrix},\qquad B(t)=\begin{bmatrix} C(t) & M(t)\\ M(t) & 0\end{bmatrix}, \tag{12}$$

we see that the entries of $\mathcal{L}(t)$ and $\mathcal{R}(t)$ should satisfy:

$$R_{12} = -DM, \tag{13}$$
$$R_{21} = DK, \tag{14}$$
$$L_{12} = D^\top M^\top, \tag{15}$$
$$L_{21} = -D^\top K^\top, \tag{16}$$
$$L_{11}-L_{22} = D^\top C^\top, \tag{17}$$
$$R_{11}-R_{22} = -DC, \tag{18}$$

where $D\in\mathbb{R}^{n\times n}$ is an arbitrary matrix parameter. Also hidden implicitly in (17) and (18) are the other two free matrix parameters. There are several possible ways to choose the parameters and to arrange the diagonal blocks of $\mathcal{L}(t)$ and $\mathcal{R}(t)$. For instance, corresponding to the choice,

$$\mathcal{L} = \begin{bmatrix} D^\top & 0\\ 0 & D^\top\end{bmatrix}\begin{bmatrix} \frac{C^\top}{2} & M^\top\\ -K^\top & -\frac{C^\top}{2}\end{bmatrix}+\begin{bmatrix} N_L^\top & 0\\ 0 & N_L^\top\end{bmatrix}, \tag{19}$$

$$\mathcal{R} = \begin{bmatrix} D & 0\\ 0 & D\end{bmatrix}\begin{bmatrix} -\frac{C}{2} & -M\\ K & \frac{C}{2}\end{bmatrix}+\begin{bmatrix} N_R & 0\\ 0 & N_R\end{bmatrix}, \tag{20}$$

an isospectral flow of the triplet $(M(t),C(t),K(t))$ can be defined by the autonomous system:

$$\begin{aligned}\dot{K} &= \frac{1}{2}(CDK-KDC)+N_L^\top K+KN_R,\\ \dot{C} &= (MDK-KDM)+N_L^\top C+CN_R,\\ \dot{M} &= \frac{1}{2}(MDC-CDM)+N_L^\top M+MN_R.\end{aligned} \tag{21}$$

Furthermore, by assuming $N_R(t)=N_L(t)$, the symmetry specified for the matrix parameter D in Table 1 will preserve the symmetry for the flow $(M(t),K(t),C(t))$ defined by the dynamical system (21).

The remaining task is to control the free matrix parameters in such a way that the structure preserving isospectral flow $(A(t),B(t))$ is also a gradient flow for a certain properly selected objective function. Our idea is based on the scenario that

$D(t)$	$M(t)$	$C(t)$	$K(t)$
skew-symmetric	symmetric	symmetric	symmetric
symmetric	symmetric	skew-symmetric	symmetric
symmetric	skew-symmetric	skew-symmetric	skew-symmetric
skew-symmetric	skew-symmetric	symmetric	skew-symmetric

TABLE 1. Preserving symmetries of $(M(t), C(t), K(t))$ by $D(t)$, if $N_R(t) = N_L(t)$.

given a sufficiently smooth objection function $f : \mathbb{R}^n \to \mathbb{R}$ whose state variable $\mathbf{x} \in \mathbb{R}^n$ is constrained to the integral curve of $\dot{\mathbf{x}} = g(\mathbf{x})\mathbf{u}$ starting with $\mathbf{x}(0) = \mathbf{x}_0$ where $\mathbf{u}(t)$ is the control, perhaps one way we can do is to choose the control $\mathbf{u}$ so that the vector $\dot{\mathbf{x}}$ is as close to $-\nabla f(\mathbf{x})$ as possible. This amounts to the selection of the least squares solution $\mathbf{u}$ defined by

$$\mathbf{u}(t) = -g(\mathbf{x}(t))^\dagger \nabla f(\mathbf{x}(t)), \tag{22}$$

where $g(\mathbf{x})^\dagger$ stands for the Moore-Penrose generalized inverse of $g(\mathbf{x})$. In this way, the closed-loop dynamical system,

$$\dot{\mathbf{x}} = -g(\mathbf{x})g(\mathbf{x})^\dagger \nabla f(\mathbf{x}), \tag{23}$$

defines a descent flow $\mathbf{x}(t)$ for the objective function $f(\mathbf{x})$. This scenario fits us perfectly if we seek matrix parameters N_R, N_L and D to minimize the function,

$$\begin{aligned} f(K, C, M) &:= \frac{1}{2}\left\{\|\text{offdiag}(M)\|_F^2 + \|\text{offdiag}(C)\|_F^2 + \|\text{offdiag}(K)\|_F^2\right\} \\ &+ \delta h(\text{diag}(M), \text{diag}(C), \text{diag}(K)), \end{aligned} \tag{24}$$

subject to the condition that $(M(t), C(t), K(t))$ is governed by the differential system (21). Our purpose in designing the objective function is to minimize the off-diagonal entries of (M, C, K) while using the function h to monitor the behavior of the diagonal entries by a factor of δ. The free matrix parameters D, N_L and N_R are used as controls to direct the flow and can be obtained as the least squares solution to the equation:

$$\begin{bmatrix} \frac{1}{2}(K \otimes C - C \otimes K) & K \otimes I & I \otimes K \\ K \otimes M - M \otimes K & C \otimes I & I \otimes C \\ \frac{1}{2}(C \otimes M - M \otimes C) & M \otimes I & I \otimes M \end{bmatrix} \begin{bmatrix} \mathbf{vec}(D) \\ \mathbf{vec}(N_L^\top) \\ \mathbf{vec}(N_R) \end{bmatrix} = \begin{bmatrix} \mathbf{vec}(-\text{offdiag}(K) - \delta \frac{\partial h}{\partial K}) \\ \mathbf{vec}(-\text{offdiag}(C) - \delta \frac{\partial h}{\partial C}) \\ \mathbf{vec}(-\text{offdiag}(M) - \delta \frac{\partial h}{\partial M}) \end{bmatrix}$$

Since the gradient flow can be tracked by available ODE integrator, it is feasible for numerical computation. Computer simulations seem to suggest the working of this approach.

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A numerical method for Hamiltonian systems based on piecewise smooth space-approximations

Philippe Chartier
(joint work with Erwan Faou)

Consider a Hamiltonian system

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H(q,p), \\ \dot{p} & = & -\nabla_q H(q,p), \end{array} \right. \tag{1}$$

where $(q,p) \in \boldsymbol{R}^d \times \boldsymbol{R}^d$, and with a separable Hamiltonian H of the form

$$H(q,p) = \frac{1}{2} p^T p + V(q),$$

where $V(q)$ is the potential function. In many applications, such as for instance molecular dynamics, it is of importance that the numerical flow used to compute the solution of (1) preserves the volume form and the Hamiltonian. However, it is generally admitted that no standard method can satisfy both requirements, apart from exceptional situations such as for instance a quadratic Hamiltonian. In the case of *multi-quadratic* potentials as considered by R. Quispel and R.I. McLachlan in [5], a possible approach consists in solving in sequence the d Hamiltonian systems with Hamiltonians

$$\begin{array}{rcl} H^{[i]}(q_i,p_i) & = & \frac{1}{2} p_i^2 + V^{[i]}(q_i) + \frac{1}{2} \sum_{j \neq i} \bar{p}_j^T \bar{p}_j, \\ V^{[i]}(q_i) & = & V\left(\bar{q}_1, \ldots, \bar{q}_{i-1}, q_i, \bar{q}_{i+1}, \ldots, \bar{q}_d\right), \end{array}$$

obtained by freezing all components (denoted with a bar) except the two conjugate coordinates q_i and p_i. If each subsystem is then solved exactly and the same step-size is used for all, the resulting "numerical" method preserves the desired quantities, since each sub-step is symplectic and preserves $H^{[i]}$ (and thus H).

In order to retain the possibility of solving exactly each sub-system and at the same time to cover more general situations, we give up the requirement of exact Hamiltonian preservation and we consider a multi-quadratic piecewise approximation of H. If instead of (1) we now solve

$$\left\{ \begin{array}{rcl} \dot{q} & = & \nabla_p H^\tau(q,p), \\ \dot{p} & = & -\nabla_q H^\tau(q,p), \end{array} \right. \tag{2}$$

where $H^\tau(q,p) = \frac{1}{2}p^T p + V^\tau(q)$ is a $C^{1,1}$ multi-quadratic approximation of H, the aforementioned procedure applied with exact solution of the sub-systems gives a first-order method which preserves H^τ exactly as well as the volume form. If $\sup_K |H - H^\tau| \leq C_K\ \tau^2$ for a compact subset K of $\boldsymbol{R}^d \times \boldsymbol{R}^d$ containing the numerical solution, then H is conserved up to an error of size τ^2 over arbitrarily long intervals of integration (including infinite ones).

In this talk, we describe the implementation of the method with quadratic B-splines only for the case of separable Hamiltonians and prove the following properties of the flow of piecewise polynomial Hamiltonian systems:

Theorem 1. *Let H be a continuously differentiable scalar function defined on $\boldsymbol{R}^{2d}$ such that $f = J^{-1}\nabla H$ is Lipschitz over the whole space $\boldsymbol{R}^{2d}$ and consider the flow φ_t associated with f. Then, for a fixed $t \in \boldsymbol{R}$, φ_t satisfies the following properties:*

- *(iii) for any $y \in \boldsymbol{R}^{2d}$, $H(\varphi_t(y)) = H(y)$, that is to say φ_t is Hamiltonian-preserving.*
- *(iv) φ_t is a.e. differentiable on $\boldsymbol{R}^{2d}$.*
- *(vi) $(\varphi_t')^T J \varphi_t' = J$ a.e. on $\boldsymbol{R}^{2d}$.*
- *(vii) $|det(\varphi_t')| = 1$ a.e. on $\boldsymbol{R}^{2d}$.*

An explicit expression of the exact solution is given for the two-dimensional case that serves as a basis for higher dimensions and the numerical scheme used here is shown to be of order 1 and becomes an order 2 method when composed with its adjoint, though in a slightly weaker sense than usual:

Theorem 2. *Let φ_t be the exact flow of the system (1) and $\varphi_{i,t}^\tau$ the exact flow of the Hamiltonian system with Hamiltonian $H^{[i,\tau]}$. The numerical flow Φ_h^τ as defined above with stepsize $h > 0$ and space discretization parameter τ is of the form $\Phi_h^\tau = \varphi_{1,h}^\tau \circ \dots \varphi_{d,h}^\tau$ and satisfies the following estimate for all Lipschitz function g with compact support:*

$$|\langle \varphi_h - \Phi_h^\tau | g \rangle| \leq C(h\tau + h^2 \|g\|_{L^1}) \tag{3}$$

for a constant C depending on V, and for sufficiently small h and τ.

If the systems for the $H^{[i,\tau]}$ are solved for $i = 1, \dots, d$ and then for $i = d, \dots, 1$ in reverse order, the resulting method $\Phi_{h/2}^\tau \circ \left(\Phi_{h/2}^\tau\right)^*$ is symmetric and

$$|\langle \varphi_h - \Phi_{h/2}^\tau \circ \left(\Phi_{h/2}^\tau\right)^* |g\rangle| \leq C(h\tau + h^3 \|g'\|_{L^1}). \tag{4}$$

Eventually, we present numerical results for three different test problems, for which the usual behaviour of symplectic integrators is exhibited and no resonances occur: the Kepler problem, Fermi-Pasta-Ulam mechanical system and the Sine-Gordon equation.

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Integral–preserving Integrators

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(joint work with D.I. McLaren[1])

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Many systems of differential equations possess so–called geometric properties, for example one or more first integrals, symplectic structure, volume preservation, and others. Numerical solution of such systems is usually best effected using a geometric integrator, i.e. one that can preserve this property exactly (i.e. up to round–off accuracy) [1, 2, 3].

In this extended abstract we are particulary interested in integral–preserving integrators (IPIs) which are designed to provide exact preservation of any first integral possessed by a system of ordinary differential equations (ODEs), e.g. momentum, angular momentum, energy, etc. We concentrate here on IPIs using so–called discrete gradients [4, 5, 6, 7, 8].

Consider thus an ODE

$$\frac{dx}{dt} = f(x) \quad x \in \mathbb{R}^n \tag{1}$$

which possesses a first integral $I(x)$, i.e.

$$\frac{dI(x)}{dt} = 0 \tag{2}$$

provided x satisfies (1).

Under conditions that are generally satisfied, (1) and (2) are equivalent to the existence of a skew matrix $S(x)$ such that (1) can be rewritten*

$$\frac{dx}{dt} = S(x)\nabla I(x). \tag{3}$$

An IPI for (3) is given by

$$\frac{x' - x}{h} = \bar{S}(x, x')\bar{\nabla} I(x, x'). \tag{4}$$

Here h denotes the time step, and

$$x := x(nh), \quad x' := x((n+1)h),$$

and $\bar{S}$ and $\bar{\nabla}$ denote a "discrete skew matrix" resp a "discrete gradient".

Discrete gradients must satisfy

$$I(x') - I(x) =: \bar{\nabla} I(x, x') \cdot (x' - x)$$

Discrete skew matrices must be skew, otherwise the only conditions on $\bar{S}$ and $\bar{\nabla}$ are that they must be consistent, i.e. in the limit $h \to 0$, i.e. $x' \to x$, they must go to S resp. ∇.

*Note that in general $S(x)$ does **not** satisfy the Jacobi identity.

It follows that $\bar{S}$ and $\bar{\nabla}$ are not at all unique. Many examples of discrete gradients have been constructed [5, 6], here we give two in $\mathbb{R}^2$:

$$\bar{\nabla}_1 I(x,x') := \begin{pmatrix} \frac{I(x_1',x_2)-I(x_1,x_2)}{x_1'-x_1} \\ \\ \frac{I(x_1',x_2')-I(x_1',x_2)}{x_2'-x_2} \end{pmatrix}$$

Here $x =: (x_1, x_2),\ x' =: (x_1', x_2')$.

A second example is given by

$$\bar{\nabla}_2 I(x,x') := \frac{\bar{\nabla}_1 I(x,x') + \bar{\nabla}_1 I(x',x)}{2}$$

In general, the above will give a numerical integration method of first–order accuracy.

There are various ways to obtain IPIs of higher order of accuracy. One method that we have developed constructs a method of order $n+1$ from a method of order n. For the sake of simplicity we here only give the construction of a second–order IPI from a first–order one:

Let $\dfrac{x'-x}{h} = S_1 \bar{\nabla} I(x,x')$ be a first–order IPI, with $S_1 := S = S(x)$, then a second–order IPI is given by

$$\frac{x'-x}{h} = S_2 \bar{\nabla} I(x,x'),$$

where

$$S_2 := S + h\left(\mathrm{SQS} + \frac{1}{2}C\right).$$

Here C and Q are skew matrices given by:

$$C^{ij} := \frac{\partial S^{ij}}{\partial x_m} S^{ml} \frac{\partial I}{\partial x_l}$$

and

$$Q := \frac{1}{2}(B^T - B),$$

where B is defined by

$$\bar{\nabla} =: \nabla I + B(x)\cdot(x'-x) + O\left(\|x'-x\|^2\right)$$

Similarly one obtains higher–order IPIs.

Concluding, we remark that

(1) Multiple integrals are preserved similarly.
(2) We are currently studying N–dimensional systems with $N-1$ integrals.
(3) Some generalizations of the above ideas to PDEs exist.

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Splitting Methods in Geometric Numerical Integration

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(joint work with Fernando Casas, Ander Murua)

A widely used technique in the geometric numerical integration of differential equations is the splitting idea: if the differential equation can be split into two or more parts that are either solvable or simpler to integrate than the original system, it is also possible to build integrators by composition of the corresponding flows. They are frequently used in celestial mechanics, quantum mechanics, molecular dynamics, accelerator physics and, in general, for solving numerically Hamiltonian systems, as well as Poisson systems and reversible differential equations [6, 7, 8, 9]. They can be adapted to many different problems and frequently can be combined in a natural way with other techniques to improve their performances. In addition, many problems can be split in many different ways leading to systems differing in the following aspects: (i) the geometric properties which are preserved; (ii) the cost for evaluating each part; (iii) the magnitude of the error when using a given method; (iv) the alternative techniques to combine with splitting (modified vector fields, processing, etc.); (v) the families of splitting methods which can be used. Then, the knowledge of the algebraic structure a given problem in many cases helps to choose highly efficient methods from the literature, or to build new methods tailored for a given family of problems. This is well illustrated by the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x)\right)\psi(x,t). \tag{1}$$

After a semidiscretization, we have to solve the following linear system of ODEs

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t), \qquad \mathbf{c}(0) = \mathbf{c}_0 \in \mathbb{C}^N \tag{2}$$

with formal solution $\mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}_0$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{R}^{N\times N}$ is an Hermitian matrix. Fourier methods are frequently used to approximate the solution because $(\mathbf{Vc})_i = V(x_i)c_i$ is computed with N products and $\mathbf{Tc} = \mathcal{F}^{-1}\mathbf{D}_T\ \mathcal{F}\mathbf{c}$, where $\mathcal{F}$ is the fast Fourier transform (FFT) and $\mathbf{D}_T$ is a diagonal matrix, can be computed with $\mathcal{O}(N\log N)$ operations. Notice that $\left(e^{\tau\mathbf{V}}\mathbf{c}\right)_k = e^{\tau V(x_k)}c_k, \quad k = 0, 1, \ldots, N-1$ where the exponentials are computed only once at the beginning of the integration and they are stored, so their cost can be safely neglected. Similarly, for the kinetic part we have that $e^{\tau\mathbf{T}}\mathbf{c} = \mathcal{F}^{-1}e^{\tau\mathbf{D}_T}\mathcal{F}\mathbf{c}$. Then, standard splitting methods, for a time step, $\tau = -i\triangle t$, and preserving unitarity read as follows

$$\mathbf{U}_n(\tau) = \prod_{j=1}^{m} \mathcal{F}^{-1}e^{b_j\tau\mathbf{D}_T}\mathcal{F}e^{a_j\tau\mathbf{V}}. \tag{3}$$

In addition, for this family of problems we can also consider that the commutator, $[\mathbf{V}, [\mathbf{T}, \mathbf{V}]]$, is a diagonal matrix. Since the cost of the algorithm (3) is dominated by the FFTs, we can add these terms to the potentials, without increasing the cost, to improve the performance. Higher order terms can also be considered as well as new terms can be added to the kinetic energy in case the potential is a low degree polynomial. In addition, the processing technique is very easy to use in this problem. It decompose the method $\mathbf{U}_n(\tau)$ as follows: $\mathbf{U}_n = \mathbf{U}_P\mathbf{U}_K\mathbf{U}_P^{-1}$ so, for p steps $\mathbf{U}_n^p = \mathbf{U}_P\mathbf{U}_K^p\mathbf{U}_P^{-1}$, where $\mathbf{U}_K$ is the kernel and $\mathbf{U}_P$ is the processor or corrector (see [1, 2] and references therein).

Alternatively, Eq. (2) can also be split in two parts with a completely different structure, allowing to use different techniques and methods. Consider $\mathbf{c} = \mathbf{q} + i\mathbf{p}$, then Eq. (2) can be rewritten as a classical Hamiltonian system with Hamiltonian: $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q} = A + B$. This splitting has a very particular property with respect to the Poisson brackets: $\{A, \{A, \{A, B\}\}\} = \{B, \{B, \{B, A\}\}\} = 0$. This property drastically reduces the number of order conditions allowing to reach high order methods with a relatively small number of stages, preserving symplecticity.

This problem illustrates how flexible the splitting methods are and the many tools which can be used to obtain efficient methods. A large number of methods have recently appeared in the literature, and tailored for many different families of problems. At this point, we make a review about the last fifteen years for some of the most popular families of methods: (i) Composition of second order symmetric methods; (ii) Composition of a first order methods with its adjoint, which is equivalent to splitting in two general parts; (iii) splitting Nyström methods when the kinetic energy is quadratic in momenta; (iv) splitting Nyström methods using modified potentials; (v) Near-integrable systems; and (vi) Linear separable oscillatory systems with the property $\{A, \{A, \{A, B\}\}\} = \{B, \{B, \{B, A\}\}\} = 0$. A great effort in the search of methods has been done by many different authors leading to highly efficient methods for all these families of problems. Most reviewed methods can also be found in [2, 4, 5, 6, 7, 8, 9].

If we return to the classical representation of the Schrödinger equation, we find that it fits in case (vi) (as well as many other important oscillatory linear systems like e.g. the Maxwell equations). The best methods from the previous review

appear mainly in [5]. However, using the processing technique and due to the structure of this problem, we noticed that it is very easy to build methods at any order. In addition, it is possible to consider additional stages in the composition to improve simultaneously both accuracy and stability [3, 4], a fact very unusual for general problems. Following these procedures we build methods up to order twenty which outperform the previous schemes. We also build a new family of second order methods whose coefficients are chosen in order to get both large stability domain and high accuracy (making use of Chevishev techniques), and this occurs even for very large time step. Some of these methods reach round off accuracy nearly for all time steps inside the stability domain. These new methods have nearly the same stability as the symmetric second order decomposition (which attain the maximum stability among splitting methods of this family) and outperform all other schemes for all time steps and accuracies desired.

The analysis is carried out for the harmonic oscillator, and this toy problem allowed us to build highly efficient methods for non trivial problems like the Schrödinger equation. These methods are tested in the one-dimensional problem (1) with a Morse potential showing the performance expected from the theoretical analysis.

As a result, we conclude: (I) Splitting methods are powerful methods for many problems; (II) It is very important to use the most appropriate methods for each problem; and (III) In some cases we can also build methods tailored for particular problems which outperform the existing methods from the literature.

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Splitting methods for the harmonic oscillator

Ander Murua
(joint work with Sergio Blanes, Fernando Casas)

We consider the application of splitting methods to linear problems of the form

$$\dot{q} = Mp, \quad \dot{p} = Nq. \tag{1}$$

Such linear systems arise when space discretization of different linear partial differential equations, for instance, the time-dependent Schrödinguer equation [2, 4, 1]. Studying the behaviour of splitting methods applied to such linear systems is also of interest as a mean to understand the stability of splitting methods applied to non-linear systems of the form

$$\dot{q} = g(p), \quad \dot{p} = f(q). \tag{2}$$

Note that a linear system of the form (1) is obtained after linearization around a stationary point of (2). In this sense, it is of interest the construction of splitting methods with extended stability properties [3].

Application of a splitting method to the system (1) is equivalent to approximating the exponential

$$\exp\begin{pmatrix} 0 & hM \\ -hN & 0 \end{pmatrix}$$

by means of a product of the form

$$\mathbf{K}(h) = \begin{pmatrix} I & 0 \\ -hb_mN & I \end{pmatrix}\begin{pmatrix} I & ha_mM \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -hb_1N & I \end{pmatrix}\begin{pmatrix} I & ha_1M \\ 0 & I \end{pmatrix},$$

with appropriately chosen values of the real parameters a_i, b_i.

The stability of $\mathbf{K}(h)$ is related to the stability polynomial $p(x)$ of the splitting method [3, 2, 4], which is a polynomial in even powers of x that approximates $\cos(x)$.

We show that, for a given even polynomial $p(x)$, there exists a finite number of symmetric splitting methods (that is, a finite number of different choices of the parameters $\{a_i, b_i \ : \ 1 \le i \le m\}$) that have $p(x)$ as a stability polynomial, and we give a step by step algorithm that explicitly give all such methods.

We construct families of stability polynomials with extended stability intervals and very good accuracy properties that allow, together with the aforementioned algorithm, the construction of very stable and efficient splitting methods with processing for the numerical solution of linear systems of the form (1).

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Using additivity in numerical integration of DAEs

Laurent O. Jay

We report on extensions of Gauss methods and the Hilber-Hughes-Taylor (HHT) method for differential-algebraic equations (DAEs) arising in mechanics.

Gauss methods have not been considered as having much practical interest for the numerical solution of DAEs. This has been mainly due to poor convergence properties of these methods when applied in a standard direct way. Stiffly accurate methods have generally better convergence properties to solve DAEs [1, 3, 5]. However, in the context of geometric numerical integration of ODEs, e.g., for Hamiltonian or Lagrangian systems, Gauss methods have excellent theoretical properties [2]. It was an open problem and a question of interest to know if there was any way of generalizing and developing methods based on Gauss coefficients that would lead to methods of high order and quality for DAEs while preserving geometric properties of DAEs. It was shown recently that such generalizations are indeed possible for DAEs of index 2 [6, 10] and index 3 [7, 8].

Let us consider DAEs of the form

$$y' = v(t,y,z), \tag{1a}$$

$$(p(t,y,z))' = f(t,y,z) + r(t,y,\psi), \tag{1b}$$

$$0 = g(t,y), \tag{1c}$$

where in mechanics the quantities y, v, p, f, and r represent respectively generalized coordinates, generalized velocities, generalized momenta, generalized forces, and reaction forces due to the holonomic constraints $g(t,y) = 0$ ($r(t,y,\psi) = -g_y^T(t,y)\psi$). Differentiating (1c) once one obtains additional velocity constraints

$$0 = g_t(t,y) + g_y(t,y)v(t,y,z). \tag{1d}$$

The matrices $p_z(t,y,z)$ and $g_y(t,y)v_z(t,y,z)p_z^{-1}(t,y,z)r_\psi(t,y,\psi)$ are assumed to be invertible. The above formulation generalizes both Hamiltonian ($p = z$) and Lagrangian systems ($v = z$) with holonomic constraints. Applied to the system (1) one step with stepsize h of the standard 1-stage Gauss RK method is divergent in general even when $p(t,y,z) = z$ and $r(t,y,\psi)$ is linear in the algebraic variables ψ.

The modified method based on the implicit midpoint rule that we propose reads

$$\begin{aligned} Y_1 &= y_0 + \frac{h}{2} v(T_1, Y_1, Z_1), \\ p(T_1, Y_1, Z_1) &= p(y_0, z_0) + \frac{h}{2} f(T_1, Y_1, Z_1) + \frac{h}{2} r(t_0, y_0, \Psi_0), \\ y_1 &= y_0 + h v(T_1, Y_1, Z_1), \\ 0 &= g(t_1, y_1), \\ p(t_1, y_1, z_1) &= p(t_0, y_0, z_0) + h f(T_1, Y_1, Z_1) + \frac{h}{2} r(t_0, y_0, \Psi_0) + \frac{h}{2} r(t_1, y_1, \Psi_1), \\ 0 &= g_y(t_1, y_1) v(t_1, y_1, z_1), \end{aligned}$$

where h is the stepsize, $T_1 := t_0 + h/2$, and $t_1 := t_0 + h$. We call this method the $(1,1)$-*Gauss-Lobatto specialized partitioned additive Runge-Kutta (SPARK) method*. It mixes coefficients from the midpoint rule with those from the trapezoidal rule to treat holonomic constraints properly. It makes use of the additivity of the differential equations (1b). Note that the quantity Ψ_0 above is an internal algebraic variable, it is not an initial condition or a value ψ_0 coming from the previous step. We can generalize these ideas to obtain higher order schemes based on Gauss coefficients mixed with Lobatto coefficients. The family of Gauss-Lobatto SPARK methods makes great use of the partitioning and additive structure of the equations (1). We summarize our findings in the following theorem [7, 8]:

Theorem 1: *For the overdetermined system of DAEs (1) the (s,s)-Gauss-Lobatto SPARK methods are constraint-preserving, symmetric, and of maximal order $2s$. For holonomically constrained Hamiltonian systems and Lagrangian systems these methods are also symplectic and variational.*

The HHT method is widely used in structural dynamics [4]. The HHT method for $y'' = f(t, y, y')$ or equivalently for

$$y' = z, \qquad z' = f(t, y, z),$$

can be expressed as an implicit non-standard one-step method as follows

$$\begin{aligned} y_1 &= y_0 + h z_0 + \frac{h^2}{2} \left((1 - 2\beta) a_0 + 2\beta a_1 \right), \\ z_1 &= z_0 + h \left((1 - \gamma) a_0 + \gamma a_1 \right), \\ a_1 &= (1 + \alpha) f(t_1, y_1, z_1) - \alpha f(t_0, y_0, z_0), \end{aligned}$$

where a_0 and a_1 are approximations to the acceleration $a(t) := f(t, y(t), z(t))$ at $t_0 + \alpha h$ and $t_1 + \alpha h$ respectively. The coefficients α, β, γ are taken according to $\alpha \in [-1/3, 0], \beta = (1 - \alpha)^2/4, \gamma = 1/2 - \alpha$. We have extended the HHT method to the DAEs (1) with $v = p = z$, i.e., to DAEs of the form

$$(2) \quad y' = z, \quad z' = f(t, y, z) + r(t, y, \psi), \quad 0 = g(t, y), \quad 0 = g_t(t, y) + g_y(t, y) z.$$

Given (y_0, z_0, a_0) we define the extended HHT method for (2) as follows

$$\text{(3a)} \quad y_1 = y_0 + hz_0 + \frac{h^2}{2}\left((1-2\beta)a_0 + 2\beta a_1\right) + \frac{h^2}{2}((1-b)R_0 + bR_1),$$

$$\text{(3b)} \quad z_1 = z_0 + h\left((1-\gamma)a_0 + \gamma a_1\right) + \frac{h}{2}\left(R_0 + R_1\right),$$

$$\text{(3c)} \quad a_1 = (1+\alpha)f(t_1, y_1, z_1) - \alpha f(t_0, y_0, z_0),$$

where $b \neq 1/2$ is a new free coefficient,

$$\text{(3d)} \qquad R_0 = r(t_0, y_0, \Psi_0), \qquad R_1 = r(t_1, y_1, \Psi_1),$$

and Ψ_0 is not a value ψ_0 coming from the previous step or an initial condition, but Ψ_0 and Ψ_1 are internal algebraic variables determined by the two sets of constraints

$$\text{(3e)} \qquad 0 = g(t_1, y_1), \qquad 0 = g_t(t_1, y_1) + g_y(t_1, y_1)z_1.$$

Once again we make use of the additivity of the differential equations for z' in (2). To make the method less implicit, one can replace R_1 by $r(t_1, y_0 + hz_0, \Psi_1)$ in (3d). Theorem 2 below remains valid in this situation. One can show global convergence of order 2 of the extended HHT method [9]:

Theorem 2: *Consider the overdetermined system of DAEs (2) with initial conditions (y_0, z_0, a_0) at t_0 satisfying*

$$g(t_0, y_0) = 0, \quad g_t(t_0, y_0) + g_y(t_0, y_0)z_0 = 0, \quad a_0 - a(t_0 + \alpha h) = O(h).$$

Then the numerical solution (y_n, z_n, a_n) at t_n to the system of equations (3) satisfies for $0 \leq h \leq h_0$ and $t_n - t_0 = nh \leq Const$

$$y_n - y(t_n) = O(h^2), \qquad z_n - z(t_n) = O(h^2), \qquad a_n - a(t_n + \alpha h) = O(h^2),$$

where $(y(t), z(t))$ is the exact solution to (1) at t passing through (y_0, z_0) at t_0.

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Explicit, volume preserving splitting methods for divergence-free polynomial vector fields

Antonella Zanna

(joint work with Robert I. McLachlan, Hans Z. Munthe-Kaas and G. R. W. Quispel)

In this talk we address the problem of the numerical integration of divergence-free vector fields by volume-preserving methods. It is well known that devising methods which preserve volume is quite a hard task. To-date the general techniques consist in splitting the given vector field into the sum of two-dimensional volume-preserving systems and solve those by symplectic methods (Feng Kang) or by solving for $n-1$ variables and then correct for the last one in order to obtain a volume-preserving method (Shang Zai-jiu, 1994, Quispel 1995). However, these methods are generally implicit and expensive. Explicit methods exist for particular problems, for instance trigonometric ones.

We address the case of polynomial vector fields.

The main idea is to split the given divergence free vector field into the sum of pieces that

- Can be integrated exactly easily, or
- Can be integrated in a volume preserving manner by simple explicit methods (a.k.a. Forward Euler) and whose adjoint is also explicit.

Then, the basic split terms can be combined to obtain higher order integrator, either by Yoshida's technique, or by other symmetric composition methods.

Several new methods are presented for linear and quadratic problems. Roughly, these can be divided into two classes: i) methods that distinguish the diagonal part (all the terms in equation i that include the variable x_i, for $i = 1, 2 \ldots, n$), and ii) methods that do not distinguish the diagonal part. The diagonal part is generally more difficult to treat as its coefficient are interconnected as a result of volume-preservation, however it is computationally less expensive, as the off-diagonal part requires computations of a order of n higher.

Among the methods for the diagonal part, we mention the splitting in d shears, where d is the degree of the polynomial vector field, and exponentiation. As for the off-diagonal part, we consider splitting in strictly lower triangular systems (as these can be integrated in a volume-preserving manner by any Runge–Kutta method) by permutations, as well as splitting in n natural shears, which are integrated exactly by a step of Forward Euler. As for methods that do not distinguish the diagonal part, we consider a splitting in $n + d$ shears. The splitting in shears has been

successfully used in the context of Hamiltonian integration in particle accelerator physics.

Stability analysis of symplectic methods

Zaijiu Shang

We study linear stability of numerical methods for Hamiltonian systems. For analytic methods, the linear stability can be analyzed in the framework of Dahlquist, and a well known result is that symmetric analytic methods are I-stable. Note that an analytic symplectic method is always I-stable because it is symmetric when applying to linear Hamiltonian systems. As a consequence, Symplectic Runge-Kutta methods are I-stable. For non-analytic methods (e.g., partitioned methods), the linear stability was only analyzed for very few symplectic integrators of lower order in literature [1, 2, 6].

We give a careful analysis of the linear stability of symplectic Euler methods of arbitrarily high order. We prove that the stability interval of a symplectic Euler method shrinks as the order increases. The limit of the interval, as the order approaches infinity, is $[-\frac{\pi}{2}, \frac{\pi}{2}]$, which is just the connected component containing the origin of the set on which the *cosine* function takes non-negative real values. The first order symplectic Euler method has stability interval $[-2, 2]$, which is biggest in the class of symplectic Euler methods.

We also analyze the linear stability of other partitioned symplectic methods. For Lobatto IIIA-IIIB Pairs, we find that the stability set is bounded and is expanding as the order increases. The number of connected components of the stability set of the Lobatto IIIA-IIIB Pairs is finite and equal to $m - 1$, where m is the order of the methods. The limit of the set is the whole real line. The Lobatto IIIA-IIIB Pairs have much better stability than symplectic Euler methods.

We also explore some relationships between linear stability and nonlinear stability of symplectic methods for stable Hamiltonian systems.

The detailed results about this topic are referred to [5] and [7]. For nonlinear stability analysis of symplectic methods, see [3, 4].

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Efficient strong integration of linear stochastic systems

Simon J.A. Malham
(joint work with Gabriel Lord, Anke Wiese)

We are interested in designing efficient numerical schemes for the strong approximation of linear Stratonovich stochastic differential equations driven by two Wiener processes and with non-commutative vector fields. One solution to such systems is the Neumann series obtained by successive Picard iteration. The logarithm of the Neumann expansion is known as the Magnus expansion, and this provides an alternative solution ansatz. For ease of exposition, we also specialize to the still non-trivial case when the coefficient matrices are constant.

Classical numerical schemes such as the Euler-Maruyama and Milstein methods correspond to truncating the stochastic Taylor expansion to generate global strong order 1/2 and order 1 schemes, respectively. Numerical schemes based on deterministic Runge–Kutta methods have also been derived—see Kloeden & Platen (1999) and Talay (1995). At the linear level, the Neumann, stochastic Taylor and Runge–Kutta type methods are equivalent. In the stochastic context, Magnus integrators have been explored by Castell & Gaines (1995), Burrage (1999) and Misawa (2001).

We will present numerical schemes based on truncated Neumann and Magnus expansions. Higher order multiple Stratonovich integrals are approximated across each time-step by their expectations conditioned on the increments of the Wiener processes on suitable subdivisions (see Gaines & Lyons 1997).

We prove that for linear SDEs driven by two Wiener processes:

(1): Superior accuracy is provided for a given stepsize by a modified class of order one Magnus integrators.

(2): Accuracy of all stochastic integrators asymptotically scales like the square-root of the computational cost for small stepsizes.

Our first statement reflects that the exponential of the Magnus series is a natural solution ansatz for linear SDEs. Magnus integrators should therefore be preferable to classical stochastic numerical schemes or Neumann integrators provided the cost of computing the matrix exponential is not significant.

Our second statement naturally arises in the time-ordered integration of information generated at infinitesimally small scales by the two driving Wiener signals. In particular, for small stepsizes the accurate representation of the Lévy area (chordal area process) between the two Wiener processes dominates the computational cost for all methods of order one and higher. Coincidentally, half-order methods, which do not require the Lévy area, also obey this square-root scaling.

There are several potential sources of cost contributing to the overall computational effort of a stochastic numerical integration scheme. The main ones are the efforts associated with:

(A): Quadrature: the accurate representation of multiple integrals;
(B): Evaluation: computing and combining the individual terms and special functions such as the matrix exponential.

In the fixed time-step scenario, stochastic numerical schemes of order 1/2 do not invoke any quadrature effort because they only involve increments of the Wiener processes across each time-step. When two or more Wiener processes are present, to obtain a higher order stochastic integrator we need to include the Lévy area. In the variable time-step scenario, order 1/2 integrators do not necessarily converge to the correct solution (see Gaines & Lyons 1997) and a successful integrator must include the Lévy area (see Lyons 1998, who proves that the solution is continuously controlled by the driving processes and the Lévy area).

Our research/presentation is outlined as follows. We start by reviewing convergence results for the Neumann and Magnus expansions. Then we present the Neumann and Magnus integrators for linear systems. In particular we show that high order Magnus stochastic integrators are simple and concise, and that both Neumann and Magnus integrators can be expressed using a computationally favourable basis of high order stochastic multi-dimensional integrals. We compute the global truncation errors associated with both types of methods, and use these to reduce each method to their canonical forms. We compare the local truncation errors for the Magnus and Neumann integrators, and the non-trivial extension to the corresponding global comparison. We prove that the order 1/2 Magnus integrator is globally more accurate than the order 1/2 Neumann integrator for the same stepsize. Further, we prove that a given modified order 1 Magnus integrator is globally more accurate than the corresponding Neumann scheme.

In the second part, we show how to approximate multiple Stratonovich integrals by their conditional expectations (Gaines & Lyons 1997). For numerical methods up to global strong order 2, the multiple Stratonovich integrals approximated in this way are only single sums and therefore relatively cheap to compute. We show that the accurate representation of the Lévy area dominates the quadrature effort resulting in the square-root scaling law between the global error and computational effort. Then we present numerical experiments that reflect our theoretical predictions, and in particular the superior accuracy of Magnus methods. Also we apply both the Neumann and Magnus integrators to a stochastic Riccati differential system that can be linearized. Lastly we discuss the implications of our conclusions on Neumann and Magnus integrators to dynamic programming applications such as filtering problems.

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Semi-Lagrangian methods and new integrators for convection dominated problems

Elena Celledoni

In this talk we consider nonlinear convection diffusion problems with a dominating convection term. For example of the type,

$$\frac{\partial}{\partial t}u(\mathbf{x},t) + \mathbf{V}\cdot\nabla u(\mathbf{x},t) = \nu\nabla^2 u + f(\mathbf{x}), \tag{1}$$

with $\mathbf{x}\in\Omega\subset\mathbb{R}^d$ and $\mathbf{V}:\mathbb{R}^d\times[0,T]\to\mathbb{R}$ is a given vector field, $u:\mathbb{R}^d\times[0,T]\to\mathbb{R}^d$, and $u(\mathbf{x},0)=u_0(\mathbf{x})$. We can distinguish between two important special cases of the above equation. The first case arises when u is a conserved passive scalar, $f(x)=0$, u can represent temperature, or salt concentration in the water, $\mathbf{V}$ is known a priori. The second case is given by the Navier–Stokes equations where u is a vector field, $\mathbf{V}=u$, and $f(x)=-\nabla p$, with the constraint $\nabla\cdot u=0$.

The case when the parameter ν tends to zero is particularly interesting and very challenging from the numerical point of view.

If we semidiscretize (1) in space with a finite element or finite difference method we obtain a system of ordinary differential equations of the type

$$y_t - C(y)y = Ay + f, \qquad y(0)=y_0. \tag{2}$$

Here C is the discretized convection operator, A corresponds to the linear diffusion term, often negative definite.

A typical approach for solving numerically the semidiscretized equations is to treat convection and diffusion separately, the diffusion with an implicit approach and the convection with an explicit integrator possibly of higher order, see for example [1], [3].

We propose here a new class of integration methods particularly suited for convection diffusion problems. These methods are exponential integrators and their peculiarity is that they allow for the computation of exponentials of the linearized convection term of (2). This means that terms of the form $W(h)\cdot g =$

$\exp(\gamma h C(w)) \cdot g$, where w and g are fixed vectors in $\mathbf{R}^n$, and γ is a parameter of the integration method, appear as building blocks for the methods.

A simple example is the following first order integrator for (2),

$$y_{n+1} = \exp(hC(y_n))y_n + hAy_{n+1} + hf. \tag{3}$$

The goal here is to present and analyze higher order methods which share some of the features of (3). The main reason for developing this type of methods is that as it turns out they can be applied to the numerical integration of the considered PDEs in a semi-Lagrangian fashion. The main challenge in the numerical approximation of convection dominated phenomena is to avoid the occurence of spurious oscillations in the numerical solution, (numerical dispersion), without adding too much artificial diffusion. This task is achieved nicely by semi-Lagrangian methods, [Pi], [HE], [RM], [2]. In these methods linear convective terms are integrated *exactly* by computing first the characteristics corresponding to the grid points of the adopted discretization, and then producing the numerical approximation via a simple although expensive interpolation procedure.

The exponential $\exp(\gamma h C(w)) \cdot g$ is the solution of the semidiscretized equation

$$v' = C(w)v, \qquad v(0) = g, \quad \text{in } [0, h], \tag{4}$$

which corresponds to the pure convection problem

$$\begin{aligned} &\gamma_t + \mathbf{V} \cdot \nabla\gamma = 0, \qquad \gamma(x_i, 0) = g_i, \quad \text{in } [0, h] \times \Omega, \text{ i.e.} \\ &\tfrac{D\gamma}{Dt} = 0, \qquad \gamma(x_i, 0) = g_i, \quad \text{in } [0, h] \times \Omega, \end{aligned} \tag{5}$$

where x_i are the nodes of the space discretization, $\mathbf{V} = \mathbf{V}(x_i) = w_i$, and $\frac{D\cdot}{Dt}$ is the total derivative. If we apply (3) directly to the problem (1) before discretizing in space, and we make the exponential $\exp(hC(y_n))y_n$ correspond to the exact integration of a pure convection problem, we obtain the following transport-diffusion algorithm studied in [Pi],

$$\begin{aligned} &\tfrac{Du_{n+\frac{1}{2}}}{Dt} = 0, \;\; u_{n+\frac{1}{2}}(x, t_n) = u_n(x), \;\; \text{on } [t_n, t_n + h] \\ &u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h) \\ &u_{n+1} = u_{n+\frac{1}{2}} + h\nu\nabla^2 u_{n+1} + hf, \end{aligned} \tag{6}$$

the convecting vector field is $\mathbf{V}(x) = u_n(x)$. The exact integration of the pure convection problem in (6) can be obtained by introducing characteristics, we get

$$\begin{aligned} &u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h) = u_n(X(t_n)) \\ &\tfrac{dX}{d\tau} = u_n(X(\tau)), \;\; X(t_n + h) = x, \end{aligned} \tag{7}$$

and the equation for the characteristics $X(\tau)$ must by integrated backwards in time, either exactly or with a suitable numerical integrator. Now substituting the result in the second equation of (6) we have

$$\begin{aligned} &\tfrac{dX}{d\tau} = u_n(X(\tau)), \;\; X(t_n + h) = x, \\ &u_{n+1} = u_n(X(t_n)) + h\nu\nabla^2 u_{n+1} + hf. \end{aligned} \tag{8}$$

The outlined correspondence between (3) and (8) motivates the use of exponentials of the linearized semidiscrete convection operator of (2) in the integrators.

This work is also related to the methods presented in [MPR], and [XK] for the disretization of the Navier-Stokes equations. Previous preliminary work has also been presented in [5].

If we consider the semidiscretized ordinary differential equation

$$\dot{y} - C(y)y = Ay, \quad y(0) = y_0, \tag{9}$$

where for the sake of simplicity, but without loss of generality we have dropped the forcing term f compared to (2). The general format for the considered methods is

for $i = 1 : s$ do

$$Y_i = \varphi_i y_n + h \sum_{j=1}^{i} a_{i,j} \varphi_i \varphi_j^{-1} A Y_j$$

$$\varphi_i = \exp(h \textstyle\sum_k \alpha_{iJ}^k C(Y_k)) \cdots \exp(h \sum_k \alpha_{i1}^k C(Y_k))$$

end

$$y_{n+1} = \varphi_{n+1} y_n + h \sum_{i=1}^{s} b_i \varphi_{n+1} \varphi_i^{-1} A Y_i$$

$$\varphi_{n+1} = \exp(h \textstyle\sum_k \beta_J^k C(Y_k)) \cdots \exp(h \sum_k \beta_1^k C(Y_k))$$

These methods can be directly interpreted as transport-diffusion algorithms for convection diffusion equations.

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Conserved quantities of some Hamiltonian wave equations after full discretization

Begoña Cano

It is well known that some differential systems have some invariants which would be good to conserve after numerical integration. More precisely, I have concentrated on some Hamiltonian wave equations, like the nonlinear wave and Schrödinger ones. Let us assume that the standard method of lines is the one used to integrate these systems, first discretizing in space and then in time.

I have studied how a symmetric space discretization makes that the space discretized system also has some invariants or 'nearly' invariants which well approximate the continuous ones. When an even number of derivatives turn up in each of the terms of an invariant quantity, the natural discretization of the invariant, which is the one which uses the same space discretization as that used to construct the space discretized system, is also an invariant of the latter. However, in other case, the approximation of the invariant must be done through a pseudospectral discretization. Some results were already obtained in the literature concerning the momentum for the nonlinear wave equation and for a particular difference scheme and using variational techniques [4]. As distinct here, we arrive at similar conclusions, but for any symmetric space discretization, with more direct techniques, and the conclusions obtained are also valid for other quantities in nonlinear Schrödinger equation.

Then, integrating in time, the question which arises is whether geometric integrators (which behave so well in the numerical conservation of invariants for ODEs [2, 3, 5]) also behave in the same advantageous way in the numerical integration of these space discretized systems, which become arbitrarily stiff when the space grid is refined. Numerical experiment seem to suggest so. Then, some conjectures are given (difficult to prove precisely but justified heuristically and corroborated numerically) such that, taking them as hypotheses, some theorems are obtained on a proper behaviour with time of the discretized invariants after at least moderate times.

A more detailed description of the results can be seen in [1].

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Euler-Poincaré integrators: variational construction and integrability

Yuri B. Suris

After recalling the most famous example of Euler–Poincaré equations on a semi-direct product Lie algebra, – the equations of motion of a d-dimensional heavy top (rigid body with a fixed point), two questions have been posed:

(1) Why do semi-direct products appear in this context? In particular, what has $\mathrm{E}(d)$ to do with rotation around a fixed point (one would expect $\mathrm{SO}(d)$)?
(2) How can one find symplectic (Poisson) discretizations of Euler-Poincaré equations on semi-direct products?

The most elegant solutions to both problems are claimed to be based on the Lagrangian mechanics (with reduction): with continuous time (on TG) for the first problem, and with discrete time (on $G \times G$) for the second one. The main ingredients for the Lagrangian reduction procedure, leading to Euler-Poincaré equations on semi-direct products, are:

- G – Lie group (configuration space), with the Lie algebra $\mathfrak{g}$.
- $\Phi : G \times V \to V$ – representation of G on a vector space V:

$$\Phi(g) \cdot v \quad \text{für} \quad g \in G, \;\; v \in V.$$

- $\phi : \mathfrak{g} \times V \to V$ – corresp. representation of $\mathfrak{g}$ on V:

$$\phi(\xi) \cdot v = \frac{d}{d\epsilon}\Big(\Phi(e^{\epsilon\xi}) \cdot v\Big)\Big|_{\epsilon=0} \quad \text{for} \quad \xi \in \mathfrak{g}, \;\; v \in V.$$

- Bilinear map $\diamond : V^* \times V \to \mathfrak{g}^*$: for $v \in V$, $y \in V^*$

$$\langle y \diamond v, \xi \rangle = -\langle y, \phi(\xi) \cdot v \rangle \qquad \forall \xi \in \mathfrak{g}.$$

- Fix $p \in V$ and let $G^{[p]}$ be its isotropy subgroup:

$$G^{[p]} = \{h \,:\, \Phi(h) \cdot p = p\} \subset G.$$

- Continuous time Lagrange function $\mathrm{L} : TG \to \mathbb{R}$ (discrete time Lagrange function $\mathbf{L} : G \times G \to \mathbb{R}$), *invariant* w.r.t. left multiplication of $G^{[p]}$:

$$\mathrm{L}(g, \dot{g}) = \mathcal{L}^{(l)}(\Omega, P), \quad \mathbf{L}(g, \widehat{g}) = \Lambda^{(l)}(W, P),$$
$$\Omega = g^{-1}\dot{g}, \quad W = g^{-1}\widehat{g}, \quad P = \Phi(g^{-1}) \cdot p.$$

- Reduced configuration space: $\mathfrak{g} \times O_p$, resp. $G \times O_p$, where $O_p \subset V$ is the G-orbit of $p \in V$ under Φ.

Theorem 1. [1] *Reduced Euler-Lagrange equations take the* Euler–Poincaré *form:*

$$\begin{cases} \dot{M} = \mathrm{ad}^*\,\Omega \cdot M + d_P\mathcal{L}^{(l)}(\Omega, P) \diamond P, \\ \dot{P} = -\phi(\Omega) \cdot P, \end{cases}$$

where

$$M = d_\Omega \mathcal{L}^{(l)}(\Omega, P) \in \mathfrak{g}^*$$

(this is the Legendre transformation $\mathfrak{g} \times O_p \to \mathfrak{g}^* \times O_p$, $(\Omega, P) \mapsto (M, P)$*). The above system is Hamiltonian w.r.t. Poisson bracket*

$$\{F_1, F_2\}^{(l)}(M, P) = \langle M, [d_M F_1, d_M F_2] \rangle + \langle P, \phi^*(d_M F_2) \cdot d_P F_1 - \phi^*(d_M F_1) \cdot d_P F_2 \rangle$$

(Lie-Poisson bracket of the semi-direct product $\mathfrak{g} \ltimes V^*$ *for the representation* $-\phi^*$ *of* $\mathfrak{g}$ *on* V^**), with the Hamilton function*

$$H^{(l)}(M, P) = \langle M, \Omega \rangle - \mathcal{L}^{(l)}(\Omega, P).$$

Theorem 2. [2] *Reduced discrete Euler-Lagrange equations take the* discrete Euler-Poincaré *form:*

$$\begin{cases} M_{n+1} = \mathrm{Ad}^* W_n \cdot \Big(M_n + d_P \Lambda^{(l)}(W_n, P_n) \diamond P_n \Big), \\ P_{n+1} = \Phi(W_n^{-1}) \cdot P_n, \end{cases}$$

where

$$M_n = D'_W \Lambda^{(l)}(W_{n-1}, P_{n-1}) \in \mathfrak{g}^*$$

(discrete Legendre transformation $G \times O_p \to \mathfrak{g}^* \times O_p$, $(W_{n-1}, P_{n-1}) \mapsto (M_n, P_n)$*). Evolution* $(M_n, P_n) \mapsto (M_{n+1}, P_{n+1})$ *is Poisson w.r.t. Lie-Poisson bracket of the semi-direct product* $\mathfrak{g} \ltimes V^*$*.*

These results lead to a **recipe for constructing Euler-Poincaré integrators**:

▶ For a given system of Euler-Poincaré equations, find a Lagrangian formulation with a $G^{[p]}$-invariant continuous time Lagrange function on a Lie group G,

$$\mathrm{L}(g, \dot{g}) = \mathcal{L}^{(l)}(\Omega, P),$$

with $\Omega = g^{-1}\dot{g}$, $P = \Phi(g^{-1}) \cdot p$.

▶ Take *any* $G^{[p]}$-invariant discrete time Lagrange function on G,

$$\mathbf{L}(g_n, g_{n+1}) = \Lambda^{(l)}(W_n, P_n),$$

with $W_n = g_n^{-1} g_{n+1}$, $P_n = \Phi(g_n^{-1}) \cdot p$, and such that

$$\Lambda^{(l)}(W, P) = h\mathcal{L}^{(l)}(\Omega, P) + O(h^2)$$

as $W = I + h\Omega + O(h^2)$ (approximation).

▶ Compute corresponding discrete Euler-Poincaré equations.

These recipe has been illustrated by two *integrable* examples [3].

A. Dynamically symmetric top is a heavy top with an isotropic tensor of inertia $J = \frac{1}{2} I$ and with the Lagrange function

$$\mathrm{L}(g, \dot{g}) = \mathcal{L}^{(l)}(\Omega, P) = \frac{1}{2}\langle \Omega, \Omega \rangle - \langle P, A \rangle.$$

Legendre transformation: $M = \Omega$. Equations of motion:

$$\begin{cases} \dot{M} = A \wedge P, \\ \dot{P} = -MP. \end{cases}$$

Hamilton function: $H(M,P) = \frac{1}{2}\langle M,M\rangle + \langle P,A\rangle$. This system is completely integrable, due to a Lax representation $\dot{L}(\lambda) = [U(\lambda), L(\lambda)]$, with the Lax matrix

$$L(\lambda) = \begin{pmatrix} M & \lambda P - \lambda^{-1}A \\ \lambda P^{\mathrm{T}} - \lambda^{-1}A^{\mathrm{T}} & 0 \end{pmatrix}.$$

An *integrable discretization of the symmetric top* is generated by the following discrete Lagrange function:

$$\mathbf{L}(g_n, g_{n+1}) = \Lambda^{(l)}(W_n, P_n) = -\frac{1}{h}\,\mathrm{tr}\log(2I + W_n + W_n^{-1}) - h\langle P_n, A\rangle.$$

One should note a non-trivial discretization of the kinetic energy. Legendre transformation (coming to replace $M = \Omega$):

$$M_{n+1} = \frac{2}{h}\cdot\frac{W_n - I}{W_n + I} \quad \Leftrightarrow \quad W_n = \frac{I + (h/2)M_{n+1}}{I - (h/2)M_{n+1}}$$

Theorem 3. *Discrete Euler-Lagrange equations:*

$$\begin{cases} M_{n+1} = M_n + hA \wedge P_n\,, \\ \\ P_{n+1} = \dfrac{I - (h/2)M_{n+1}}{I + (h/2)M_{n+1}}\,P_n\,. \end{cases}$$

This explicit map is Poisson w.r.t. Lie-Poisson bracket on $\mathrm{e}(d)^*$*, and is completely integrable, due to Lax representation* $L_{n+1}(\lambda) = V_n(\lambda)L_n(\lambda)V_n^{-1}(\lambda)$*, with*

$$L_n(\lambda) = \begin{pmatrix} M_n & \lambda Q_n - \lambda^{-1}A \\ \lambda Q_n^{\mathrm{T}} - \lambda^{-1}A^{\mathrm{T}} & 0 \end{pmatrix},$$

where $Q_n = (I + \frac{h}{2}M_n)P_n + \frac{h^2}{4}A$*. One of integrals of motion:*

$$H_h(M,P) = \frac{1}{2}\langle M,M\rangle + \langle P,A\rangle + \frac{h}{2}\langle M, P\wedge A\rangle$$

(deformation of the original Hamiltonian).

B. Clebsch case of the rigid body motion in an ideal fluid

One (simplest) flow of the hierarchy (B – a diagonal $d\times d$ matrix):

$$\mathrm{L}(g,\dot{g}) = \mathcal{L}^{(l)}(\Omega,P) = \frac{1}{2}\langle\Omega,\Omega\rangle + \frac{1}{2}\langle P, BP\rangle.$$

Legendre transformation: $M = \Omega$. Equations of motion:

$$\begin{cases} \dot{M} = P\wedge(BP), \\ \dot{P} = -MP. \end{cases}$$

Hamilton function: $H(M,P) = \frac{1}{2}\langle M,M\rangle - \frac{1}{2}\langle P,BP\rangle$. Completely integrable, due to Lax representation $\dot{L}(\lambda) = [U(\lambda), L(\lambda)]$, with

$$L(\lambda) = \lambda B + M + \lambda^{-1}PP^{\mathrm{T}}.$$

An *integrable discretization of the Clebsch case* is generated by the following discrete Lagrange function:

$$\mathbf{L}(g_n, g_{n+1}) = \Lambda^{(l)}(W_n, P_n)$$
$$= -\frac{1}{h}\,\mathrm{tr}\log(2I + W_n + W_n^{-1}) + \frac{4}{h}\,\log\Big(1 + \frac{h^2}{4}\langle P_n, BP_n\rangle\Big).$$

Note a non-trivial discretization of both the kinetic and the potential energy. Legendre transformation (coming to replace $M = \Omega$):

$$M_{n+1} = \frac{2}{h}\cdot\frac{W_n - I}{W_n + I} \quad \Leftrightarrow \quad W_n = \frac{I + (h/2)M_{n+1}}{I - (h/2)M_{n+1}}$$

Theorem 4. *Discrete Euler-Lagrange equations:*

$$\begin{cases} M_{n+1} = M_n + h\,\dfrac{P_n \wedge (BP_n)}{1 + (h^2/4)\langle P_n, BP_n\rangle}\,, \\[2ex] P_{n+1} = \dfrac{I - (h/2)M_{n+1}}{I + (h/2)M_{n+1}}\,P_n\,. \end{cases}$$

This explicit map is Poisson w.r.t. Lie-Poisson bracket on $\mathrm{e}(d)^*$*, and is completely integrable, due to Lax representation* $L_{n+1}(\lambda) = V_n(\lambda)L_n(\lambda)V_n^{-1}(\lambda)$*, with*

$$L_n(\lambda) = \Big(I + \frac{h^2}{4}B\Big)^{-1}(\lambda B + M_n + \lambda^{-1}\mathcal{P}_n),$$

where $\mathcal{P}_n = (I + \frac{h}{2}M_n)P_nP_n^{\mathrm{T}}(I - \frac{h}{2}M_n)$*. Integrals of motion are* $O(h)$*-deformations of the original ones.*

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Stability of rigid body motions (and numerical integrations)

Francesco Fassò

1. Introduction. It is well known that the proper rotations of an Euler top (a rigid body with a fixed point and no forces acting on it) about the minimum and maximum axes of inertia are stable. This talk describes some recent results on the stability of these special motions for a rigid body with a fixed point subject to small ($\sim \epsilon$) conservative forces [4]. This study is rooted in an asymptotic theory of the long–term dynamics of small perturbations of the Euler top based on Nekhoroshev theory [3]. At variance from KAM theory, Nekhoroshev theory [11] permits the study of resonant motions, even though its results are valid only for a finite, but

very long, time scale $T_\epsilon = \exp(1/\epsilon^\bullet)$ (the bullet stands for some positive constant). The problem has geometric, dynamical and numerical aspects.

2. Geometry. The unperturbed system, the Euler top, is a a superintegrable system: it has three degrees of freedom, but four integrals of motion. Accordingly, motions are quasi–periodic on two–dimensional tori. The symplectic geometry of the fibration by these tori is of interest in itself and important for the comprehension and the study of the perturbed dynamics. For a review, see [8].

In short, the existence of the four integrals of motion produces a doubly fibered invariant structure of the phase space. The first fibration is given by the Hamiltonian K and by the norm G of the angular momentum vector, or equivalently, by the frequencies of the quasi–periodic motions. Each fiber F_{KG} of this fibration is a four–dimensional manifold which contains all tori with frequencies determined by K and G; in view of the rotational invariance of the system, the tori in F_{KL} are determined by the direction μ of the angular momentum vector in space. In fact, F_{KG} is fibered by the two–tori, with base the two–dimensional sphere $|\mu| = 1$.

The (symplectic) geometric properties of this structure play a key role in the formulation of Nekhoroshev theorem for superintegrable systems [7], which in the present case ensures that K and G are (nearly) constant and that the motion is approximately quasi–periodic on the time scale T_ϵ. In other words, the motion is approximately an Euler top motion around the istantaneous direction of the angular momentum vector, which however moves in space.

Thus, all the interesting dynamics takes place on the base S^2 of the toric fibration of F_{KG}. Accordingly, the theory focusses on the properties of the long–term motion of μ on the unit sphere—which is clearly relevant in applications.

3. Dynamics. The motion of μ, on the time scale T_ϵ, can be studied via the normal forms constructed within the Nekhoroshev approach. As it turns out, the properties of the motion of μ depend crucially on the resonance properties of the frequencies. As shown in [3], for any initial data (not too close to the unstable manifold of the rotation around the middle axis of inertia) and for times T_ϵ:

(i) If the frequencies are nonresonant (up to a certain order), then the motion of μ is regular. In particular, μ stays close to a level curve of a differentiable function on S^2, and the Lyapunov exponents are exponentially small.

(ii) If the frequencies are in a (low order) resonance, instead, then μ can undergo wide chaotic movements and wander unpredictably through an extended, essentially two–dimensional, region of S^2. The maximal Lyapunov exponent is positive, though small ($\sim \epsilon^\bullet$).

Numerical computations in sample cases provide a clear evidence of the existence of these chaotic movements in resonance [2].

Assume now that, at the initial time, the angular momentum vector is nearly aligned with the maximum or minimum axis of inertia. Then, for times T_ϵ, nonresonant motions are still of the type (i), but resonant motions are more stable than in (ii): even though the motion remains chaotic, with positive Lyapunov exponent, μ stays close to a level curve of a differentiable function, as in the nonresonant

case [4]. Thus, the stability of proper rotations consists in the spatial localization of chaos.

4. Numerics. This research has relayed over extensive numerical investigations, both to test the optimality of the theory and to be guided in the formulation of a precise conjecture, subsequently proved, about the stability of proper rotations, which was unknown [2, 5]. Numerical integrations used a Strang splitting "kinetic + potential" and fourth order compositions [9]. Within such an approach it is important, particularly for perturbation theory, that the flow of the integrable part be integrated exactly [10]. The exact integration of the flow of an Euler top is easy in the case of a kinetically symmetric body (two equal moments of inertia), because the flow involves only elementary functions [6, 1]. Correspondingly, [2, 5] dealt only with that case. Current work is focussing on the, significantly more difficult, exact integration of the flow of an Euler top with three distinct moments of inertia. It is known that the flow can be expressed in terms of theta functions, but explicit, workable expressions of the flow seem not to be available in the classical literature.

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Geodesic Flows on Manifolds and their Discretizations

Anthony Bloch

I describe here related pieces of work on the geometry and dynamics of geodesic flows on various manifolds of interest. This is joint work with P. Crouch, A. Iserles, J. Marsden, T. Ratiu and and A. Sanyal. In particular we are interested in representations of integrable flows and their discretizations.

Some of this work concerns continuous and discrete versions of the generalized rigid body equations and the role of these equations in numerical analysis, optimal control and integrable Hamiltonian systems. In particular, we consider a symmetric representation of the rigid body equations on the Cartesian product $SO(n) \times SO(n)$ and study its associated symplectic structure. We describe the relationship of these ideas with the Moser-Veselov theory of discrete integrable systems and with the theory of variational symplectic integrators.

In their paper on discrete analogues of some classical systems such as the rigid body and the geodesic flow on an ellipsoid, Moser and Veselov introduced their analysis in the general context of flows on Stiefel manifolds. Recently we have analyzed a general class of continuous time, quadratic cost, optimal control problems on Stiefel manifolds, which in the extreme dimensions again yield these classical physical geodesic flows. In this work we extend the symmetric representation to the geodesic flow on the ellipsoid and the more general Stiefel manifold case. The metric we choose on the Stiefel manifolds is the same as that used in the symmetric representation of the rigid body flow, and that used by Moser and Veselov. In the extreme cases of both the ellipsoid and the rigid body, the geodesic flows are known to be integrable. We obtain the extremal flows using both variational and optimal control approaches, and elucidate the structure of the flows on general Stiefel manifolds. We also discuss discrete representations of these flows.

In some related work we show that the left-invariant geodesic flow on the symplectic group with metric given by the Frobenius norm is an integrable system that is not contained in the Mishchenko-Fomenko class of integrable systems. We show that this system may be expressed as a flow on symmetric matrices and that the system is bi-Hamiltonian. We analyze the Poisson structure of this system and list the Casimirs. This flow on symmetric matrices is in some sense dual to the flow of the generalized rigid body equations which flow on the space of skew symmetric matrices. It has a Lax pair structure which differs by a sign from the double bracket equations which define another integrable system on symmetric matrices, the Toda lattice.

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Exponential integrators for highly oscillatory differential equations

Volker Grimm

(joint work with Marlis Hochbruck)

The subject of my talk is the study of differential equations of type

$$y'' = -Ay + g(y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \tag{1}$$

where A is a symmetric and positive semi-definite real matrix of arbitrarily large norm. The large norm of A introduces an oscillatory solution and therefore differential equations of this type are called oscillatory or highly oscillatory. Oscillatory differential equations of this type arise in many different applications, for example in semidiscretisations of wave equations, and are currently a subject of high interest.

The nature of oscillatory solutions is such that one needs to apply standard methods with a step size smaller than the inverse of the largest frequency, which is the square root of the largest eigenvalue of A. The idea to overcome this step-size restriction is to preserve the oscillations intrinsic to the equation by solving exactly linear problems and allowing approximations only to the smoother function g. Since this involves the evaluation of a matrix exponential, these methods are called exponential integrators.

The superior performance of exponential integrators for oscillatory differential equations could be theoretically confirmed by error bounds that are not dependent on the norm of A or higher derivatives of the solution. This is especially important for semidiscretisations of partial differential equations. For example, the Gautschi-type exponential integrator possesses error bounds independent of the frequencies (cf. [5]) and of the dimension of the system to be solved (cf. [2]), that is, the accuracy of the Gautschi-type method in time is independent of the grid chosen in space. Another example is the mollified impulse method, introduced in [1]. No standard methods are known to share this favourable property.

In this talk, joint work with Marlis Hochbruck (cf. [3]) is presented that unifies the error analysis known for some exponential integrators to the whole family of exponential integrators proposed in [4].

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Highly oscillatory Hamiltonian systems

David Cohen

We consider Hamiltonian systems where high-frequency oscillations are generated by a linear part. In the first part of the talk, we give a short review of the results obtained so far for Hamiltonian function of the form:

$$H(p,q) = \frac{1}{2}p^T p + \frac{1}{2\varepsilon^2} q^T \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} q + U(q), \tag{1}$$

where $0 < \varepsilon \ll 1$ and U is a smooth potential with bounded derivatives. As a classical model problem, we consider the modified Fermi-Pasta-Ulam problem (see [7]).

We present a class of numerical methods (the *trigonometric methods* see [6], [8], [5] and more generally [7]) designed for such problems (explicit, use of large step size). Moreover, these methods nearly conserve the total energy of the system and the oscillatory energy

$$I(p,q) = \frac{1}{2}||p_2||^2 + \frac{1}{2\varepsilon^2}||q_2||^2, \tag{2}$$

with partitions $p = (p_1, p_2)$ and $q = (q_1, q_2)$ (according to the partition of the matrix in (1)) over long time intervals.

It is now time to enlarge the class of problems studied, namely by considering the following Hamiltonian function

$$H(p,q) = \frac{1}{2}p_1^T M_1(q)^{-1} p_1 + \frac{1}{2}p^T R(q) p + \frac{1}{2}p_2^T p_2 + \frac{1}{2\varepsilon^2} q_2^T q_2 + U(q), \tag{3}$$

with a symmetric positive definite matrix $M_1(q)$ and a symmetric matrix $R(q)$ with $R(q_1, 0) = 0$. Surprising applications, such as the planar elastic dumbbell spacecraft of [9] or the motion of a triatomic molecule (the water molecule, for example) can now be considered.

For such Hamiltonian problems, we develop new numerical methods (based on the trigonometric methods). We present a frequency expansion of the numerical solution: *the modulated Fourier expansion*. We also discuss two invariants of the system that determines its coefficients. These invariants are related to the total energy and the oscillatory energy of the original system. This allows us to prove the near-conservation of the total and the oscillatory energy over very long time intervals.

We finally give some words on the application of the trigonometric methods for some nonlinear wave equation.

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Adiabatic integrators for highly oscillatory differential equations

Katina Lorenz

(joint work with Christian Lubich)

The aim of my research work is to develop integrators for highly oscillatory differential equations in classical mechanics, with the general case of Hamiltonians

$$H(p,q) = \frac{1}{2} p^T M(q)^{-1} p + U(q) + \frac{1}{\epsilon^2} V(q), \tag{1}$$

where a constraining potential $\frac{1}{\epsilon^2} V(q)$ penalizes some directions of motion.
In this talk, we present an approach in which we first consider the case of a time-dependent Hamiltonian

$$H(p,q,t) = \frac{1}{2} p^T M(t)^{-1} p + U(q,t) + \frac{1}{2\epsilon^2} q^T A(t) q, \tag{2}$$

with a symmetric positive definite matrix $M(t)$, a symmetric positive semidefinite matrix $A(t)$ and a sufficiently smooth Potential $U(q,t)$. The matrices and their derivatives are supposed to be bounded independently of ϵ.
In this time-dependent case, we found some useful transformations to reach an almost-separation of our problem into slow and fast movements [1]. After again transforming the fast subsystem to smoother, so-called adiabatic variables, we develop adiabatic integrators showing order two in the positions and one in some momenta, and another two numerical integrators of global second order, called the adiabatic midpoint rule and the adiabatic Magnus method.
In [2], we prove that these integrators can be used with significantly larger step sizes than those required by traditional schemes and we illustrate this in the talk by

applying them to some testproblems, where an almost-crossing of eigenfrequencies takes place. We also present an adaptive step size control succesfully used in the case of almost-crossings and nonadiabatic transitions. Stating the good long-time-step behaviour of the adiabatic integrators, we shortly look at the frequency-dependent case (1). We expect a similar accuracy of the integrators, but in the case of an almost-crossing of frequencies, the problem shows a chaotic behaviour (the so-called Takens chaos) and will surely raise new aspects.

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Highly oscillatory quadrature, the one dimensional case

Syvert P. Nørsett

(joint work with Arieh Iserles)

The quadrature of highly oscillatory problems has been a numerical challenge for years. Already in 1928 Filon [1] gave the clue on how it could be handled. Later on little serious were done with such problems, except for using Filon's method in a naive fashion. Only Håvie [2] did work using the ideas of Filon. A lot of papers were written, but with the wrong ideas: trying to banish oscillation by sampling on a finer grid, rather than using oscillation to improve computation. In 2003–4 Iserles and Nørsett started to look into this challenging problem.

The present talk will focus on the problem:

$$I[f] = \int_0^1 f(x) exp^{i\omega g(x)} dx \tag{1}$$

Here ω is a real positive number and G is a given real function.

The multidimensional case will be taken care of by Iserles in the following talk.

We start our talk by giving an example of how bad it becomes if one uses Gauss quadrature on the whole interval [0,1]. For example with Gauss quadrature of order 40 we get an error of $\mathcal{O}(1)$ for $\omega \geq 60$.

Next we give an asymptotic expansion for I[f], leading to an asymptotic method.

The Filon methods from 1928 exhibit excellent results for all positive ω . Filon used a quadratic interpolation for f in (1). The general idea is then to interpolate f with a polynomial p based on the interpolation points $c_1, \ldots, c_\nu \in [0, 1]$.

We will show that the best result is obtained obtain by using $c_1 = 0$ and $c_\nu = 1$. In other words we should use Filon–Lobatto quadrature. The asymptotic error is then equal to $\mathcal{O}(\omega^{-2})$

From the asymptotic expansion we also see that using Hermite interpolation at both at 0 and 1 for the function and its derivatives give us an error asymptotic equal to $\mathcal{O}(\omega^{-r})$ where r is related to the number of derivatives at 0 and 1.

Next we study which effect the interpolation points have on the asymptotic error. We will show that by using interpolation just to f, but letting interpolation points depend on ω, we obtain an asymptotic error as if we had used derivatives.

The error in the Filon-method can be estimated by using interpolation for f by a polynomial of higher order than in the method itself.

To get the Filon-method to work we have assumed that the moments can be found exactly. This can be a shortcoming of the Filon method. However, based on some ideas of Levin [3] and Olver [4] we will indicate how to rectify this problem.

A third approach has recently been given by Huybrechs and Vandewalle[5]. They solve (1) by finding an integration path in the complex plane. We will indicate their approach.

Material for the background of this talk can be found in Iserles and Nørsett [6],[7].

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Multivariate highly oscillatory quadrature

Arieh Iserles

(joint work with Syvert P. Nørsett)

We commence where Syvert Nørsett's talk left: the quadrature of univariate integrals of the form

$$I[f,(a,b)] = \int_a^b f(x)e^{i\omega g(x)}dx,$$

where f and g are real, non-oscillatory, sufficiently smooth functions and $\omega \gg 1$. The challenge being to 'transplant' the theory into a multivariate setting, we let

$\Omega \subset \mathbb{R}^d$ be a bounded, open, nonempty domain with piecewise-smooth boundary, let f and g be smooth $\operatorname{cl}\Omega \to \mathbb{R}$ functions and consider

$$I[f,\Omega] = \int_\Omega f(x) e^{i\omega g(x)} dV.$$

Exactly like in the univariate case, the key to understanding highly oscillatory quadrature is the asymptotics of I for $\omega \gg 1$. The behaviour of I for large ω depends on the function f and its derivatives at three types of *critical points* [5]:

(1) **Stationary points** $x_0 \in \operatorname{cl}\Omega$**,** where $\nabla g(x_0) = 0$;
(2) **Resonance points** $x_0 \in \partial\Omega$**,** where $\nabla g(x_0)$ is normal to the boundary; and
(3) **Vertices** $x_0 \in \operatorname{cl}\Omega$**,** where the boundary has a discontinuity and cone of outward normals is of full diemnsion.

Commencing from the asymptotic expansion

$$I[f,\Omega] \sim -\sum_{m=0}^{\infty} \frac{1}{-i\omega)^{m+1}} \int_{\partial\Omega} n^\top(x) \nabla g(x) \frac{f_m}{\|\nabla g(x)\|^2} e^{i\omega g(x)} dS,$$

where

$$f_0 = f, \qquad f_m = \nabla^\top \left[\frac{f_{m-1}}{\|\nabla g\|^2} \nabla g \right], \quad m \in \mathbb{N}.$$

Suppose that all the critical points are $\xi_1, \ldots, \xi_r$. We represent $f = \sum_{k=0}^r f_k$, where each f_k for $k = 1, \ldots, r$ is a C^∞ *bump function,* equalling 1 in a neighbourhood of ξ_k and 0 outside a larger neighbourhood. Since $I[f_0]$ decays exponentially fast with $\omega \gg 1$, it is enough to consider the contribution of each ξ_k individually and to sum them up [3].

(1) **Stationary points:** Let ξ_j be a nondegenerate point: $\nabla g(\xi_j) = 0$ and $\det\left(\frac{\partial^2 g(\xi_j)}{\partial x_k \partial x_l}\right) \neq 0$. Then, according to a theorem of Hörmander,

$$I[f,\Omega] \sim e^{i\omega g(\xi_j)} \sum_{m=0}^{\infty} \frac{a_m[f]}{\omega^{m+d/2}},$$

where a_m depends on derivatives of f at ξ_j.
(2) **Resonance points:** Essentially, a resonance pojnt $\xi_j \in \partial\Omega$ is nothing else but a stationary point in the $(d-1)$-dimensional manifold $\partial\Omega$, therefore

$$I[f,\Omega] \sim e^{i\omega g(\xi_j)} \sum_{m=0}^{\infty} \frac{b_m[f]}{\omega^{m+(d-1)/2}},$$

where the b_ms depend again on derivatives of f at ξ_j.
(3) **Vertices:** Here the one-dimensional framework scales up immediately,

$$I[f,\Omega] \sim \sum_{m=0}^{\infty} \frac{c_m[f]}{(-i\omega)^{d+1}},$$

where c_m depends on f and its derivatives at the vertex.

The full asymptotic expansion now follows from $I[f,\Omega] = \sum_{k=1}^{r} I[f_k,\Omega]$. Note that (although this is possible in principle, using a theorem by Fedoryuk) we do not seek an explicit asymptotic expansion, since it is exceedingly complex and difficult to implement in practice. What matter to us is not the precise form of expansion coefficients but *the pattern and nature of information, in terms of functions and derivative values, that they require.* Our approach to approximating $I[f,\Omega]$ can be summed up in the *Filon paradigm,* paying tribute to the pioneering contribution of Louis Napoleon Georges Filon [2, 3]. Thus, we seek a quadrature formula Q such that $Q[f,\Omega] = I[f,\Omega] + O(\omega^{-s})$ for some $s \geq 1$ and $\omega \gg 1$. To this end

(1) Given Ω and g, identify the nature of critical points $\xi_1,\ldots,\xi_r \in \mathrm{cl}\,\Omega$.
(2) At each ξ_k identify how many derivatives of f are required, once the integral is applied to the relevant bump function, for error $O(\omega^{-s})$ in the asymptotic expansion. *Note that we do not care what the asymptotic expansion is, only how many derivatives it requires!*
(3) Find a function (typically, a polynomial) ϕ that interpolates (in a Hermite, or perhaps Birkhoff–Hermite sense) f and its derivatives, up to the order that we have identified in *(2),* at each ξ_k. Note that ϕ might interpolate f at further points: although this does not change s, typically this practice results in much reduced error.
(4) Set $Q[f,\Omega] = I[\phi,\Omega]$. Therefore,

$$Q[f,\Omega] - I[f,\Omega] = I[\phi - f,\Omega] = O(\omega^{-s}), \qquad \omega \gg 1.$$

The above approach works exceedingly well in practice, *provided that* $I[\phi,\Omega]$ *can be computed exactly.* If ϕ is a polynomial, this is equivalent to the requirement that the *moments* $I[x^i,\Omega]$, where $x^i = x_1^{i_1}x_2^{i_2}\cdots x_d^{i_d}$, can be computed exactly for relevant multi-indices i. This is often, but not always, the case. Thus, it is only fair to mention two competing approaches, both available in a multivariate setting. Firstly, the *Levin-type methods* of Sheehan Olver, that, in place of interpolation, collocate the function f and its derivatives at the critical points [4]; and secondly, the *numerical stationary phase technique* of Daan Huybrechs and Stefan Vandewalle, that uses Laguerre-type quadrature along non-oscillatory paths in the complex plane [1]. Each of the three techniques – Filon-type, Levin-type and numerical stationary phase – has its own advantages and disadvantages and work is in progress to clarify further these issues.

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Integration and applications of generalized Euler equations

Robert I. McLachlan

Many Hamiltonian partial differential equations, for example the Camassa–Holm equations, the Landau–Lifshitz equation, and (Arnold's celebrated discovery of 1966) the Euler fluid equations, have the form of so-called *generalized Euler equations*, the (reduced) equations of geodesics on an infinite-dimensional group with respect to an invariant metric. The talk explored some analytic and numerical features of the Euler equations associated with the group of all diffeomorphisms of the plane. The metric, typically an H^k metric of the form $\langle u, v\rangle = \iint \langle u, (1-\nabla^2)^k v\rangle \, dx\, dy$, is allowed to vary. The equations of motion are usually written in Lie–Poisson form as

$$\dot{m} + u \cdot \nabla m + \nabla u^T \cdot m + m(\nabla \cdot u) = 0$$

where the momentum m is the Legendre transform of the velocity u; in the example above, $m = (1-\nabla^2)^k u$. A striking feature of Euler equations in $\mathbb{R}^n$ is that they admit singular solutions in which the momentum is concentrated on delta functions on submanifolds of lower dimension m. In the Euler fluid case these correspond when $(m, n) = (0, 2)$ to point vortices; $(0, 3)$ to vortex sticks; $(1, 2)$ or $(2, 3)$ to vortex sheets; and $(1, 3)$ to vortex filaments. (In the codimension 2 and 3 cases the evolution is singular and has to be regularized.) These are used both to understand fluid motion and to simulate general fluid flows, as in the point vortex method. For our equation singular solutions take the form

$$m(x,t) = \int_M p(s)\delta(x - q(s,t))\, ds$$

where the submanifold M is either a set of curves or points. They are Hamiltonian on T^*Q (the cotangent bundle of the embeddings $Q = \mathrm{Emb}(M, \mathbb{R}^2)$ of the points or curves in the plane) with Hamiltonian

$$H = \iint_{M\times M} p(s)G(\|q(s) - q(u)\|)p(u)\, ds\, du,$$

the integrals reducing to sums in the case of point particles. Here G is the Green's function of the metric, i.e. $u = G * m$. Numerical evidence of Holm and Staley suggests that smooth initial momentum distributions with compact support evolve towards a sum of such momentum sheets. They appear to be attracting, at least in a neighbourhood. Therefore one should first understand the motion of momentum sheets themselves, and the talk described a first look at the stability and well-posedness of straight and circular momentum sheets. Unlike the parallel (and ill-posed) case of vortex sheets, which undergo the Kelvin–Helmholtz instability ending in a finite-time singularity, momentum sheets are well-posed but generally vulnerable to a high-frequency instability. This is the opposite to what one might expect, because the metric is chosen to specifically filter out the high frequencies in the momentum. Even more remarkably, an important special case, of a straight

momentum sheet moving normal to itself under the H^1 (Helmholtz) metric, is in fact linearly stable. Circular sheets are always weakly (algebraically) unstable [2].

Generalized Euler equations can be solved numerically in Eulerian or Lagrangian form. The first is a Lie–Poisson PDE on $\mathit{diff}(\mathbb{R}^2)^*$ and has no known Hamiltonian discretizations; Holm and Staley use a mimetic finite difference scheme. The second is a canonical Hamiltonian PDE on $T^*\mathit{Diff}(\mathbb{R}^2)$ and can be discretized by the point particle solutions described above. These can be used to simulate smooth solutions (many particles are needed, but the calculation can be speeded up by the Marker-and-Cell method), momentum sheets (place particles on the sheets), or just the point particle solutions themselves, as is done in the application to image registration. In all cases one has a Hamiltonian system with Hamiltonian $H = \sum\sum p_i G(\|q_i - q_j\|)p_j$, for which only implicit symplectic integrators are available. However, the equations of motion do have the feature that, once $\|q_i - q_j|$ and G have been calculated, the Jacobian derivative of the vector field can be calculated essentially for free. (G is a Gaussian or Bessel function.) This can be exploited in the iterative solver. For $\dot{x} = f(x)$ and the midpoint rule $x_0 \mapsto x_1 := x_0 + \Delta t z$, we have to solve $g(z) := z - f(x_0 + \frac{1}{2}\Delta t z) = 0$. The standard iteration is $z^{k+1} = z^k - g(z^k)$ while Newton's method is $z^{k+1} = z^k - (I-A)^{-1}g(z^k)$, $A = \frac{1}{2}\Delta t f'(z^k)$. The new iteration is $z^{k+1} = z^k - (\sum_{i=0}^{M} A^i)g(z^k)$, which uses one vector field and Jacobian evaluation and M Jacobian–vector multiplies. In practice M is determined dynamically using a suitable termination criterion, and z^0 is given by polynomial extrapolation from previous time steps, the order determined dynamically. The iteration is advantageous both for N-particle and for lattice (e.g. semidiscrete PDE) systems. In practice only a few (typically 1–3) evaluations of the vector field are needed per time step [1]. Open problems in the momentum sheet application include finding a high-order regularization of singular Green's functions that does not introduce a temporal instability, conserving the so-called potential vorticity, and integrating the normal motion of straight sheets; these are degenerate, having a double zero eigenvalue in each Fourier mode, which is split by the particle method. The last two problems can be fixed by first reducing by the particle-relabelling symmetry $G = \mathrm{Diff}(\mathbb{R})$ to obtain a Lie–Poisson system on $T^*(Q/G) \oplus \mathfrak{g}^*$, but a Hamiltonian discretization on this space is more difficult.

A second application is to image registration (warping, morphing) [4]. One is given two images f and g and seeks a diffeomorphism φ that minimizes $\|f - g \circ \varphi\|$. φ is induced by the motion of point particles. This gives an optimization problem with respect to the initial momenta (and positions, if desired) of the particles, constrained by the equations of motion. Constrained optimization relies on accurate satisfaction of the constraints, indicating the use of a shooting method, where all our knowledge of fast solution of initial value problems can be applied. The iteration described above works even better on optimization, control, and boundary value problems, because excellent initial guesses are available; this again favours implicit over explicit methods. The numerical results are encouraging but a major open problem is to find a direct link between the symplecticity of the integrator and the behaviour of the optimization problem.

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Discussion

Some open problems in Geometric Numerical Integration

- The implicit midpoint rule applied to $y' = J\nabla H(y)$ is a Poisson map. For more general Poisson systems $y' = J(y)\nabla H(y)$, does there exist any nonstandard generalization of the implicit midpoint rule that is at least conjugate to a Poisson map for a perturbed matrix $\widetilde{J}(y)$? One can use for example the multiplicative structure of the equations to obtain nonstandard generalizations of the implicit midpoint rule, e.g.,

$$y_{n+1} = y_n + \frac{h}{2}(J(y_n) + J(y_{n+1}))\nabla H\left(\frac{y_n + y_{n+1}}{2}\right).$$

  [Laurent O. Jay]
- To give a lower bound on the complexity of approximating the solution of a differential equation, where (in contrast to standard complexity theory) the algorithm can depend on the differential equation. Hence divide differential equations into natural complexity classes. *[Robert McLachlan]*
- The use of fixed-point iterations enlarges the class of functions that can be computed quickly and also enlarges the class of numerical methods, for example to include implicit Runge-Kutta methods. Fixed point iterations with degenerate fixed points, for example $(x, y) \mapsto (f(x, y), g(x, y))$ where $(x, x) \mapsto (x, x)$, define a function by mapping an initial condition (x_0, y_0) to a limit (x^*, x^*) which depends on the initial condition. Examples are the AGM (Arithmetic-Geometric Mean) used in computing elliptic functions and an algorithm for the matrix sign function. The problem asks whether such iterations can be used in numerical integration of differential equations. *[Robert McLachlan]*

- Construct a volume-preserving integrator that preserves all symmetries and reversing symmetries of the AAA flow:

$$\begin{aligned} \frac{dx}{dt} &= A\sin z + A\cos y \\ \frac{dy}{dt} &= A\sin x + A\cos z \\ \frac{dz}{dt} &= A\sin y + A\cos x \end{aligned}$$

  or prove that such a construction is impossible. *[G. Reinout W. Quispel]*
- What (if any) are the benefits of symplectic in space and time integrators for Hamiltonian wave equations. *[Sebastian Reich]*
- Backward error analysis for ODEs is well-developed and has been used very successfully in the analysis of numerical methods, for example to explain long time approximate energy conservation of symplectic discretizations of Hamiltonian systems. Recently there has been some progress in the development of a backward error analysis for multisymplectic discretizations of semilinear Hamiltonian PDEs and approximate momentum and energy conservation of symplectic discretiztions could be explained. However a backward error analysis for fully nonlinear PDEs - modelling for example problems from continuum mechanics like fluid dynamics and elastodynamics - is still missing, and this poses a challenging problem for the Geometric Integration community. *[Claudia Wulff]*

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