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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 structure preservation affects the long-time behaviour of numerical methods.

Mathematics Subject Classification (2010): 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, including Lie group methods and integrators for constrained Hamiltonian mechanics, and methods for problems with highly oscillatory solutions. The unifying theme is 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 arises independently in such diverse areas of research as astronomy, molecular dynamics, mechanics, theoretical physics, control theory, and numerical analysis with important contributions from other areas of both applied and pure mathematics. Moreover, it turns out that the 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.

Geometric numerical integration has developed into an active and interdisciplinary research area in the last two decades. While the core of the subject, for ordinary differential equations, is presented in the monographs

E. Hairer, Ch. Lubich, G. Wanner, Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations. Springer, Berlin, 2002,

and

B. Leimkuhler, S. Reich, Geometric Integrators in Hamiltonian Mechanics. Cambridge Univ. Press, 2004,

recent progress in the development and long-time theory of geometric integrators for classes of partial differential equations is documented in the book

E. Faou, Geometric numerical integration and Schrödinger equations. Zurich Lectures in Advanced Mathematics 15, European Math. Soc., Zürich, 2012.

In addition to the construction of geometric integrators, an important aspect of geometric integration is the explanation of 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, where 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 seamlessly translate into structure preservation on the level of the modified equation. Much insight and rigorous 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 backward error analysis has been very successful for ordinary differential equations, it does not extend directly to highly oscillatory systems and geometric integrators for partial differential equations. Only fairly recently, versions of backward error analysis based on Birkhoff normal form theory or on modulated Fourier expansions have allowed to explain favourable long-time energy behaviour for geometric integrators for some Hamiltonian partial differential equations. Highly oscillatory systems is another area with substantial recent progress where yet much remains to be understood and explored.

The workshop addressed the recent developments in theory and applications of geometric numerical integration and reflected the multidisciplinary nature of the topic.

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Workshop: Geometric Numerical Integration

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Abstracts

Numerical methods for wave equation in heterogenous media

Assyr Abdulle

In this report we discuss recent developments of numerical methods for the wave equation in a bounded polygonal domain Ω

$$\partial_{tt} u_\varepsilon - \nabla \cdot (a_\varepsilon(x) \nabla u_\varepsilon) = F \text{ in } \Omega \times]0,T[\tag{1}$$

$$u_\varepsilon(x,0) = g^1(x), \partial_t u_\varepsilon(x,0) = g^2(x), \ u_\varepsilon = 0 \text{ on }]0,T[\times \partial\Omega, \tag{2}$$

where $g^1 \in H^1(\Omega)$, $g^2 \in L^2(\Omega)$, $F \in L^2(0,T;L^2(\Omega)$. The family of symmetric tensors satisfy $a_\varepsilon \in (L^\infty(\Omega))^{d\times d}$ and is assumed to be uniformly elliptic and bounded. Here we think of ε as an abstract parameter $0 < \varepsilon << 1$. Furthermore, the derivative of a^ε is assumed to be large and unbounded as $\varepsilon \to 0$ (e.g., $\|a'_\varepsilon\| = \mathcal{O}(\varepsilon^{-1})$). We consider two situations that require different numerical modelling.

Heterogenenous media without scale separation. For the discrete approximation, we pick a piecewise linear finite element space V_h and consider the following problem: find $u_h : [0,T] \to V_h$ such that $\forall v_h \in V_h$ and a.e. $t > 0$

$$\langle \partial_{tt} u_h, v_h \rangle + (a_\varepsilon(x) \nabla u_h(\cdot,t), \nabla v_h)_{L^2(\Omega)} = (F(\cdot,t), v_h)_{L^2(\Omega)},$$

with appropriate discrete initial value. Following the best approximation result of Baker [7] we have ($u^\varepsilon \in C^0(0,T;H^1(\Omega))$ is the solution to the weak form of (1))

$$\|u_\varepsilon - u_h\|_{L^\infty(L^2)} \leq C(T)(\|u_\varepsilon - \Pi_h(u_\varepsilon)\|_{L^\infty(L^2)} + \|\partial_t u_\varepsilon - \partial_t \Pi_h(u_\varepsilon)\|_{L^1(L^2)}),$$

where $\Pi_h : H^1_0(\Omega) \to V_h$ is the Ritz-projection on V_h, i.e., the $(a_\varepsilon \nabla\cdot, \nabla\cdot))$-orthogonal projection. An a priori error estimate of the projection error involves the norm of the derivative of a_ε and leads to a rate of convergence that cannot scale better than $C(T)(h/\varepsilon)$ leading to a computational complexity of $\mathcal{O}(h^{-d})$ with $h < \varepsilon$. In what follows, we construct a multiscale space following [11]. We consider a coarse grid V_H and assume that the fine space V_h is obtained by refinement of V_H with $h < \varepsilon << H$. We then consider the decomposition

$$V_h = V_H^{ms} \oplus W_h,$$

where $W_h = Ker(I_H)$ and $I_H : V_h \longrightarrow V_H$ is the L^2 projection. The multiscale space is defined by

$$V_{H,k}^{ms} = \{\Phi_z + Q_{h,k}(\Phi_z), \Phi_z \text{ nodal macro basis fct}\},$$

where $\Phi_z \in V_H$ is a macroscopic basis function and for each $K \in \text{supp}(\Phi_z)$, $Q_{h,k}(\Phi_z) \in W_h(U_k(K))$ is the solution the solution of a localized fine scale elliptic problem in an environment $U(K)$ around K. We can then show [4]

Theorem 1. *Under the regularity assumptions for the wave equation stated above, we have*

$$\|u_\varepsilon - u_{H,k}^{ms}\|_{L^\infty(L^2)} \leq C(T)(\|u^\varepsilon - \Pi_{H,k}^{ms}(u^\varepsilon)\|_{L^\infty(L^2)} + \|\partial_t u^\varepsilon - \partial_t \Pi_{H,k}^{ms}(u^\varepsilon)\|_{L^1(L^2)}).$$

Assuming in addition $\partial_t u_\varepsilon \in L^1(H^1)$ *then*

$$\|u_\varepsilon - \Pi^{ms}_{H,k}(u_\varepsilon)\|_{L^\infty(L^2)} \leq C(T)H\|u_\varepsilon\|_{L^\infty(H^1)}$$
$$\|\partial_t u_\varepsilon - \partial_t \Pi^{ms}_{H,k}(u_\varepsilon)\|_{L^1(L^2)} \leq C(T)H\|\partial_t u_\varepsilon\|_{L^1(H^1)}.$$

One issue in the above estimate that also appears in other multiscale methods developed so far (see the references in [4]) is the boundedness of $\|\partial_t u_\varepsilon\|_{L^1(H^1)}$. A standard a priori error estimates yields $\|\partial_t u_\varepsilon\|_{L^1(H^1)} = \mathcal{O}(\varepsilon^{-1})$. Using a perturbation argument together with $G-$convergence we show in [4] that this term can be bounded and we obtain $\|u_\varepsilon - u^{ms}_{H,k}\|_{L^\infty(L^2)} \leq C(T)(H + r(\varepsilon))$, with C independent of ε and $\lim_{\varepsilon\to 0} r(\varepsilon) = 0$.

Heterogenenous media with scale separation. Using $G-$convergence, one can show there exists a subsequence of solution of (1) that converges weakly* in $L^\infty(H^1_0)$ to a homogenized function u_0 solution of

$$\partial_{tt} u_0 - \nabla \cdot (a_0(x)\nabla u_0) = F \text{ in } \Omega\times]0,T[$$
$$u_0(x,0) = g^1(x), \partial_t u_0(x,0) = g^2(x),\ u_0 = 0 \text{ on }]0,T[\times\partial\Omega,$$

where a^0 is again uniformly elliptic and bounded but independent of the small scale ε [8]. For periodic (or locally periodic) coefficients, a^0 is obtained from d solutions $\chi^1, \ldots, \chi^d$ of so-called cell problems (localized elliptic problems).

Finite element heterogeneous multiscale method. We pick a standard macroscopic finite element space V_H and define a sampling domain K_δ (of size δ comparable to ε) within each macro element K. We consider then the following problem: find $u_H : [0,T] \to V_H$ such that

$$(\partial_{tt} u_H, v_H) + B_H(u_H, v_H) = (F, v_H) \qquad \forall v_H \in V_H, \tag{3}$$

with appropriate projection of the true initial conditions, where $B_H(u^H, v^H) = \sum_{K\in\mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x)\nabla u^h_K \cdot \nabla v^h_K dx$ and u^h_K (respectively v^h_K) are solutions of a micro problem in a localized sampling domain $K_\delta \subset K$ with $\delta \simeq \varepsilon$. A generalized version of the above method is shown to converge in [1] towards the homogenized solution u^0. However, with increasing time, due to dispersive effects, the true solution, u^ε, deviates from the classical homogenized limit u^0 [13, 10]. In [5] the solutions of the following family of effective equations

$$\partial_{tt}\tilde{u} = a^0\partial_{xx}\tilde{u} - \varepsilon^2\big(\tilde{a}^2\partial_{xxxx}\tilde{u} - \tilde{b}^0\partial_{xx}\partial_{tt}\tilde{u}\big) \quad \text{in } (0,T^\varepsilon]\times\Omega, \tag{4}$$

is shown to capture the dispersive effects over time $\mathcal{O}(\varepsilon^{-2})$. This generalizes results in [10, 9]. In the above equation, we assume $x \mapsto \tilde{u}(t,x)$ is Ω periodic.

Theorem 2. Under appropriate regularity assumptions of the data, for any $\mu = \langle\chi\rangle$ and any real numbers $\tilde{b}^0, \tilde{a}^2$ such that $\tilde{b}^0 = b^0 + \langle\chi\rangle^2$, $b^0 = \langle(\chi - \langle\chi\rangle)^2\rangle$, $\tilde{a}^2 = a^0\langle\chi\rangle^2$ the solution of the effective equation

$$\partial_{tt}\tilde{u} - a^0\partial_{xx}\tilde{u} + \varepsilon^2(\tilde{a}^2\partial_{xxxx}\tilde{u} - \tilde{b}^0\partial_{ttxx}\tilde{u}) = F,$$

is an effective equation that satisfies $\|u^\varepsilon - \tilde{u}\|_{L^\infty(0,\varepsilon^{-2}T;L^2(\Omega))} \leq C\varepsilon$, over longtime $\varepsilon^{-2}T$, where C is independent of ε.

Next following [3], we consider the FE-HMM-L method obtained from (3) by replacing $(\partial_{tt}u^H, v^H)$ with $(\partial_{tt}u^H, v^H)_Q$ where

$$(u_H, v_H)_Q = (u_H, v_H) + \sum_{K\in\mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} (u_K^h - u_H)(v_K^h - v_H)dx,$$

where u_K^h (respectively v_K^h) are the micro functions already in (3). A fully discrete a prior error analysis over long-time has been obtained for the FE-HMM-L in [5].

Theorem 3. Under suitable regularity assumptions we have

$$\|u^\varepsilon - u_H\|_{L^\infty(0,\varepsilon^{-2}T;L^2(\Omega))} \leq C\left(\varepsilon + \left(h/\varepsilon^2\right)^2 + H/\varepsilon\right),$$

where C is independent of ε. Generalization to higher order macro elements and higher order estimates are also derived (the term H/ε can be replaced by H^ℓ/ε). As error estimates for classical resolved FEM yields a bound of the type $C(h/\varepsilon^3)$, the FE-HMM-L achieves significant reduction in the computational complexity (the size of the linear system of ODEs scale as $\mathcal{O}((tol\cdot\varepsilon^3)^{-1})$ for a resolved FEM while it only scale as $\mathcal{O}((tol\cdot\varepsilon)^{-\ell})$ for the FE-HMM-L). A seneralization to multi-dimensional wave problems has been obtained in [6].

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References

[1] A. Abdulle and M. J. Grote. Finite element heterogeneous multiscale method for the wave equation. *Multiscale Model. Simul.*, 9(2):766–792, 2011.

[2] A. Abdulle, M. J. Grote, and C. Stohrer. FE heterogeneous multiscale method for long-time wave propagation. *C. R. Math. Acad. Sci. Paris*, 351(11-12):495–499, 2013.

[3] A. Abdulle, M. J. Grote, and C. Stohrer. Finite element heterogeneous multiscale method for the wave equation: long-time effects. *Multiscale Model. Simul.*, 12(3):1230–1257, 2014.

[4] A. Abdulle, P. Henning. Localized orthogonal decomposition method for the wave equation with a continuum of scales *to appear in Math. Comp.*

[5] A. Abdulle, T. Pouchon. A priori error analysis of the finite element heterogenenous multiscale method for the wave equation over long time *to appear in SIAM J. Numer. Anal.*.

[6] A. Abdulle, T. Pouchon. Effective models for the multidimensional wave equation in heterogeneous media over long time *preprint 2016.*

[7] G. A. Baker. Error estimates for finite element methods for second order hyperbolic equations. *SIAM J. Numer. Anal.*, 13(4):564–576, 1976.

[8] S. Brahim-Otsmane, G. A. Francfort, and F. Murat. Correctors for the homogenization of the wave and heat equations. *J. Math. Pures Appl.*, 71(3):197–231, 1992.

[9] T. Dohnal, A. Lamacz, and B. Schweizer, *Bloch-wave homogenization on large time scales and dispersive effective wave equations*, Multiscale Model. Simul., 12 (2014), pp. 488–513.

[10] A. Lamacz. Dispersive effective models for waves in heterogeneous media. *Math. Models Methods Appl. Sci.*, 21(9):1871–1899, 2011.

[11] A. Målqvist and D. Peterseim. Localization of elliptic multiscale problems. *Math. Comp.*, 83(290):2583–2603, 2014.

[12] A. Pankov. *G-convergence and homogenization of nonlinear partial differential operators*, volume 422 of *Mathematics and its Applications*. Kluwer Academic Publishers, Dordrecht, 1997.

[13] F. Santosa and W. W. Symes. A dispersive effective medium for wave propagation in periodic composites. *SIAM J. Appl. Math.*, 51(4):984–1005, 1991.

Zassenhaus splitting and semi-classical Schrödinger equations

Philipp Bader

(joint work with A. Iserles, P. Singh, K. Kropielnicka)

We consider the efficiency of Yoshida's composition method versus a Zassenhaus decomposition to construct high-order integrators for the (semi-classical) Schrödinger equation,

$$\partial_t u(x,t) = -\frac{\mathrm{i}}{\varepsilon} H u(x,t) = \mathrm{i}\left(\varepsilon\Delta - \varepsilon^{-1}V(x)\right) u(x,t),\ x \in [-1,1],\ t \geq 0,$$

equipped with an initial condition $u(x,t) = u_0(x)$, and periodic boundary conditions and potential V. Several numerical methods exist in the literature, mostly based on splitting (reviewed in [2]), Hagedorn wavepackets [3] and the Zassenhaus expansion [1]. Splitting methods are efficient since the Laplacian can be solved with Fast Fourier Transforms (FFTs). Similarly, the related Zassenhaus decomposition relies on the fast computation of spatial derivatives using FFTs and the two methods complement each other: Splitting methods are particularly efficient for low orders of accuracy since very few FFTs are involved, however, for higher orders, the quadratic growth in cost for the Zassenhaus approach soon becomes superior to the exponential growth in cost for the splitting methods.

We introduce a hybrid method that combines the benefits of the two families showcasing the versatility of the Zassenhaus decomposition versus the standard composition technique due to Yoshida [7], Suzuki [6] and others. Since higher order methods permit the use of larger time-steps which can compensate the higher computational effort per step, we elaborate on the optimal choice thereof.

For low orders of accuracy, the order conditions can be solved directly and splitting methods are highly efficient. They approximate the flow of an IVP $u' = A(u) + B(u),\ u(t_0) = u_0$, by composing the individual flow maps, $\varphi_t^{[A]}$, $\varphi_t^{[B]}$ and furthermore, if both flows preserve certain geometric properties, such as symplecticity, unitarity, energy, etc., so will their composition. An m-stage method of order p takes the form $\Phi_h^{[p]} = \varphi_{a_m h}^{[A]} \circ \varphi_{b_m h}^{[B]} \circ \cdots \circ \varphi_{a_1 h}^{[A]} \circ \varphi_{b_1 h}^{[B]}$ for some coefficients $a_i, b_j \in \mathbb{R}$ which can be obtained from the Baker–Campbell–Haussdorf (BCH) formula (for sufficiently small h)

$$\mathrm{e}^{hA}\mathrm{e}^{hB} = \mathrm{e}^{\mathrm{BCH}(hA,hB)} = \mathrm{e}^{h(A+B)+\frac{1}{2}h^2[A,B]+\cdots} \tag{1}$$

As the order increases, the number of equations to satisfy grows exponentially together with the dimension of the graded Lie algebra generated by A, B and different approaches are needed.

Before we go into further details, a few words on the peculiarities of the semi-classical Schrödinger equation and its discretisation are in place: The semi-classical SE involves three small parameters, the step-size h, the grid-size $2/N$ where N is the number of grid points and the external parameter ε. From WKB analysis, it is clear that oscillations of size $1/\varepsilon$ will occur and require $N = \mathcal{O}(1/\varepsilon)$. We also express the step-size and the desired error in the same parameter $h = \varepsilon^\sigma$ and ε^κ, respectively.

Yoshida's device. Let Φ_h be a symmetric method of order $2p$ for a time-step h. Then, the order can be risen by $2k$ in k steps in by the sequence $S_0(h) = \Phi_h$, $\{S_k\}_{k=1,\dots,m}$, where S_k is of order $2(p+k)$ using

$$S_{k+1}(h) = S_k((1+\alpha_k)h) \circ S_k((-1-2\alpha_k)h) \circ S_k((1+\alpha_k)h),$$

tripling the computational effort per step. In order to establish the overall error, we need to look at the size of the leading error constants using the symmetric BCH formula. Because of Theorem 1 below and (1), we have a leading local error of $\mathcal{O}(\varepsilon^{(p+1)\sigma-1})$ for a $2p$th order splitting with cost c_p per step and after m repetitions of the Yoshida process starting from $\Phi_h = \Phi_h^{[2p]}$, we get $S_m(h) - \mathrm{e}^{-\frac{\tau}{\varepsilon}H} = \mathcal{O}(\varepsilon^{(2m+2p+1)\sigma-1})$. Expressing σ as a function of κ and m, the total cost per unit interval $c_p \times 3^m/\varepsilon^\sigma$ is minimised with respect to the number of steps at $\sigma_{opt.} = \sqrt{-\frac{\kappa+1}{2\log\varepsilon}\log 3}$, and the total cost is $\mathrm{cost}(S_{\sigma_{opt}}(\Phi_h)) = \frac{c_p}{3^p}\mathrm{e}^{\sqrt{\log 9}\sqrt{(1+\kappa)(-\log\varepsilon)}}$. The optimal time-step size is independent of the order of the underlying method and the cost grows exponentially with the precision $\sqrt{\kappa}$.

Hybrid Zassenhaus. We propose a hybridised Zassenhaus expansion based on the Zassenhaus method [1] in a way that incorporates both optimised splittings and cheap order increase using commutators. We start from some efficient (symmetric) splitting method $\Phi_h^{[2p]}$ of order $2p$ and write it as a single exponential using the sBCH formula as follows: $\Phi_h^{[2p]} = \mathrm{e}^{-\frac{\tau}{\varepsilon}\tilde{H}} = \mathrm{e}^{A+B+\sum_{k=p}\mathcal{W}_0^{[k]}}$ where $\tilde{H}$ is a *modified Hamiltonian* and $\mathcal{W}_0^{[k]} = \mathcal{O}(\varepsilon^{(2k+1)\sigma-1})$. The idea is to cancel the largest error term $\mathcal{W}_0^{[p]}$ by extracting it,

$$\mathrm{e}^{-\frac{\tau}{\varepsilon}H+\sum_{k=p+1}\mathcal{W}_1^{[k]}} = \mathrm{e}^{\mathrm{sBCH}(-\mathcal{W}_0^{[p]},-\frac{\tau}{\varepsilon}H)} = \mathrm{e}^{-\mathcal{W}_0^{[p]}/2}\Phi_h\mathrm{e}^{-\mathcal{W}_0^{[p]}/2},$$

and proceeding in the same way, the order is increased gradually

$$\begin{aligned}\mathrm{e}^{-\frac{\tau}{\varepsilon}H+\sum_{k=p+2}\mathcal{W}_2^{[k]}} &= \mathrm{e}^{\mathrm{sBCH}(-\mathcal{W}_1^{[p+1]},\mathrm{sBCH}(-\mathcal{W}_0^{[p]},-\frac{\tau}{\varepsilon}\tilde{H}))}\\ &= \mathrm{e}^{-\frac{1}{2}\mathcal{W}_1^{[p+1]}}\mathrm{e}^{-\frac{1}{2}\mathcal{W}_0^{[p]}}\Phi_h^{[p]}\mathrm{e}^{-\frac{1}{2}\mathcal{W}_0^{[p]}}e^{-\frac{1}{2}\mathcal{W}_1^{[p+1]}}.\end{aligned}$$

since we can ensure that $\mathcal{W}_l^{[k]} = \mathcal{O}\left(\varepsilon^{(2k+1)\sigma-1}\right)$.

An important feature of the Zassenhaus split is to defer the spatial discretisation to the latest possible step and derive the method in the Lie algebra. This means that we compute commutators symbolically and group the result by size in powers of ε yielding the $\mathcal{W}_l^{[k]}$ and at the same time ensuring stability. For efficient

computation and analysis, we need to work in the appropriate algebra of angle brackets, introduced in [5]. For some functions $f, g : \mathbb{R} \to \mathbb{C}$ and $n \in \mathbb{N}$, define the operator $\langle f \rangle_n = \frac{1}{2}\left(f\partial_x^n + \partial_x^n f\right)$. This bracket hence forms an anti-commutator with the nth spatial derivative. Furthermore, angle-brackets are closed under commutation and changes parity, i.e., if the sum of indices $k + l$ in $[\langle f \rangle_k, \langle g \rangle_l]$ is even (odd), all resulting angle brackets will have odd (even) indices which will yield a unitary integration scheme and the maximal degree of the derivatives is lowered to $k + l - 1$.

Theorem 1. *Let* $\mathfrak{g}$ *be in the Lie algebra generated by* $\{\varepsilon\partial_x^2, \varepsilon^{-1}V\} \Rightarrow \mathfrak{g} = \mathcal{O}\left(\varepsilon^{-1}\right)$.

Therefore, any commutator of length $2k + 1$ with elements $\{\tau\varepsilon\partial_x^2, \tau\varepsilon^{-1}V\}$ is of size $\mathcal{O}\left(\varepsilon^{(2k+1)\sigma-1}\right)$ and the terms $\mathcal{W}_0^{[k]}$ contain all commutators of this length in the sBCH formula. Since a commutator is smaller than the product of its constituents, we only need to examine the number of angle brackets than can appear at a given order in ε in order to find the optimal combination of time-step and order. From $\mathcal{W}_0^{[k]} = \mathcal{O}\left(\varepsilon^{(2k+1)\sigma-1}\right)$, we already know that $\mathcal{W}_l^{[p+l]}$ includes commutators of length $2(p + l) + 1$. The proof of Theorem 1 lets us conclude that commuting the largest angle-brackets of a given degree in the derivative will not change the size and since the construction begins with brackets applied to $\langle \tau V \rangle_0, \langle \tau \rangle_2$, it follows that the largest derivative of degree $2k$ is constructed when using $2k$ Laplacians and only one potential, this implies that the exponent generated in the kth step, $\mathcal{W}_k^{[p+k]}$ contains $p + k$ angle brackets. To reach global error $\mathcal{O}(\varepsilon^\kappa)$ using m Zassenhaus steps (computing up to $\mathcal{W}_{m-1}^{[m-1+p]}$), $\mathcal{O}(\varepsilon^\kappa) = \mathcal{O}\left(\mathcal{W}_m^{[m+p]}/\varepsilon^\sigma\right) \Longrightarrow \kappa = (2(m + p) + 1)\sigma - 1 - \sigma = 2(m + p)\sigma - 1$ we need a time step σ of $\sigma = \frac{\kappa+1}{2(m+p)}$. In each step, we evaluate the underlying method once and $2m$ exponentials $\mathrm{e}^{\frac{1}{2}\mathcal{W}_k^{[p+k]}}, k = 0, \ldots, m - 1$. Since the latter decrease rapidly in size with k, we employ the Arnoldi method which preserves unitarity of the exponential and requires only a small number of Krylov iterations. In order to approximate $\mathrm{e}^{\frac{1}{2}\mathcal{W}_k^{[p+k]}} = \mathcal{O}\left(\exp(\varepsilon^{(2(p+k)+1)\sigma-1})\right)$ up to the local error $\mathcal{O}(\varepsilon^{\kappa+\sigma})$, we require r_k Krylov iterations [4, 1], where r_k has to satisfy $r_k \geq \left\lceil \frac{\kappa+\sigma}{(2(k+p)+1)\sigma-1} \right\rceil$.

Recalling that $\mathcal{W}_k^{[p+k]}$ contains $p+k$ angle brackets which have to be evaluated, each Krylov iteration comes with a price tag of $(3(k+p)+1)$ FFTs . With this result, we can establish the cost of an exponential to $\mathrm{cost}(\mathrm{e}^{\mathcal{W}_k^{[p+k]}}) = r_k(3(k+p)+1)$. Summing up terms, we can show that using a high-order optimised splitting method as building block, the Zassenhaus splitting is superior to Yoshida's composition technique in computational efficiency.

References

[1] P. Bader, A. Iserles, K. Kropielnicka, and P. Singh. Effective approximation for the semiclassical Schrödinger equation. *Found. Comput. Math.*, 14(4):689–720, 2014.

[2] W. Bao, S. Jin, and P. A. Markowich. On time-splitting spectral approximations for the Schrödinger equation in the semiclassical regime. *J. Comput. Phys.*, 175:487–524, 2002.

[3] E. Faou, V. Gradinaru, and C. Lubich. Computing semiclassical quantum dynamics with Hagedorn wavepackets. *SIAM J. Sci. Comp.*, 31:3027–3041, 2009.
[4] M. Hochbruck and C. Lubich. On Krylov subspace approximations to the matrix exponential operator. *SIAM J. Numer. Anal.*, 34:1911–1925, 1997.
[5] P. Singh. Algebraic theory for higher-order methods in computational quantum mechanics, 2015. arXiv:1102.1622v1 [math.NA].
[6] M. Suzuki. General theory of fractal path integrals with applications to many-body theories and statistical physics. *J. Math. Phys.*, 32:400–407, 1991.
[7] H. Yoshida. Construction of higher order symplectic integrators. *Phys. Lett. A*, 150:262–268, 1990.

Nonrelativistic limit of the nonlinear Klein-Gordon equation: dynamics over long times

Dario Bambusi
(joint work with S. Pasquali)

We study the nonrelativistic limit of the nonlinear Klein Gordon equation

$$\frac{1}{c^2}u_{tt} - \Delta u + c^2 u = -\lambda u^3 \ , \quad x \in M \ , \quad c \to \infty \ , \tag{1}$$

M compact manifold or $\mathbb{R}^d$ with the goal of obtaining an effective equation describing the dynamics for times which are as long as possible. It is well known that at first order in $1/c^2$ the solutions are, at least formally, described by solutions of the nonlinear Schrödinger equation

$$i\dot{\phi} = -\frac{1}{2}\Delta\phi + \lambda|\phi|^3 \ , \tag{2}$$

in the sense that, up to higher order corrections, $u = \Re(e^{-ic^2t}\phi(t))$. For the case $M = \mathbb{R}^d$, rigorous results showing that this is actually true for times of order 1 have been obtained in a series of papers (see in particular [4]). A similar result (with loss of smoothness) has been obtained in the case of $M = \mathbb{T}^d$ in [3].

In this talk I have discussed the problem in the case of more general manifolds and the possibility of getting estimates valid over longer times, namely times of order c^r with an arbitrary r.

In order to get the result for general manifolds, the idea is to use a Hamiltonian approach. Indeed the system is Hamiltonian, and, in suitable variables, its Hamiltonian takes the form

$$H = \int_M c \left| \langle\nabla\rangle_c^{1/2}\psi \right|^2 + \frac{\lambda}{4}\left[\left(\frac{c}{\langle\nabla\rangle_c} \right)^{1/2} \frac{\psi + \bar{\psi}}{\sqrt{2}} \right]^4 dx \tag{3}$$

where

$$\langle\nabla\rangle_c := (c^2 - \Delta)^{1/2} \ ,$$

which after expansion and time rescaling becomes

$$H = \int_M |\psi|^2 dx + \frac{1}{c^2}\int_M \left(\frac{1}{2}|\nabla\psi|^2 + \frac{\lambda}{2}\left(\psi + \bar{\psi}\right)^4 \right) dx + h.o.t. \tag{4}$$

For $c = \infty$ the Hamiltonian reduces to the generator of the Gauge group $\psi \mapsto e^{-it}\psi$ which has always period 1 in time. Thus one can see (4) as a (singular) perturbation of a completely resonant system and apply the standard methods of canonical perturbation theory (for example see [1]). More precisely, for any r one can construct a canonical transformation $\psi = \mathcal{T}^{(r)}(\phi)$ which conjugates the Hamiltonian (3) to a new Hamiltonian which is in normal form (namely has a form which is as simple as possible) plus a remainder of order c^{-r}. The equation of the normal form turns out to be a perturbation of (2).

Then, following the ideas of [1], one can show that the solution of the normal form equation (in which the remainder is neglected) are c^{-r} close to the solutions of the true equations for times of order 1. This is the first result presented in the talk.

In general it is not possible to improve the time scale. The reason is strictly related to the fact that the distance between two solutions of the original problem can increases exponentially in time with a rate of order 1.

One can get a result valid over longer time scales in the case of $\mathbb{R}^d$. Indeed, in this case one can exploit dispersion and in particular Strichartz estimates in order to show that in this case there is no exponential divergence of the solutions of the original equation. This was already exploited in [2].

In order to state a Theorem denote by ϕ the solution of the normal form equations (described above).

Theorem 2. *Fix $k \geq 0$ and a large r, then there exists large k_* and c_*, with the following property: assume $c > c_*$, take an initial datum such that the solution ϕ of the normalized equation exists for all times and has the structure*

$$\phi(x,t) = \phi_{rad}(x,t) + \sum_{l=1}^{N} \eta_l(x - v_l t) \tag{5}$$

with some $\eta_l \in \mathcal{S}$, $v_l \in \mathbb{R}^3$ and $\phi_{rad} \in L^p_t W^{k_*,q}_x$ with (p,q) any Schrödinger admissible pair; denote $\psi_a(t) := \mathcal{T}^{(r)}(e^{ic^2 t}\phi(t))$. Let $\psi(t)$ be the solution of the Hamilton equation of (3) with the corresponding initial datum, then one has

$$\|\psi_a(t) - \psi(t)\|_{H^k} \preceq \frac{1}{c}\ , \quad |t| \preceq c^r\ .$$

References

[1] D. Bambusi, *Galerkin averaging method and Poincaré normal form for some quasilinear PDEs*, Ann. Sc. Norm. Super. Pisa Cl. Sci. **4** (2005), 669–702.

[2] D. Bambusi, A. Maspero, *Freezing of Energy of a Soliton in an External Potential*, Commun. Math. Phys. To appear.

[3] E. Faou, K. Schratz, *Asymptotic preserving schemes for the Klein-Gordon equation in the non-relativistic limit regime*. Numer. Math. **126** (2014), 441–469.

[4] N. Masmoudi, K. Nakanishi, *From nonlinear Klein-Gordon equation to a system of coupled nonlinear Schrödinger equations*, Math. Ann. **324** (2002), 359–389.

Multiscale Methods and Analysis for Highly Oscillatory Nonlinear Dispersive Partial Differential Equations

Weizhu Bao
(joint work with Yongyong Cai, Xuanchun Dong, Xiaofei Zhao)

Nonlinear dispersive partial differential equations (PDEs) have become fundamental and the most significant and important mathematical models for problems arising from quantum physics without/with Einstein's general relativity, plasma physics, nonlinear optics, molecular dynamics, degenerate quantum gas, etc. Typical examples are such as the nonlinear Schrodinger equation for many-body dynamics with quantum effect, the Klein-Gordon equation for spinless relativistic particles or superfluid universe, the Zakharov system and Klein-Gordon-Zakharov system for plasma physics, the Dirac equation for spin particles and/or graphene, etc. These equations are nonlinear and dispersive, and their solutions are usually highly oscillatory in space and/or time. From a numerical and mathematical point of view, the appearance of nonlinear terms and highly oscillatory solutions bring up fundamental and significant new difficulties in efficient numerical computation and mathematical analysis.

Multiscale methods and analysis have been become the most efficient and powerful numerical and mathematical tools for solving problems with multiscale phenomena, such as highly oscillatory solutions in nonlinear dispersive PDEs. Recently, tremendous progress have been advocated for a good mathematical understanding for some highly oscillatory nonlinear and dispersive PDEs, such as the Klein-Gordon equation in the nonrelativisitc limit regime, the nonlinear Schrodinger equation with wave operator, the Klein-Gordon-Zakharov system in the high-plasma-frequency and subsonic limit regime, the Dirac equation in the nonrelativisitc limit regime, etc.

Recently, we have proposed and analyzed several multiscale methods for highly oscillatory nonlinear dispersive PDEs. For the Gross-Pitaevskii/nonlinear Schrödinger with nonlocal dipole-dipole interaction and anisotropic confinement, we obtained new mathematical models in lower dimensions via multiscale analysis [1, 2, 11]. For the nonlinear Schrödinger equation with wave operator involving a small parameter, we obtained uniform error estimates for the finite difference time domain (FDTD) methods regarding the small parameter [3], and proposed an exponential wave integrator spectral (EWI-SP) method and established optimal and uniform error bounds for the problem [4]. For the Klein-Gordon equation in the nonrelativistic limit regime, we analyzed FDTD methods and EWI-SP method and obtained error bounds which depends explicitly on the small parameter [8, 9]; in addition, by adapting the fast-slow wave decomposition, we proposed and analyzed a uniformly accurate mutliscale time integrator spectral (MTI-SP) method [7]. Furthermore, we extended these multiscale methods and analysis to the mathematical and numerical study of the Dirac equation in the nonrelativistic limit regime [5, 6], the Klein-Gordon-Schrödinger equations in the nonrelativistic

limit regime [12], the Klein-Gordon-Zakharov system in the high-plasma-frequency limit regime [9].

References

[1] W. Bao, Mathematical models and numerical methods for Bose-Einstein condensation, Proceedings of the International Congress of Mathematicians (Seoul 20140), **IV** (2014), 971–996.

[2] W. Bao, N. Ben Abdallah and Y. Cai, Gross-Pitaevskii-Poisson equations for dipolar Bose-Einstein condensate with anisotropic confinement, SIAM J. Math. Anal., **44** (2012), 1713–1741.

[3] W. Bao and Y. Cai, Uniform error estimates of finite difference methods for the nonlinear Schrödinger equation with wave operator, SIAM J Numer. Anal., **50** (2012), 492–521.

[4] W. Bao and Y. Cai, Uniform and optimal error estimates of an exponential wave integrator sine pseudospectral method for the nonlinear Schrödinger equation with wave operator, SIAM J. Numer. Anal., **52** (2014), 1103–1127.

[5] W. Bao, Y. Cai, X. Jia and Q. Tang, Numerical methods and comparison for the Dirac equation in the nonrelativistic limit regime, arXiv: 1504.02881.

[6] W. Bao, Y. Cai, X. Jia and Q. Tang, A uniformly accurate (UA) multiscale time integrator pseudospectral method for the Dirac equation in the nonrelativistic limit regime, SIAM J. Numer. Anal., to appear (arXiv: 1507.04103).

[7] W. Bao, Y. Cai and X. Zhao, A uniformly accurate multiscale time integrator pseudospectral method for the Klein-Gordon equation in the nonrelativistic limit regime, SIAM J. Numer. Anal., **52** (2014), 2488–2511.

[8] W. Bao and X. Dong, Analysis and comparison of numerical methods for Klein-Gordon equation in nonrelativistic limit regime, Numer. Math., **120** (2012), 189–229.

[9] W. Bao, X. Dong and X. Zhao, An exponential wave integrator pseudospectral method for the Klein-Gordon-Zakharov system, SIAM J. Sci. Comput., **35** (2013), A2903–A2927.

[10] W. Bao, X. Dong and X. Zhao, Uniformly accurate multiscale time integrators for highly oscillatory second order differential equations, J. Math. Study, **47** (2014), 111–150.

[11] W. Bao, H. Jian, N. J. Mauser and Y. Zhang, Dimension reduction of the Schrödinger equation with Coulomb and anisotropic confining potentials, SIAM J. Appl. Math., **73** (2013), 2100–2123.

[12] W. Bao and X. Zhao, A uniformly accurate (UA) multiscale time integrator Fourier pseoduspectral method for the Klein-Gordon-Schrödinger equations in the nonrelativistic limit regime, arXiv: 1505.00083.

Exponential integrators for the Schrödinger equation with time-dependent Hamiltonian

Sergio Blanes

(joint work with Fernando Casas, Ander Murua, Mechthild Thalhammer)

We consider the numerical integration of the linear non-autonomous problem

$$i\frac{du}{dt} = H(t)\,u, \qquad t \in (t_0, T]\,, \qquad u(t_0) = u_0 \in \mathbb{C}^d, \tag{1}$$

associated to the Schrödinger equation with time-dependent Hamiltonian where $d \gg 1$ and $H(t)$ stands for the Hermitian Hamiltonian operator. Except for simple academic examples, it is not possible to find analytical solutions of (1) and so one has to call on numerical procedures. Among them, exponential time integration methods have shown to be particularly useful in approximating the

exact solution, since the exponential function captures some of the most relevant properties of the solution, such as oscillations or damping, whereas preserving qualitative properties of the system. One of the simplest exponential integrators is the so-called exponential midpoint rule,

$$u_{n+1} = \mathrm{e}^{-i\tau H(t_n+\tau/2)}\, u_n, \qquad t_0 \le t_n < t_{n+1} = t_n + \tau \le T \tag{2}$$

and $u_n \approx u(t_n)$. Exponential integrators must be implemented with efficient algorithms to approximate the action of the exponential on a vector instead of computing the exponential itself (see [10, 11] and references therein) i.e. procedures that involve only vector-matrix products to approximate the action of the exponential on a vector (e.g., Chebyshev or Krylov algorithms).

The solution provided by scheme (2) is at most of second order in the time step τ and we look for higher order approximations. There exist high order methods in the literature as for example the referred (t, t') method that considers the time as an independent variable and transforms the system into a linear autonomous problem, but of higher dimension and the computational cost is exceedingly high. One of the most efficient methods correspond to composition methods (products of exponentials) where the time is considered as a dependent variable. Alternatively, one can use a Magnus integrator where the time-dependency is averaged, but a naive application turns very expensive.

We consider new exponential methods based on composition of exponentials that use similar averages as in the Magnus integrators and the simplicity in the implementation of composition methods. We first consider the general case in which $H(t)$ is a complex matrix and next we consider the particular case in which $H(t)$ is a real symmetric matrix. We also assume that the computational cost to compute the product $H(t_1)u$ is similar to the cost of the product $(H(t_1)+H(t_2))u$.

Case I: $H(t)$ **is a complex matrix.** We consider the class of commutator-free methods defined by a composition of several exponentials of linear combinations of H at certain nodes. Specifically, a method of order r is formulated as

$$u_{n+1} = S_J^{[r]}(\tau)u_n = \mathrm{e}^{B_J} \cdots \mathrm{e}^{B_1} u_n, \qquad B_j = -i\tau \sum_{k=1}^{K} a_{jk}\, H(t_n + c_k\tau)\,, \tag{3}$$

$1 \le j \le J$, with real $c_k \in [0, 1]$. Different integrators of this type have been constructed and analyzed in [1, 7, 13]. In particular, in [1] optimized methods of orders 4, 6 and 8 have been proposed and tested. In the limit in which H is constant, the composition (3) simplifies to

$$S^{[r]}(\tau) = \mathrm{e}^{-ia_J H} \cdots \mathrm{e}^{-ia_1 H}\,, \qquad \text{with} \qquad a_j = \sum_{k=1}^{K} a_{jk}\,, \qquad 1 \le j \le J\,. \tag{4}$$

In this way, the algorithm is suitable to be used for parabolic problems or dissipative quantum systems as long as

$$\mathrm{Re}(a_j) > 0, \qquad \text{for all } j. \tag{5}$$

It has been noticed that all previous methods from the literature of order 6 and higher have real coefficients and involve at least one negative a_j coefficient and thus present a poor stability when applied to driven open quantum systems [2]. In [9] we propose new 5th- and 6th-order CF methods with complex coefficients that only require $J = 3$ and $J = 4$ respectively and such that condition (5) is satisfied. Since H is a complex matrix, the computational cost does not increases when considering complex coefficients. In addition, the schemes show higher accuracy and better stability properties when applied to non-reversible problems. We have also considered schemes that involve one commutator as follows (with similar computational cost as a 5-exponential CF method)

$$u_{n+1} = \mathrm{e}^{B_5}\, \mathrm{e}^{B_4}\, \mathrm{e}^{[B_{3,1},B_{3,2}]}\, \mathrm{e}^{B_2}\, \mathrm{e}^{B_1}\, u_n$$

where condition (5) is satisfied. The new methods have shown to be superior to previous optimised CF methods on several numerical examples in [9].

The coefficients a_{ij} proposed for all methods in [9] (as well as in [3] for the case in which H is real) are given for the nodes c_1, c_2, c_3 of the 6th-order Gauss-Legendre quadrature nodes, $K = 3$. If a different quadrature rule is used, say $\{\hat{b}_i, \hat{c}_i\}_{i=1}^{K}$, the same algorithms can be used by replacing in (8) the nodes $c_i,\ i = 1, 2, 3$ by $\hat{c}_i,\ i = 1, \ldots, K$, and the corresponding coefficients $\hat{a}_{i,j},\ i = 1, 2, 3,\ j = 1, \ldots, K$ are easily obtained from the coefficients $a_{i,j}$.

Case II: $H(t)$ is a real symmetric matrix. If we consider the split $u = q + ip$, the d-dimensional linear complex system (1) with $A = -iH$ and $H(t)$ real and symmetric can be written as the $2d$-dimensional real system

$$q' = H(t)p, \qquad p' = -H(t)q, \tag{6}$$

which can be considered as the classical Hamiltonian equations associated to the classical Hamiltonian

$$\mathcal{H}(q, p, t) = \frac{1}{2} p^T H(t) p + \frac{1}{2} q^T H(t) q = T(p, t) + V(q, t) \tag{7}$$

that is separable into two solvable parts [12]. We propose new splitting methods that take, on each internal stage, an appropriate average (over the whole time step) of the time-dependent part of $T(p, t)$ and $V(q, t)$, respectively. For one time step, from t_h to $t_{n+1} = t_n + h$, the method is given by the following algorithm

$$\begin{aligned} &\textbf{do}\ \ i = 1, m \\ &\quad q_i = q_{i-1} + h\,(a_{i,1}H_1 + a_{i,2}H_2 + a_{i,3}H_3)\, p_{i-1} \\ &\quad p_i = p_{i-1} - h\,(b_{i,1}H_1 + b_{i,2}H_2 + b_{i,3}H_3)\, q_i \\ &\textbf{enddo} \end{aligned} \tag{8}$$

where $q_0 = Re(u_n),\ p_0 = Im(u_n),\ H_i = H(t_n + c_i h),\ i = 1, 2, 3$ and $u_{n+1} = q_m + ip_m$. In [4] it is analysed how to build splitting symplectic methods in the autonomous case (H independent of t) and in [6] an algorithm with a sufficiently large number of methods is built such that for all accuracies and problems shows better performance than the Chebyshev method under the same conditions (the same input data). In [5] this technique is extended to the non-autonomous case and

in [3] the study is completed and a set of methods tailored for different accuracies is presented. Different 4th- and 6th-order schemes are considered with up to $m = 15$ so, the computational cost for one time step is similar to the computational cost of the action of one or two exponentials on a vector and have shown better performance for this problem than previous schemes.

References

[1] A. Alvermann and H. Fehske, *High-order commutator-free exponential time-propagation of driven quantum systems*, J. Comp. Phys. **230** (2011), 5930–5956.

[2] A. Alvermann, H. Fehske, and P. B. Littlewood, *Numerical time propagation of quantum systems in radiation fields*, New. J. Phys. **14**, 105008 (2012).

[3] S. Blanes, F. Casas, and A. Murua, *Propagators for the Schödinger equation with time-dependent Hamiltonian*. To be submitted.

[4] S. Blanes, F. Casas, and A. Murua, *Error analysis of splitting methods for the time dependent Schrodinger equation*, SIAM J. Sci. Comput. **33** (2011), 1525–1548.

[5] S. Blanes, F. Casas, and A. Murua, *Splitting methods in the numerical integration of non-autonomous dynamical systems*, RACSAM **106** (2012), 49–66.

[6] S. Blanes, F. Casas, and A. Murua, *An efficient algorithm based on splitting for the time integration of the Schrödinger equation*, J. Comput. Phys. **303** (2015), 396–412.

[7] S. Blanes and P. C. Moan, *Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems*. Appl. Numer. Math. **56** (2006), 1519–1537.

[8] S. Blanes, F. Casas, J. A. Oteo, and J. Ros, *The Magnus expansion and some of its applications*, Physics Reports **470** (2009), 151–238.

[9] S. Blanes, F. Casas, and M. Thalhammer, *High-order exponential integrators for non-autonomous linear evolution equations*. To be submitted.

[10] M. Hochbruck and A. Ostermann, *Exponential integrators*, Acta Num. **19** (2010), 209–286.

[11] C. Lubich, *From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis*, European Mathematical Society, (2008).

[12] J.M. Sanz-Serna and A. Portillo, *Classical numerical integrators for wave-packet dynamics*, J. Chem. Phys. **104** (1996), 2349–2355.

[13] M. Thalhammer, *A fourth-order commutator-free exponential integrator for nonautonomous differential equations*. SIAM J. Numer. Anal. **44** (2006), 851–864.

Two different approaches to highly oscillatory problems

Simone Buchholz

(joint work with L. Gauckler, V. Grimm, M. Hochbruck, T. Jahnke)

We consider the second order linear differential equation

$$q'' = -\Omega^2 q + Gq \tag{1}$$

for a matrix Ω being symmetric and positive definite with large norm $\|\Omega\| \gg 1$. The norm of the matrix G is assumed to be moderate, i.e., $\|G\| \ll \|\Omega\|$, and independent of Ω. In the literature, e.g., [1, 2, 4] and also [3], trigonometric integrators have been proposed and analyzed to solve such problems. The analysis shows that using appropriate filter functions, one can design methods which can be used with step sizes τ being much larger than $\|\Omega\|^{-1}$. However, using these integrators without filter functions leads to resonances in the global error as illustrated in

the following Figure 1. In the worst case, this means that we do not even have convergence for certain step sizes.

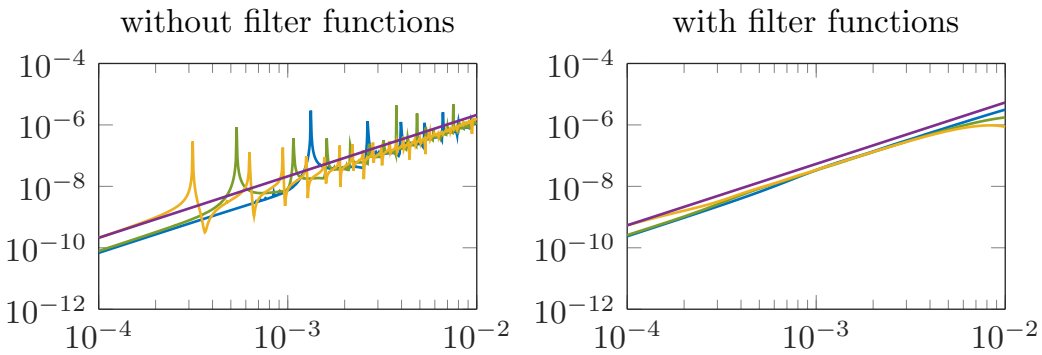


FIGURE 1. Global error of the trigonometric integrator over time step size. The different colors illustrate different matrices Ω (blue: $\|\Omega\| = 5000$, green: $\|\Omega\| = 12500$, yellow: $\|\Omega\| = 20000$, lilac: τ^2 reference line).

A different point of view is to interpret trigonometric integrators applied to the linear second order problem (1) as splitting methods applied to the first order equation

$$\widetilde{u}' = (A + \widetilde{B})\widetilde{u}, \tag{2}$$

where

$$A = \begin{bmatrix} 0 & I \\ -\Omega^2 & 0 \end{bmatrix}, \qquad \widetilde{B} = \begin{bmatrix} 0 & 0 \\ \widetilde{G} & 0 \end{bmatrix}, \qquad \widetilde{G} = \Psi G \Phi,$$

and $\Psi = \psi(\tau\Omega)$ and $\Phi = \phi(\tau\Omega)$. ψ and ϕ are suitably chosen filter functions. The symmetric Strang splitting $e^{\tau\tilde{B}/2}e^{\tau A}e^{\tau\tilde{B}/2}$ applied to (2) results in a scheme being equivalent to a trigonometric integrator mentioned above.

Standard Lie and Strang splitting methods were analyzed before in [5] in a different framework without filter functions. However, the analysis does not carry over to highly oscillatory problems. Our project aims at generalizing the splitting analysis such that it applies to problems of that kind. In order to do so, a first step is to prove that the distance between the solution of the filtered equation (2) and the solution of (1) is in $\mathcal{O}(\tau^2)$ with a constant being independent of $\|\Omega\|$. We then use a new representation of the local error, for which the main part can be handled using Lady Windermere's fan, and we show that the remaining terms can be bounded with the help of a modified version of Lady Windermere's fan. In the end, we show convergence of order two independent of $\|\Omega\|$ for the splitting method applied to the linear problem (1). Interestingly, the new proof yields different conditions on the filter functions than in [2].

References

[1] B. García-Archilla and J. M. Sanz-Serna and R. D. Skeel, *Long-Time-Step Methods for Oscillatory Differential Equations*, SIAM J. Sci. Comput. **20** (1998), 930–963.

[2] V. Grimm and M. Hochbruck, *Error analysis of exponential integrators for oscillatory second-order differential equations*, J. Phys. A **39** (2006), 5495–5507.

[3] E. Hairer, Ch. Lubich and G. Wanner, *Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics **31** (2006).

[4] M. Hochbruck and C. Lubich, *A Gautschi-type method for oscillatory second-order differential equations*, *Numer. Math.*, **83** (1999), 403–426.

[5] T. Jahnke and Ch. Lubich, *Error bounds for exponential operator splittings*, BIT **40** (2000), 735–744.

Avoiding order reduction when integrating nonlinear Schrödinger equation with Strang method

Begoña Cano

(joint work with Nuria Reguera)

In the talk, a technique is suggested in order to integrate nonlinear Schrödinger equation with non-homogeneous Dirichlet boundary conditions in such a way that no order reduction is shown [2]. The technique consists of applying firstly the discretization in time of the problem and then the discretization in space. In such a way, suitable boundary functions must be suggested for the linear partial differential equation which arises when applying Strang method. The key is to consider an asymptotic Taylor expansion of first order for the boundary of the function which is to be approximated when solving that linear part. We have justified that this boundary can be calculated in terms of the data of the original problem. Moreover, we have seen that an asymptotic Taylor expansion of second order cannot be calculated directly in terms of data.

Theoretical results have been given which show that local order 2 is obtained in time under suitable assumptions of regularity. After full discrezation in space, some results have also been shown for that local error. Finally, using a summation-by-parts argument and some more regularity assumptions which allow to use bounds already established in [1] for nonlinear Schrödinger equation, a result on the global error is given. This one proves that no order reduction is observed with the suggested technique.

As this technique does not conserve the symmetry of the method, a slight modification of it has also been suggested in order to conserve the symmetry while order reduction is still avoided. We have seen that the symmetry is also conserved under any diagonallizable discretization of the Laplacian.

Finally, we have posed the following problem for possible future research: From a qualitative point of view, it is good to conserve the symmetry of the method because, in such a way, the reversibility of the equation is also conserved. However, from a quantitative point of view, the advantages of symmetry are not so clear

as when integrating Hamiltonian ordinary differential equations or partial differential equations with periodic or homogeneous boundary conditions. In the latter case, the good approximation of certain invariants of the problem with symmetric methods leads to advantageous results on error growth with time. However, when the boundary conditions are not homogeneous, the continuous problem lose those invariants and it is not so easy to deduce advantageous quantitative results.

References

[1] G. Dujardin, *Exponential Runge-Kutta methods for the Schrödinger equation*, Appl. Numer. Math. **59** (2009), 1839–1857.

[2] B. Cano and N. Reguera, *Avoiding order reduction when integrating nonlinear Schrödinger equation with Strang method*, submitted for publication.

Splitting methods (with processing) for near-integrable problems

Fernando Casas

(joint work with S. Blanes, A. Farrés, J. Laskar, A. Murua, J. Makazaga)

In the previous "Geometric Numerical Integration" workshop held in Oberwolfach in 2011, Jacques Laskar proposed to construct more accurate and efficient numerical integrators for the integration of the Solar System over long time spans. The specific goals were to achieve round off error (in extended arithmetic) with the new schemes with the minimum computational cost. In addition, the methods should be symplectic and specially adapted to the particular structure of the Hamiltonian problem. This was the the starting point for a collaboration that has materialized (until now) in the papers [2, 3].

A very simplified model for the Solar System consists in considering it as a non-relativistic gravitational N-body problem. In this setting one is concerned with the motion of $n+1$ particles (the Sun, with mass m_0, and N planets with masses m_i, $i = 1, \ldots, N$) only affected by their mutual gravitational interaction. The system is then described by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=0}^{N} \frac{\|\mathbf{p}_i\|^2}{m_i} - G \sum_{0\le i<j\le n} \frac{m_i m_j}{\|\mathbf{q}_i - \mathbf{q}_j\|} \tag{1}$$

where $\mathbf{q}_i$ and $\mathbf{p}_i = m_i\,\dot{\mathbf{q}}_i$ are, respectively, the positions and momenta of the $N+1$ bodies in a barycentric reference frame. Moreover, the planets evolve around the central mass following almost Keplerian orbits, so that, by an appropriate change of coordinates one can rewrite (1) as

$$H = K + V_I, \qquad \text{where} \qquad |V_I| \ll |K|.$$

Here K stands for a sum of independent unperturbed Kepler (2-body) problems, whereas V_I are perturbations depending on the interactions of the planets and their structure is dictated by the specific coordinate system chosen (either Jacobi

or Heliocentric coordinate systems). In any case, this constitutes a particular example of a *near-integrable Hamiltonian system*:

$$H(q,p;\varepsilon) = H^{[a]}(q,p) + \varepsilon H^{[b]}(q,p), \tag{2}$$

where $\varepsilon \ll 1$ and $H^{[a]}$ is exactly integrable. It makes sense then to take into account this special structure when designing integration methods to approximate its dynamics. *Splitting methods* are particularly well suited for dealing with this class of systems: the idea is to construct the integrator as a composition of the flows corresponding to $H^{[a]}$ and $H^{[b]}$ with appropriately chosen weights. Specifically, if $\varphi_\tau^{[a]}$ and $\varphi_\tau^{[b]}$ denote the flows corresponding to $H^{[a]}$ and $H^{[b]}$, respectively, then we seek integrators of the form

$$\psi_\tau = \varphi^{[a]}_{a_{s+1}\tau} \circ \varphi^{[b]}_{b_s\tau} \circ \varphi^{[a]}_{a_s\tau} \circ \cdots \circ \varphi^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau} \tag{3}$$

where, in particular,

$$\sum_{i=1}^{s+1} a_i = 1, \qquad \sum_{i=1}^{s} b_i = 1. \tag{4}$$

Typically, one also requires time-symmetry, so that the composition (3) is left-right palindromic: $a_{s+2-i} = a_i$, $b_{s+1-i} = b_i$. Then, if the consistency condition (4) is satisfied, the method is of order two in the step size τ.

In the analysis, one has two parameters: τ (the step size) and ε (the size of the perturbation), and one is interested in how the local error $\psi_\tau - \varphi_\tau$ decreases as $\varepsilon \to 0$ (here φ_τ represents the exact flow of the system). Thus, for any consistent symmetric method one has $\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\varepsilon\,\tau^3)$, where $x = (q,p)$. By following McLachlan's notation [4], method (3) is of generalized order $(r_1, r_2, \ldots, r_m)$ if

$$\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\varepsilon\tau^{r_1+1} + \varepsilon^2\tau^{r_2+1} + \cdots + \varepsilon^m\tau^{r_m+1}),$$

with $r_1 \geq r_2 \geq \cdots \geq r_m$. Thus, in particular, one has a method of (generalized) order

- $(8,2)$: if $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^3 + \cdots)$
- $(8,4)$: if $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^5 + \varepsilon^3\tau^5 + \cdots)$
- $(8,6,4)$: if $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^7 + \varepsilon^3\tau^5 + \cdots)$
- $(10,6,4)$: if $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^{11} + \varepsilon^2\tau^7 + \varepsilon^3\tau^5 + \cdots)$

In [2], a systematic study is carried out to get the independent generalized order conditions of this class of methods. This is done by considering a particular subset of multi-indices called *Lyndon multi-indices*. Essentially, one associates *one* order condition to *each* Lyndon multi-index, and the analytic expression of each order condition is also obtained. By solving these order conditions, methods of order $(8,6,4)$ and $(10,6,4)$ are obtained involving seven and eight stages, respectively. The same strategy can also be applied to get methods valid in Heliocentric coordinates, where V_I depends not only on coordinates, but also on their conjugate momenta.

Although the schemes thus constructed show an excellent behavior on long time integrations of the Solar System, one might ask if it is possible to construct even

more efficient integrators for this problem. A possibility consists in using the *processing technique*. The idea is consider methods of the form

$$\hat{\psi}_\tau = \pi_\tau^{-1} \circ \psi_\tau \circ \pi_\tau,$$

so that we *enhance*, *correct* or *process* the numerical scheme ψ_τ (the *kernel*) with a (near-identity) map π_τ (the *processor* or *corrector*), so that the resulting method $\hat{\psi}_\tau$ is 'better' than ψ_τ. After n steps one has

$$\hat{\psi}_\tau^n = \pi_\tau^{-1} \circ \psi_\tau^n \circ \pi_\tau.$$

When considering processed methods, it happens that many order conditions can be satisfied by π_τ, and thus ψ_τ must verify a much reduced set of conditions. Since the bulk of the computation corresponds to the kernel, one expects to reduce the computational cost by constructing kernels with less stages than standard schemes. This strategy is particularly appealing for very long time integrations when intermediate outputs are not required.

In a typical procedure, both the kernel and (an approximation to) the processor are both constructed as compositions of the form (3). There are already several processed splitting methods that involve less stages for near-integrable problems, showing an excellent behavior for simple problems [1]. In the integration of the Solar System, however, they present some drawbacks (instabilities, etc.) that can be traced back to the fact that, in the corresponding composition (3) for the processor the sum of the coefficients has to be zero. This, in turn, can produce large coefficients and error terms.

One possibility to avoid these drawbacks is the use of a *starter*. Basically, the idea is to form a new processor as a composition of the old processor with the kernel. In that way, the new scheme is also symmetric and the coefficients of this starter have to add up to 1, exactly as in the kernel. With this procedure one is able to construct methods of the form $(s, 6, 4)$ with kernels involving a minimum of three stages (instead of seven). The same strategy as in the standard case can be applied to construct schemes for Heliocentric coordinates involving one additional stages. This constitutes an ongoing research project.

References

[1] S. Blanes, F. Casas, J. Ros, *Processing symplectic methods for near-integrable Hamiltonian systems*, Celest. Mech. Dyn. Astron. **77** (2000), 17–35.

[2] S. Blanes, F. Casas, A. Farrés, J. Laskar, J. Makazaga and A. Murua, *New families of symplectic splitting methods for numerical integration in dynamical astronomy*, Appl. Numer. Math. **68** (2013), 58–72.

[3] A. Farrés, J. Laskar, S. Blanes, F. Casas, J. Makazaga and A. Murua, *High precision symplectic integrators for the Solar System*, Celest. Mech. Dyn. Astr. **116** (2013), 141–174.

[4] R.I. McLachlan, *Composition methods in the presence of small denominators*, BIT **35** (1995), 258–268.

Shape Analysis on Lie Groups with Applications in Computer Animation

Elena Celledoni, Markus Eslitzbichler, Alexander Schmeding

Shape analysis methods have in the past few years become very popular, both for theoretical exploration as well as from an application point of view. Originally developed for planar curves, these methods have been expanded to higher dimensional curves, surfaces, activities, character motions and many other objects. In this talk, we present a framework for shape analysis of curves in Lie groups for problems of computer animations. In particular, we use these methods to find cyclic approximations of non-cyclic character animations and interpolate between existing animations to generate new ones, see Figure 1 for an example.

Our starting point is the generalisation of the Square Root Velocity Transform (SRVT), [3], to curves on Lie groups.

We discuss the Riemannian geometry of the SRV transform. Let G be a (possibly infinite-dimensional) Lie group modelled on a Hilbert space and $\mathfrak{g}$ be its corresponding Lie algebra. We prove that the pull back of the L^2 inner product on the Lie algebra of curves on $\mathfrak{g}$ is a Sobolev-type metric on the infinite dimensional Lie group of curves on G, the *elastic metric*, see [1] for details. Since this

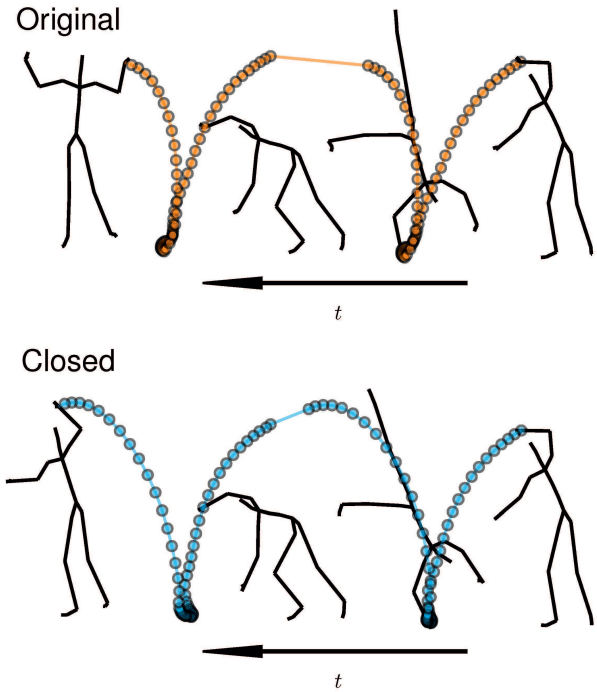


Figure 1. Application of the closing gradient flow algorithm to a cartwheel animation. Note the large difference between start and end poses, on the right and the left respectively. The motion is repeated once and suffers from a strong jerk when it repeats, especially in the left hand. In the second row, the curve closing method has been used to alleviate this discontinuity.

metric is convenient to work with, we use it in our applications. In fact, through the SRVT we transform curves on G to curves on $\mathfrak{g}$ to manipulate them (interpolate two curves, compute distances between curves using the L^2 metric) and when appropriate map the results back to the Lie group via the inverse SRVT.

We prove that the subset of closed curves on G starting at the identity is mapped through the SRVT to a split submanifold of the infinite dimensional Lie algebra of curves on $\mathfrak{g}$. We then construct a gradient flow which, given a non-closed curve as initial condition, it converges towards a nearby closed curve, see Figure 1 for results. Further information and results can be found in [1].

References

[1] E. Celledoni, M. Eslitzbichler, A. Schmeding, *Shape Analysis on Lie Groups with Applications in Computer Animation*, (2015), arXiv:1506.00783v3 [math.DG].

[2] M. Eslitzbichler, *Modelling character motions on infinite-dimensional manifolds*, The Visual Computer, **31** (2015): 1179-1190.

[3] A. Srivastava, E. Klassen, S. Joshi, and I. Jermyn, *Shape analysis of elastic curves in euclidean spaces*. Pattern Analysis and Machine Intelligence, IEEE Transactions on **33** (2011):1415–1428.

Approximation of Invariant Measure for Damped Stochastic Nonlinear Schrödinger Equation via an Ergodic Numerical Scheme

Chuchu Chen

(joint work with Jialin Hong, Xu Wang)

In this paper, we consider an initial-boundary problem of an ergodic one-dimensional damped stochastic NLSE

$$\begin{cases} du = \big(\mathbf{i}\Delta u - \alpha u + \mathbf{i}\lambda|u|^2 u\big)dt + Q^{\frac{1}{2}}dW \\ u(t,0) = u(t,1) = 0,\ t \geq 0 \\ u(0,x) = u_0(x),\ x \in [0,1], \end{cases} \tag{1}$$

where $\alpha > 0$, $\lambda = \pm 1$ and the solution u is a complex valued ($\mathbb{C}$-valued) random field on a probability space $(\Omega, \mathcal{F}, P)$. The noise term involves a cylindrical Wiener process W and a symmetric, positive, trace class operator Q such that the noise is colored in space and white in time. The operator Q is supposed to commute with Laplacian operator Δ, and the noise is in the form

$$Q^{\frac{1}{2}}dW = \sum_{m=1}^{\infty} \sqrt{\eta_m} e_m(x) d\beta_m(t), \quad \eta_m \in \mathbb{R}^+ \ \text{ and } \ \eta := \sum_{m=1}^{\infty} \eta_m < \infty,$$

where $\{\beta_m(t)\}_{m\geq 1}$, associated to a filtration $\{\mathcal{F}_t\}_{t\geq 0}$, are independent and identically distributed $\mathbb{C}$-valued Wiener processes and $\{e_m\}_{m\geq 1}$ is the orthonormal basis of $L^2(0,1)$ with homogenous Dirichlet boundary condition. The ergodicity for problem (1) has been studied in [7] by a coupling method, where the damped term ($\alpha > 0$) may be caused by the Gordon-Haus effect and is necessary for

both linear and nonlinear Schrödinger equation to be ergodic. [7] showed that the solution u of (1) possesses a unique invariant measure μ.

Our work mainly focuses on the construction of a fully discrete and uniquely ergodic numerical scheme (i.e., whose numerical solution possesses a unique invariant measure). Moreover, the estimation of error between the original invariant measure and the numerical one is also considered based on the weak error of solutions.

As the lack of compactness of the bounded and closed sets in infinite-dimensional Hilbert spaces, the Lyapunov function may be hardly chosen for SPDEs. We apply spectral Galerkin method in spatial direction to obtain a finite-dimensional SDE

$$du_N = \Big(\mathbf{i}\Delta u_N - \alpha u_N + \mathbf{i}\lambda\pi_N\left(|u_N|^2 u_N\right)\Big)dt + \pi_N Q^{\frac{1}{2}} dW. \tag{2}$$

We find a Lyapunov function by proving the uniform boundedness of u_N in L^2-norm. It ensures the existence of the invariant measure of (2). We show that the solution $u_N(t)$ is a strong Feller and irreducible process via the non-degeneracy of the noise term in (2). Hence, $u_N(t)$ possesses a unique invariant measure μ_N, which implies the ergodicity of $u_N(t)$.

Theorem 3. *Let $u_N(t,x)$ be the solution of equation (2), then u_N possesses a unique invariant measure, denoted by μ_N. Thus, u_N is ergodic.*

We would like to emphasize that the noise in the original equation do not need to be non-degenerate. This method is available when the covariance operator Q has enough nonzero eigenvalues. The error between the invariant measures μ_N and μ is transferred into the weak error of the solutions, which is required to be independent of time t. Different from conservative equations, the damped term in (1) and (2) contributes to an exponential estimate on the difference between semigroup operators $S(t)$ and $S(t)\pi_N$, where $S(t)$ is generated by the linear operator $\mathbf{i}\Delta - \alpha$. Therefore, we achieve the time-independent weak error of solutions directly, avoiding proving the exponential decay of the solution of Kolmogorov equation.

Theorem 4. *Assume that $u_0 \in \dot{H}^1$ and $\|Q^{\frac{1}{2}}\|_{\mathcal{HS}(L^2,\dot{H}^1)} < \infty$. For any $\phi \in C_b^2(L^2)$, there exists a constant $C = C(u_0,\phi,Q)$ independent of T, such that for any $T > 0$,*

$$\left|E\Big[\phi\big(u_N(T)\big)\Big] - E\Big[\phi\big(u(T)\big)\Big]\right| \le CN^{-1}.$$

This theorem implies the convergence order between invariant measures μ and μ_N:

$$\left|\int_{L^2}\phi(y)d\mu(y) - \int_{V_N}\phi(y)d\mu_N(y)\right| \le CN^{-1}. \tag{3}$$

Based on a combination of splitting-up method and finite difference method in temporal direction of (2), we propose a fully discrete scheme

$$u_N^k - e^{-\alpha\tau}u_N^{k-1} = \left(\mathbf{i}\Delta u_N^k + \mathbf{i}\lambda\pi_N\left(\frac{|u_N^k|^2 + |e^{-\alpha\tau}u_N^{k-1}|^2}{2}u_N^k\right)\right)\tau + \pi_N Q^{\frac{1}{2}}\delta W_k. \tag{4}$$

This scheme is implicit as is required for local Lipschitz SDE to be ergodic, and is proved to be solvable by denoting the discrete semigroup operator $S_\tau := (I - \mathbf{i}\tau\Delta)^{-1}e^{-\alpha\tau}$. In order to analyze the effect of the time discretization, we give the proof of its ergodicity. The fully discrete scheme (4) is specially constructed to make sure the uniform boundedness of u_N^k in L^2-norm. Together with the Brouwer fixed point theorem and properties of homogeneous Markov chains, we prove that u_N^k is uniquely ergodic.

Theorem 5. *For all τ sufficiently small, the solution $(u_N^k)_{k\in\mathbb{N}}$ of scheme (4) has a unique invariant measure μ_N^τ. Thus, it is ergodic.*

Since the weak error of the solutions is required to be independent of time and the coefficients are nonlinear for cases $\lambda = \pm 1$, existing theories establishing the weak error of numerical solutions (see e.g. [8]) do not apply. We prove the exponential decay of the difference between operators $S(t)$ and S_τ, which is a crucial condition for the solutions to have a time-independent weak error. Moreover, when considering the weak error of the solutions in temporal direction, an exponential estimation of the difference between the unbounded and nonlinear terms in spatial semi-discretization and full discretization is also required. Thus, some technical estimates are given to obtain the exponential decay of the difference between these nonlinear terms. We obtain the following result.

Theorem 6. *Assume that $u_0 \in \dot{H}^2$, $u_N^0 = u_N(0) = \pi_N u_0$ and $\|Q^{\frac{1}{2}}\|^2_{\mathcal{HS}(L^2,\dot{H}^2)} < \infty$. For the cases $\lambda = -1$, the weak errors are independent of time and of order $\frac{1}{2}$. That is, for any $\phi \in C_b^2(L^2)$, there exists a constant $C = C(u_0, \phi)$ independent of N, T and M, such that for any $T = M\tau$,*

$$\left|E[\phi(u_N(T))] - E[\phi(u_N^M)]\right| \leq C\tau^{\frac{1}{2}}.$$

Based on the time-independency of the weak error of the solutions, we show that the error of invariant measure has at least the same order as the weak error of the solutions, i.e.,

$$\left|\int_{V_N} \phi(y)d\mu_N(y) - \int_{V_N} \phi(y)d\mu_N^\tau(y)\right| \leq C\tau^{\frac{1}{2}} \tag{5}$$

References

[1] A. Abdulle, G. Vilmart, and K. C. Zygalakis. High order numerical approximation of the invariant measure of ergodic SDEs. *SIAM J. Numer. Anal.*, 52(4):1600–1622, 2014.

[2] G. D. Akrivis, V. A. Dougalis, and O. A. Karakashian. On fully discrete Galerkin methods of second-order temporal accuracy for the nonlinear Schrödinger equation. *Numer. Math.*, 59:31–53, 1991.

[3] A. D. Bouard and A. Debussche. A semi-discrete scheme for the stochastic nonlinear Schrödinger equation. *Numer. Math.*, 96:733–770, 2004.

[4] C.-E. Bréhier. Approximation of the invariant measure with an Euler scheme for stochastic PDEs driven by space-time white noise. *Potential Anal*, 40:1–40, 2014.

[5] C.-E. Bréhier and M.Kopec. Approximation of the invariant law of SPDEs: error analysis using a poisson equation for full-discretization scheme. *arXiv: 1311.7030*.

[6] C. Chen, J. Hong, and A. Prohl. Convergence of a θ-scheme to solve the stochastic nonlinear Schrödinger equation with Stratonovich noise. *Stoch. Partial Differ. Equ. Anal. Comput.*, DOI:10.1007/s40072-015-0062-x.
[7] A. Debussche and C. Odasso. Ergodicity for a weakly damped stochastic non-linear Schrödinger equation. *J. Evol. Equ.*, 5:317–356, 2005.
[8] A. Debussche and J. Printems. Weak order for the discretization of the stochastic heat equation. *Math. Comp.*, 78:845–863, 2009.
[9] L. Hörmander. Hypoelliptic second order differential equations. *Acta Math.*, 119:147–171, 1967.
[10] J. Mattingly, A. Stuart, and D. Higham. Ergodicity for SDEs and approximations: locally Lipschitz vector fields and degenerate noise. *Stochastic Process. Appl.*, 101:185–232, 2002.
[11] G. D. Prato. An introduction to infinite-dimensional analysis. *Springer Berlin Heidelberg*, 2006.
[12] D. Talay. Second order discretization schemes of stochastic differential systems for the computation of the invariant law. *Rapports de Recherche, Institut National de Recherche en Informatique et en Automatique*, 1987.

Numerical discretisations of stochastic wave equations

David Cohen
(joint work with Rikard Anton, Stig Larsson, LLuís Quer-Sardanyons, Magdalena Sigg, Xiaojie Wang)

We begin the presentation with a very concise crash course on stochastic partial differential equations (SPDEs), where we introduce, amongst other things, the main two approaches for a proper definition of SPDEs: the functional setting approach (SPDEs are seen as stochastic differential equations in a Hilbert space) and the random-field approach (the noise appearing in the problem is a multi-parameter version of a Brownian motion).

We next introduce a semilinear stochastic wave equation driven by a multiplicative noise

$$\begin{aligned} \mathrm{d}\dot{u} - \Delta u \,\mathrm{d}t = f(u)\,\mathrm{d}t + g(u)\,\mathrm{d}W \quad &\text{in } \mathcal{D}\times(0,T), \\ u = 0 \quad &\text{in } \partial\mathcal{D}\times(0,T), \\ u(\cdot,0) = u_0,\ \dot{u}(\cdot,0) = v_0 \quad &\text{in } \mathcal{D}, \end{aligned} \tag{1}$$

where $u = u(x,t,\omega)$, with $t \in [0,T]$, $\mathcal{D} \subset \mathbb{R}^d$, $d = 1,2,3$, is a bounded convex domain with polygonal boundary $\partial\mathcal{D}$. The stochastic process $\{W(t)\}_{t\geq 0}$ is an $L_2(\mathcal{D})$-valued (possibly cylindrical) Q-Wiener process on a probability space $(\Omega,\mathcal{F},\mathbb{P})$. The maps f and g, as well as the initial values u_0 and v_0 are given.

Various applications of the above stochastic wave equation and related equations can be found, for example, in [5].

An analytic solution to the stochastic wave equation (1) is, in general, not available: we thus must resort to numerical simulations in order to understand such problems!

Inspired by the construction of trigonometric schemes for highly oscillatory deterministic problems and deterministic wave equations, see [2, Chapter XIII], [1, 4] and references therein, we propose a new numerical method for the time

discretisation of (1). This explicit time integrator allows for mean-square error bounds independent of the space discretisation and thus do not suffer from a step size restriction as in the often used Störmer-Verlet leapfrog scheme. Furthermore, our stochastic trigonometric integrator satisfies an almost trace formula (i. e., a linear drift of the expected value of the energy of the problem, see below).

We now shortly describe our results.

(1) In a first step, we consider the numerical discretisation of the linear stochastic wave equation with additive noise [7]

$$\mathrm{d}\dot{u} - \Delta u \,\mathrm{d}t = \mathrm{d}W.$$

We discretise this problem first in space, using a standard linear finite element method [6], and then in time using our stochastic trigonometric method. We prove mean-square order of convergence for the full discretisation. Observe that the speed of convergence depends on the regularity of the noise. Finally, we show that the expected value of the energy of the numerical solution grows linearly with time as does the exact solution to the above problem. This is one of the first long-time result for the numerical solution of SPDEs.

(2) We next generalise the above results to the full discretisation of the semilinear stochastic wave equation driven by multiplicative noise [9]

$$\mathrm{d}\dot{u} - \Delta u \,\mathrm{d}t = f(u)\,\mathrm{d}t + g(u)\,\mathrm{d}W.$$

(3) Finally, we prove mean-square error estimates in $L^p(\Omega)$, for any $p \geq 1$, of the full discretisation of the $1d$ semilinear wave equation [8]

$$\frac{\partial^2 u}{\partial t^2}(t,x) = \frac{\partial^2 u}{\partial x^2}(t,x) + f(u(t,x)) + \sigma(u(t,x))\frac{\partial^2 W}{\partial x \partial t}(t,x).$$

A standard finite difference approximation is used in space [3] and our stochastic trigonometric method is used in time. Observe, that the above problem is based on the second definition of an SPDE, i. e. the random-field approach.

Finally, we present numerical experiments in order to support the above theoretical results. Figure 1 displays one realisation of the solution given by one of the above numerical discretisation of a semilinear stochastic wave equation.

References

[1] V. Grimm, *On the use of the Gautschi-type exponential integrator for wave equations*, Numerical Mathematics and Advanced Applications, 2006 (**110(2)**), 557–563.

[2] E. Hairer, C. Lubich and G. Wanner, *Geometric Numerical Integration*, Springer Series in Computational Mathematics, 2006 (**31**).

[3] L. Quer-Sardanyons and M. Sanz-Solé, *Space semi-discretisations for a stochastic wave equation*, Potential Anal, 2006 (**24(4)**), 303–332.

[4] D. Cohen, E. Hairer and C. Lubich, *Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations*, Numer. Math., 2008 (**110(2)**), 113–143.

[5] R.C. Dalang, *The stochastic wave equation*, A minicourse on stochastic partial differential equations, 2009 (**1962**), 39–71.

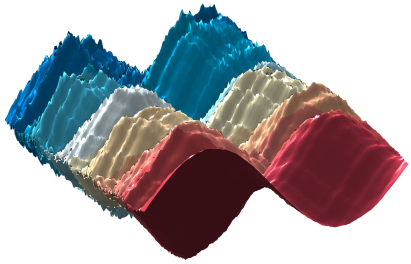


FIGURE 1. Space-time evolution of one realisation of the numerical solution of a stochastic wave equation.

[6] M. Kovács, S. Larsson and F. Saedpanah, *Finite element approximation of the linear stochastic wave equation with additive noise*, SIAM J. Numer. Anal., 2010 (**48(2)**), 408–427.
[7] D. Cohen, S. Larsson and M. Sigg, *A trigonometric method for the linear stochastic wave equation*, SIAM J. Numer. Anal., 2013 (**51(1)**), 204–222.
[8] D. Cohen and L. Quer-Sardanyons, *A fully discrete approximation of the one-dimensional stochastic wave equation*, IMA J NUMER ANAL, 2016 (**36(1)**), 400–420.
[9] R. Anton, D. Cohen, S. Larsson and X. Wang, *Full discretization of semilinear stochastic wave equations driven by multiplicative noise*, accepted for publication in SIAM J. Numer. Anal., 04.02.2016.

Structure preserving numerical methods for the Vlasov equation

LUKAS EINKEMMER

In astro- and plasma physics the behavior of a collisionless plasma is modeled by the Vlasov equation

$$\partial_t f(t,x,v) + v \cdot \nabla_x f(t,x,v) + F \cdot \nabla_v f(t,x,v) = 0.$$

The force F is given by the Lorentz force law and the electric E and magnetic B fields are self-consistently determined from the particle-density f. Thus, in the most general setting we have to solve the Vlasov equation coupled with Maxwell's equations (the so-called Vlasov–Maxwell system). In many applications, however, it is sufficient to consider the electrostatic case. That is, the Vlasov equation is only coupled to a Poisson problem

$$\Delta\phi(t,x) = \int f(t,x,v)\,\mathrm{d}v - 1.$$

The potential ϕ is then used to determine the electric field by using the relation $E = \nabla_x \phi$. This is the model that we will consider in the present report.

Solving the Vlasov–Poisson system numerically is a challenging task as

- the problem is posed in an up to six-dimensional phase space;
- the system is nonlinear;
- the characteristic time scale in many applications is on the order of picoseconds (the plasma frequency) while interesting physical phenomena can happen on much larger timescales.

Here we will focus mostly on the last point. The discrepancy in timescales implies that in order to obtain meaningful results we have to perform a large number of time steps. Therefore, it is not possible to use the numerical scheme in the asymptotic regime. Nevertheless, numerical simulations can still prove useful if they are able to capture the plasma dynamics qualitatively. Thus, in the present context the goal is to construct a numerical integrator that can capture as much of the structure of the analytic solution as possible.

In the case of the Vlasov equation it is well known that an infinite number of conserved quantities exist (for example, all L^p norms are conserved by the analytic solution). Certainly, it is unrealistic to expect that all those invariants are conserved by a numerical approximation. Thus, we focus on the physically important invariants: mass, momentum, energy, and positivity. In addition, we will include entropy and the L^2 norm as a measure of how much dissipation is introduced by the numerical scheme.

Since an explicit time stepping scheme needs to obey the CFL constraint given by $v\tau < h$ (τ is the time step size and h is the grid spacing), the splitting approach introduced by Strang & Knorr [1] has been almost universally employed. This approach conserves mass, momentum, all L^p norms, and entropy. Furthermore, an extension to the full Vlasov–Maxwell system has been proposed recently (see [2]).

In addition to the good conservation properties, the splitting approach has another decisive advantage; namely, it reduces the problem of solving the up to six-dimensional Vlasov equation to a sequence of one-dimensional advection equations of the form

$$\partial_t u(t, \xi, \eta) = a(\eta)\partial_\xi u(t, \xi, \eta).$$

For this problem it is straightforward to obtain the characteristics analytically and thus semi-Lagrangian methods have become the standard approach. Note, however, that since the feet of the characteristics not necessarily coincide with the grid used, an interpolation procedure has to be employed. Cubic spline interpolation is the most commonly used approach.

More recently, the semi-Lagrangian discontinuous Galerkin (sLdG) scheme has been introduced [7, 8, 3]. The main advantage of this approach, compared to spline interpolation (or Fourier based methods), is that the resulting numerical scheme only needs data from at most two adjacent cells in order to compute the advection. This is a particularly important feature if the numerical scheme is implemented on a parallel computer system. A convergence analysis of this method has been conduced in [6, 5].

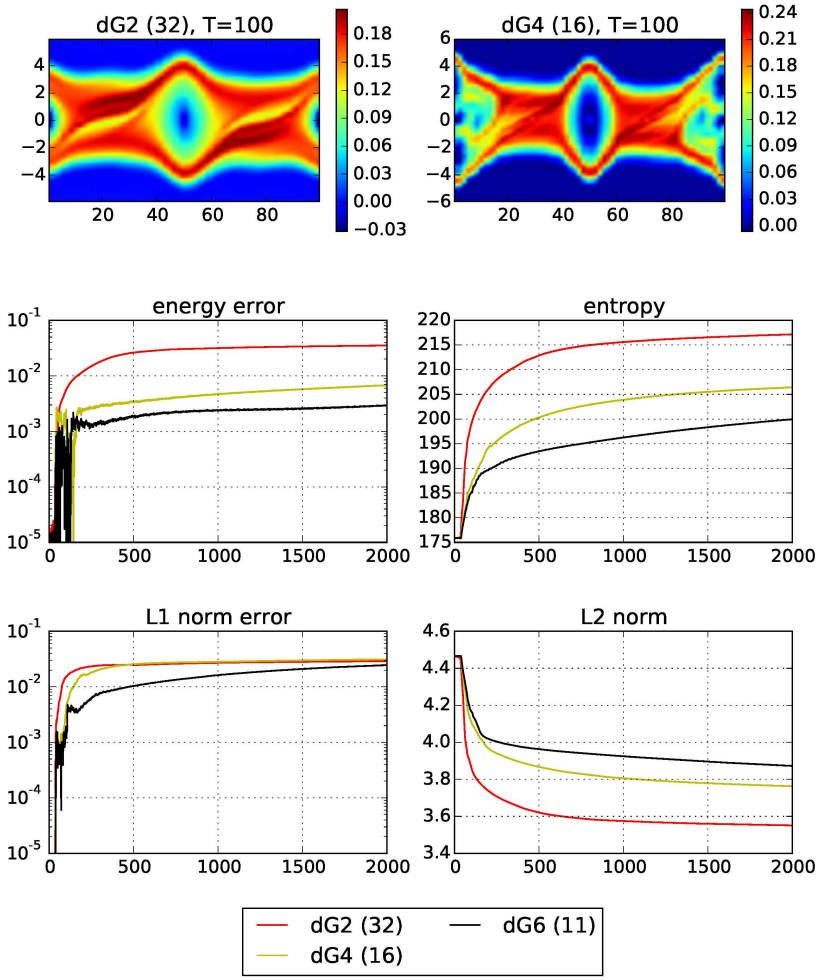


FIGURE 1. This figure shows f for $t = 100$ and the time evolution in the error of the conserved quantities energy, entropy, L^1 norm (positivity), and L^2 norm. For all numerical schemes 64 degrees of freedom are employed per space dimension. The order of the discontinuous Galerkin (dG) method is indicated and the number of cells are given in parenthesis.

Some interesting properties of the semi-Lagrangian discontinuous Galerkin approach (sLdG) should be noted.

- The error in energy includes additional error terms for the methods of order one and two. Thus, it is prudent to at least use a third order approximation in space.
- In all our simulations positivity preservation is less of an issue for the sLdG scheme compared to cubic spline interpolation. In any case, due to the local nature of the numerical method positivity limiters can be easily added (at the cost of some additional diffusion; see [8, 7])
- Numerical simulations indicate that while cubic spline interpolation violates the second law of thermodynamics (i.e. it decreases entropy), the

semi-Lagrangian discontinuous Galerkin scheme does not suffer from this deficiency. However, a proof of this statement is still missing (see [4]).
- Both for the conserved quantities and for the qualitative features of the solution there is a significant advantage in using higher order approximations (see [4]). This, however, is unexpected based on the regularity of the solution.

To illustrate some of these properties the results for the two-stream instability are shown in Figure 1.

References

[1] C. Cheng and G. Knorr. The integration of the Vlasov equation in configuration space. *J. Comput. Phys.*, 22(3):330–351, 1976.
[2] N. Crouseilles, L. Einkemmer, and E. Faou. A Hamiltonian splitting for the Vlasov–Maxwell system. *J. Comput. Phys.*, 238:224–240, 2015.
[3] N. Crouseilles, M. Mehrenberger, and F. Vecil. Discontinuous Galerkin semi-Lagrangian method for Vlasov-Poisson. In *ESAIM: Proceedings*, volume 32, pages 211–230. EDP Sciences, 2011.
[4] L. Einkemmer. On the geometric properties of the semi-Lagrangian discontinuous Galerkin scheme for the Vlasov-Poisson equation. *arXiv preprint, arXiv:1601.02280*, 2016.
[5] L. Einkemmer and A. Ostermann. Convergence analysis of a discontinuous Galerkin/Strang splitting approximation for the Vlasov–Poisson equations. *SIAM J. Numer. Anal.*, 52(2):757–778, 2014.
[6] L. Einkemmer and A. Ostermann. Convergence analysis of Strang splitting for Vlasov-type equations. *SIAM J. Numer. Anal.*, 52(1):140–155, 2014.
[7] J. Qiu and C. Shu. Positivity preserving semi-Lagrangian discontinuous Galerkin formulation: theoretical analysis and application to the Vlasov–Poisson system. *J. Comput. Phys.*, 230(23):8386–8409, 2011.
[8] J. Rossmanith and D. Seal. A positivity-preserving high-order semi-Lagrangian discontinuous Galerkin scheme for the Vlasov–Poisson equations. *J. Comput. Phys.*, 230(16):6203–6232, 2011.

Multisymplectic variational integrators for nonsmooth Lagrangian continuum mechanics

François Gay-Balmaz
(joint work with F. Demoures, T. S. Ratiu)

Numerical methods addressing contact problems are in high demand in a multitude of multibody dynamics applications. As opposed to formulations of models in smooth mechanics, contact problems must deal with the singularities separating two regions of a continuous medium, such as the contact set of colliding elastic bodies. Modeling these singularities and numerically handling them, in a way that respects the crucial inequality conditions and conserved quantities expected from the dynamics, has been an important scientific challenge. No complete satisfactory solutions meeting both physical and computational constraints exist to this day. The results presented at the workshop contribute to the solution of this long-standing problem. Our approach combines methods from nonsmooth optimization and multisymplectic field theory.

A classical point of view in physics consists in deriving the equations of motion from variational principles, i.e., by computing the critical points of an action functional. In the presence of constraints, such as impenetrability, propagation of singularities in an elastic body, solid-fluid boundaries, the critical point condition is not sufficient to derive the dynamics. One needs to consider an optimization problem for the action functional, subject to conditions appropriately derived from such type of constraints. This leads to the setting of variational analysis which provides powerful tools such as the Generalized Lagrange Multiplier Theorem, normal cone analysis, Kuhn-Tucker conditions, and, more generally, nonsmooth analysis. Developing the discrete analogue of these methods allows us to start the development of structure preserving numerical schemes for nonsmooth continuum mechanics with constraints.

The main steps underlying our approach in [2] are the following.

Step I: We formulate the smooth unconstrained problem as a multisymplectic Lagrangian field theory, by identifying the space of fields, the Lagrangian density, the spacetime Hamilton principle, and the associated Cartan forms.

Step II: We extend this multisymplectic Lagrangian formulation to a nonsmooth unconstrained setting, following [4] and identifying the types of singularities arising in the problem. This is done by using an extension of the spacetime Hamilton principle that allows for the treatment of certain types of singularities in the fields and automatically produces the needed jump conditions at the singularities. Both vertical and horizontal field variations have to be considered in the variational principle.

Step III: We include constraints in this formulation by using the generalized Lagrange multiplier approach for nonsmooth optimization [8]. This approach produces a necessary condition on the critical points of a functional restricted to a constrained subset, and is based on the concept of the normal cone. In our context, we formally apply this theory to the Lagrangian action functional relative to both vertical and horizontal variations. We show that the critical fields still verify a generalized multisymplectic form formula, as in the smooth unconstrained case, which is the spacetime extension of the symplectic property of the solution flow in classical mechanics. In addition, in presence of symmetries, a Noether theorem is still available, exactly as in the smooth unconstrained case.

Step VI: We discretize in spacetime this nonsmooth constrained variational theory. For simplicity, this is done on a 1+1 dimensional spacetime, with a discretization based on a rectangular mesh. As in the continuous case, the constraint is introduced directly at the level of the variational formulation for the discrete action functional, using the generalized Lagrange multiplier approach. Both vertical and horizontal variations are considered. The choice of the allowed horizontal variations becomes crucial in the discrete case, since it requires a spacetime grid adaptation, and the enforcement of stationarity under these horizontal variations yields discrete energy balance or discrete balance of configurational forces. In

our case, the horizontal variations are chosen to be associated to the time of impact, and therefore result in the conservation of the discrete global energy during the impact. Applying the generalized Lagrange multiplier approach with respect to the constraint in the discrete setting, relative to both vertical and horizontal variations, yields the desired numerical scheme. We show that this scheme is multisymplectic in the sense that it verifies a generalized discrete multisymplectic formula with constraints. In the presence of symmetry, we show that a discrete version of the Noether theorem is verified. Both these properties are inherited from the discrete spacetime variational character of the integrator. In absence of constraints, our schemes recover the multisymplectic integrators derived in [7]. In the particular case of classical mechanics, i.e., when spacetime reduces to time, our integrator recovers the collision variational integrators of [5].

The resulting multisymplectic scheme has been tested on two examples: the impact of an elastic beam on a rigid plate and the longitudinal impact of two elastic bars. We shall report only on the second example which is a standard benchmark example that has been widely studied in the literature (e.g., [9], [1], [6]). We tested our algorithm for identical and non-identical bars with various values for the lengths, densities, and initial velocities. In each case, we observed that the energy is conserved during and after the impact within 10^{-5} (relative energy error). Consistently with the theoretical prediction, the momentum map, associated with the invariance relative to translations, is perfectly conserved. During the persistent contact phase, we observed rapid velocity oscillations as the masses bounce rapidly against each other, especially for two identical bars. While the averaged velocity is correct, these fine-scale oscillations can be interpreted as spurious, as they do not properly capture the physical behavior. This problem has been solved by considering a slight modification of the discrete Lagrangian at the extremities of the bar that completely eliminates these spurious oscillations. Further numerical tests can be found in [3].

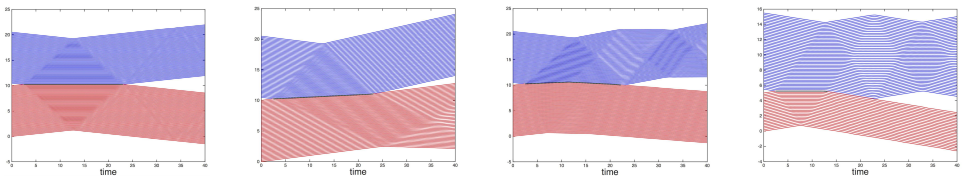


FIGURE 1. *Illustration of the displacement of the nodes of the two bars (up=bar A; down=bar B). From left to right: 1) two identical bars; 2) mass A < mass B; 3) stiffness A < stiffness B; 4) length A > length B. In each cases, energy is conserved during and after the impact within* 10^{-5}.

REFERENCES

[1] F. Cirak and M. West, *Decomposition contact response (DCR) for explicit finite element dynamics*, Internat. J. Numer. Methods Eng., **64** (2005), 1078–1110.

[2] F. Demoures, F. Gay-Balmaz, and T. S. Ratiu, *Multisymplectic variational integrators for nonsmooth Lagrangian continuum mechanics*, preprint 2016.

[3] F. Demoures, F. Gay-Balmaz, M. Desbrun, T. S. Ratiu and A. Aragon, *A multisymplectic integrator for elastodynamic frictionless impact problems*, preprint 2016.
[4] R. C. Fetecau , J. E. Marsden, and M. West, *Variational multisymplectic formulations of nonsmooth continuum mechanics*, in Perspectives and Problems in Nonlinear Science, 229–261, Springer, New York, 2003.
[5] R. C. Fetecau , J. E. Marsden, M. Ortiz, and M. West, *Nonsmooth Lagrangian mechanics and variational collision integrators*, SIAM J. Appl. Dyn. Sys., **2** (2003), 381–416.
[6] C. Glocker, *Concepts for modeling impacts without friction*, Ac. Mec., **168** (2004), 1–19.
[7] J. E. Marsden, G. W. Patrick, and S. Shkoller, *Multisymplectic geometry, variational integrators and nonlinear PDEs*, Comm. Math. Phys., **199** (1998), 351–395.
[8] R. T. Rockafellar and R. J.-B. Wets, *Variational Analysis*, Grundlehren der Mathematischen Wissenschaften, **317**, Springer-Verlag, Berlin, 1998.
[9] R. L. Taylor and P. Papadopoulos, *On a finite element method for dynamic contact/impact problems*, Internat. J. Numer. Methods Eng., **36** (1993), 2123–2140.

Growth of Sobolev norms in Hamiltonian PDEs

Benoît Grébert
(joint work with Eric Paturel, Laurent Thomann)

In the last years, much effort has been done to understand the weak turbulence phenomenon in Hamiltonian nonlinear dispersive PDEs. The central question is the following: once we have proved the global well posedness of a PDE in a Sobolev space H^{s_0}, we want to know whether

(i) the solutions remain bounded for all time and in all Sobolev norms, i.e.

$$\|u(t)\|_s \leq C_s \|u(0)\|_s, \ \forall s \geq s_0$$

at least for small initial conditions (a strong stability results for the origin),

(ii) there exist initial conditions leading to unbounded solutions, i.e.

$$\exists\, u(0) \text{ such that } \limsup_{t\to+\infty} \|u(t)\|_s = +\infty \text{ for some } s \geq s_0.$$

The first significant result in direction (ii) is due to Bourgain [6, Section 4] who showed a polynomial growth of Sobolev norms for a nonlinear wave equation in 1d with periodic boundary conditions. Later on, Colliander-Keel-Staffilani-Takaoka-Tao (see [8]), considered the cubic nonlinear Schrödinger equation, on the two dimensional torus $\mathcal{T}^2 = \left(\mathbb{R}/(2\pi\mathcal{Z})\right)^2$

$$i\partial_t u + \Delta u = |u|^2 u, \quad (t,x) \in \mathbb{R}\times\mathcal{T}^2 \tag{1}$$

and proved that for any $K \geq 1$ there exists a solution u and a time T such that $\|u(T)\|_s \geq K\|u(0)\|_s$. Of course, this result is weaker than the assertion (ii) but it suggests a possible unbounded behavior for some solutions. After that, Guardia-Kaloshin (see [16]), improving the dynamical step, proved that the time T satisfies a polynomial bound $0 < T < e^{K^c}$ for some absolute constant $c > 0$. A maybe less intuitive extension is then obtained by M. Guardia (see [15]): he proves that this

"almost unbounded" behavior is not a consequence of the exact resonances in (1), since it persists when one adds a small convolution potential V:

$$i\partial_t u + \Delta u + V \star u = |u|^2 u, \quad (t,x) \in \mathbb{R} \times \mathcal{T}^2. \tag{2}$$

In fact, in [8] (resp. in [16, 15]) the authors proved that the solutions of (1) (resp. (2)) remain close to the solution of a finite dimensional (depending on K) resonant system and they constructed an explicit solution v_K of this finite dimensional dynamical system (which also depends on K) satisfying $\|v_K(T)\|_s \geq K\|v_K(0)\|_s$. However we could expect that, since the potential V generically kills the exact resonances, the solutions of (2) would not follow the resonant dynamics. Actually in a series of paper initiated by [1, 5], Bambusi-Grébert developed a Birkhoff normal form technic that shows that, in the context of (2), assertion (i) is *almost* satisfied for a generic choice of V. Precisely they proved a stability result of kind (i) for $t \leq C\varepsilon^{-M}$ where $\varepsilon = \|u_0\|_s \ll 1$ and M is an arbitrary constant fixed from the beginning (see also [4, 3, 13] for developments or [2, 12] for a simple presentation). Notice that this stability result is even stronger in analytic regularity as conjectured in [7] and proved in [9]: if the initial datum is analytic in a strip then the solution is bounded in a strip of half width during a time of order $\varepsilon^{-\sigma|\ln\varepsilon|^\beta}$ where $\varepsilon > 0$ is the initial size of the solution and $0 < \beta < 1$. Surprisingly, the result in [15] shows that the resonant behavior in (2) may coexist with these almost stability results.

Let us also mention some interesting phenomena concerning the periodic Szegö equation introduced by Gérard and Grellier [11]. Recently, in [10] they showed the alternative (ii) for generic initial conditions, despite of an infinite number of conservation laws. Concerning the Szegö equation on the real line, Pocovnicu [18] proved (ii) by giving an explicit example.

More recently Hani-Pausader-Tzvetkov-Visciglia considered in [17] the cubic nonlinear Schrödinger equation on the wave-guide manifolds $\mathbb{R} \times \mathcal{T}^d$

$$i\partial_t u + \Delta_{\mathbb{R}\times\mathbb{T}^d} u = |u|^2 u, \quad (t,x,y) \in \mathbb{R} \times \mathbb{R} \times \mathcal{T}^d, \tag{3}$$

so they added a direction of diffusion in the PDE. Due to the dispersion along one variable, we expect that this equation is less "turbulent" than (1). Actually they proved that in the case $d = 1$ the equation (3) satisfies the assertion (i) in the alternative above, and when $2 \leq d \leq 4$ it satisfies the assertion (ii).

In a recent work ([14]) we add a convolution potential V to (3), i.e. we consider

$$i\partial_t u + \Delta_{\mathbb{R}\times\mathbb{T}^d} u + V \star u = |u|^2 u, \quad (t,x,y) \in \mathbb{R} \times \mathbb{R} \times \mathcal{T}^d \tag{4}$$

and we prove that for generic choice of the potential V assertion (i) holds true. So in that "less turbulent" case, the exact resonances are determinant to decide the limit dynamics: when we kill the exact resonances we turn off the weak turbulence phenomenon.

References

[1] D. Bambusi, *Birkhoff normal form for some nonlinear PDEs*, Comm. Math. Physics 234 (2003), 253–283.

[2] D. Bambusi, *A Birkhoff normal form theorem for some semilinear PDEs*, Hamiltonian Dynamical Systems and Applications, Springer, 2007, pp. 213–247.

[3] D. Bambusi, J.-M. Delort, B. Grébert, and J. Szeftel, *Almost global existence for Hamiltonian semilinear Klein-Gordon equations with small Cauchy data on Zoll manifolds*, Comm. Pure Appl. Math. 60 (2007), no. 11, 1665–1690.

[4] D. Bambusi and B. Grébert, Forme normale pour NLS en dimension quelconque, *Compt. Rendu. Acad. Sciences Paris* 337 (2003), 409–414.

[5] D. Bambusi and B. Grébert, Birkhoff normal form for partial differential equations with tame modulus. *Duke Math. J.* 135 (2006), no. 3, 507–567.

[6] J. Bourgain, On the growth in time of higher order Sobolev norms of smooth solutions of Hamiltonian PDE. *IMRN* 6 (1996), 277–304.

[7] J. Bourgain, Remarks on stability and diffusion in high dimensional Hamiltonian systems and PDEs. *Erg Th. and Dyn. Sys.* 24 (2004),no.5., 1331–1357.

[8] J. Colliander, M. Keel, G. Staffilani, H. Takaoka and T. Tao, Transfer of energy to high frequencies in the cubic defocusing nonlinear Schrödinger equation. *Invent. Math.*, 181 (2010), no. 1, 39–113.

[9] E. Faou and B. Grébert, A Nekhoroshev-type theorem for the nonlinear Schrödinger equation on the torus. *Anal. PDE* 6 (2013), no. 6, 1243–1262.

[10] P. Gérard and S. Grellier, On the growth of Sobolev norms for the cubic Szegö equation. *Séminaire: Équations aux Dérivées Partielles.* 2014–2015, Exp. No. XI, 20 pp.

[11] P. Gérard and S. Grellier, The cubic Szegö equation. *Ann. Sci. Éc. Norm. Supér.*, (4), 43(5) :761–810, 2010.

[12] B. Grébert, Birkhoff normal form and Hamiltonian PDEs. *Partial differential equations and applications*, 1–46, Sémin. Congr., 15, Soc. Math. France, Paris, 2007.

[13] B. Grébert, R. Imekraz and É. Paturel, Normal forms for semilinear quantum harmonic oscillators. *Commun. Math. Phys.* 291, 763–798 (2009).

[14] B. Grébert, É. Paturel and L. Thomann Modified scattering for the cubic Schrödinger equation on product spaces: the nonresonant case. To appear in *Math Res. Lett.*

[15] M. Guardia, Growth of Sobolev norms in the cubic defocusing nonlinear Schrödinger equation with a convolution potential. *Comm. Math. Phys.*, 329 (2014), no 1, 405–434.

[16] M. Guardia and V. Kaloshin, Growth of Sobolev norms in the cubic defocusing nonlinear Schrödinger equation. *J. Eur. Math. Soc*, 17 (2015), no. 1, 71–149.

[17] Z. Hani, B. Pausader, N. Tzvetkov and N. Visciglia, Modified scattering for the cubic Schrödinger equation on product spaces and applications. arXiv 1311.2275.

[18] O. Pocovnicu, Explicit formula for the solution of the Szegö equation on the real line and applications. *Discrete Cont. Dyn. Syst.* 31 (2011), 607–649.

A tale of two matrices: the Master Equations and Lie-group methods

Arieh Iserles
(joint work with Shev MacNamara)

The equation $y' = [A^{[0]}(t) + f(t)A^{[1]}(t)]y$, where $y(0) = y_0 \succ 0 \in \mathbb{R}^{N+1}$, $1^\top y_0 = 1$ and

$$A^{[0]} = \begin{bmatrix} -N & 1 & 0 & \cdots & \cdots & 0 \\ N & -N & 2 & 0 & \cdots & 0 \\ 0 & N-1 & -N & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 2 & -N & N \\ 0 & \cdots & \cdots & 0 & 1 & -N \end{bmatrix},$$

$$A^{[1]} = \begin{bmatrix} N & 1 & 0 & \cdots & \cdots & 0 \\ -N & N-2 & 2 & 0 & \cdots & 0 \\ 0 & -N+1 & N-4 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -2 & -N+2 & N \\ 0 & \cdots & \cdots & 0 & -1 & -N \end{bmatrix},$$

is a model of isomerization in a monomolecular setting. Our point of departure is the observation is that, once the ODE is solved by the Magnus method, the radius of convergence is well in excess of standard estimates [4]. We identify the eigenvalues corresponding to $A^{[k]}$ – specifically, $\sigma(A^{[0]}) = \{0, -2, -4, \ldots, -2N\}$ (with eigenvectors explicitly known), while $A^{[1]}$ is nilpotent. Moreover, $[A^{[0]}, A^{[1]}] = -2A^{[1]}$, and this implies at once that the free Lie algebra generated by $A^{[0]}$ and $A^{[1]}$ is solvable. This explains why Magnus is so good, but also why we do not need to use it: the solution is available explicitly and we present it.

This ODE is a special case of *Master Equations,* which describe the time evolution of a probability function in a chemical system,

$$y' = A(t)y, \quad t \geq 0, \qquad y(0) = y_0 \succ 0 \in \mathbb{R}^{N+1}, \quad 1^\top y_0 = 1,$$

where $1^\top A(t) \equiv 0^\top$ – it is easy to prove that $y(t) \succ 0$, $1^\top y(t)$, hence $y(t)$ is a probability distribution [3]. Often A is a graph Laplacian [2]. In numerical solution of Master Equations we need to conserve the sum $1^\top y(t)$ (easy, this being a linear invariant) and the positivity of $y(t)$. The latter is very difficult because of severe limitations on preservation of positivity by ODE methods [1].

We approach the problem of conserving positivity constructing a *flag* of methods $\{\mathcal{M}_r\}_{r=1}^{r^\star}$ such that each $\mathcal{M}_r$ is of order p_r, $p_{r+1} > p_r$, and $\mathcal{M}_{r+1}$ can be derived from $\mathcal{M}_r$ at marginal cost. The idea is that for sufficiently high order the solution is bound to be positive because of convergence, but at a great majority of steps it is sufficient to use a low-order, hence cheaper, method.

Specifically, we generate and analyse in detail a flag of Magnus methods and describe how to implement them efficiently.

References

[1] C. Bolley & M. Crouzeix, *Conservation de la positivité lors de la discrétisation des problèmes dévolution paraboliques*, RAIRO Anal. Numér. **12** (1978), 237–245.

[2] J. Gunawardena, *A linear framework for time-scale separation in nonlinear biochemical systems*, PLoS ONE **7** (2012), e36321.

[3] T. Jahnke & W. Huisinga, *Solving the chemical master equation for monomolecular reaction systems analytically*, J. Math. Biol. **54** (2007), 1–26.

[4] K. Kormann & S. MacNamara, *Error control for exponential integration of the Master Equation*, Technical Report (2015).

Adiabatic integrators for dispersion-managed nonlinear Schrödinger equations

Tobias Jahnke

(joint work with Marcel Mikl)

Data transfer through a dispersion-managed optical fiber is modelled by the semi-linear Schrödinger equation

$$\partial_t u = \frac{i}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right)\partial_x^2 u + i|u|^2 u, \qquad x \in \mathbb{T}, \quad t > 0 \tag{1}$$

with $0 < \varepsilon \ll 1$ on the one-dimensional torus $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$. The coefficient $\gamma(t) := \chi(t) + \varepsilon\alpha$ is the sum of a piecewise constant function

$$\chi(t) = \begin{cases} -\delta & \text{if} \quad t \in [m, m+1) \quad \text{with} \quad m \in \mathbb{N} \text{ even}, \\ \delta & \text{if} \quad t \in [m, m+1) \quad \text{with} \quad m \in \mathbb{N} \text{ odd} \end{cases} \tag{2}$$

and a small constant part $\varepsilon\alpha$ with parameters $\alpha, \delta > 0$; cf. [3, 4].

Typical solutions oscillate rapidly in time due to the small parameter ε. This imposes severe step-size restrictions if classical time-integrators such as splitting methods, Runge-Kutta or multistep methods are applied. The discontinuous, rapidly changing coefficient $\gamma(t/\varepsilon)$ and the nonlinearity pose additional challenges for any numerical method.

In this talk, we propose and analyze adiabatic integrators (cf. [1, 2]) which do not suffer from such a step size restriction. These integrators are based on the transformation

$$u(t,x) \mapsto \Big(y_k(t)\Big)_{k\in\mathbb{Z}}, \qquad y_k(t) := \exp\left(ik^2\phi\left(\tfrac{t}{\varepsilon}\right)\right)\hat{u}_k(t)$$

where $(\hat{u}_k)_{k\in\mathbb{Z}}$ are the Fourier coefficients of $u(t,\cdot)$ and

$$\phi(t) = \int_0^t \gamma(s)\, ds = \int_0^t \chi(s)\, ds + \varepsilon\alpha t.$$

Substituting this transform into (1) yields

$$\dot{y}_m(t) = i \sum_{j-k+\ell=m} y_j(t)\bar{y}_k(t)y_\ell(t) \exp\left(-i\omega_{[jk\ell m]}\phi\left(\tfrac{t}{\varepsilon}\right)\right), \qquad m \in \mathbb{Z}. \tag{3}$$

with $\omega_{[jk\ell m]} := j^2 - k^2 + \ell^2 - m^2$. The advantage of (3) over (1) is threefold. First, (1) involves the discontinuous function γ whereas (3) involves the continuous function ϕ. Second, the right-hand side of (1) tends to infinity as $\varepsilon \to 0$ due to the factor $1/\varepsilon$. In (3), such a factor appears only in the argument of ϕ, and since $|\exp(-i\omega_{[jk\ell m]}\phi(t/\varepsilon))| = 1$ independently of ε, the right-hand side of (3) remains bounded as long as the sequence $(y_k(t))_{k\in\mathbb{Z}}$ decays sufficiently fast. Third, it can be shown that the solution of (3) converges to a well-defined limit (cf. [3, 4]) which cannot be expected for (1).

The idea for the construction of adiabatic integrators is, roughly speaking, to freeze slowly varying variables over a time-step and to make use of the fact that oscillatory integrals of the form

$$\int_a^b \exp\left(-i\omega_{[jk\ell m]}\phi\left(\tfrac{t}{\varepsilon}\right)\right)\, dt$$

can be computed explicitly. We show that the accuracy of these integrators is not affected by ε in the sense that the time-step size is not restricted by ε, and that the constant in the error bound is independent of ε. These results are illustrated by numerical examples.

References

[1] T. Jahnke and Ch. Lubich, *Numerical integrators for quantum dynamics close to the adiabatic limit*, Numer. Math., *94(2)* (2003), 289–314.

[2] T. Jahnke, *Long-time-step integrators for almost-adiabatic quantum dynamics*, SIAM J. Sci. Comput., *25(6)* (2004), 2145–2164.

[3] S. K. Turitsyn, B. G. Bale, and M. P. Fedoruk, *Dispersion-managed solitons in fibre systems and lasers*, Physics Reports *521* (2012), 135–203.

[4] V. Zharnitsky, E. Grenier, Ch. Jones, and S. K. Turitsyn, *Stabilizing effects of dispersion management*, Physica D *152–153* (2001), 794–817.

Time-stepping of low-rank approximations with small singular values

Emil Kieri

(joint work with Christian Lubich, Hanna Walach)

We consider low-rank approximations to matrix differential equations of the form

$$\dot{A}(t) = F(t, A(t)), \qquad A(0) \in \mathbb{C}^{m\times n}.$$

Such problems appear, e.g., after spatial discretisation of time-dependent partial differential equations (PDEs) in two spatial dimensions. Higher-dimensional PDEs give rise to higher order tensor differential equations of similar form. Tensor differential equations in tensor-train format [5] are also covered by the present analysis, but for the sake of simplicity we will restrict this presentation to the matrix case.

Low-rank approximations have been used with success for high-dimensional PDEs, most predominantly in the multi-configurational time-dependent Hartree method [4]. There are, however, several open questions regarding the convergence of low-rank approximations. In this work, we answer one of these questions positively. We prove that if F has a modest Lipschitz constant and maps almost onto the tangent space of the low-rank manifold, then a recently proposed time-stepping scheme for low-rank approximations [2, 3] will give an accurate result, also in the presence of small singular values [1]. The scheme was first proposed for matrices in [2], and then extended to tensors in tensor-train format in [3].

In the vicinity of small nonzero singular values, the manifold $\mathcal{M}_r \subset \mathbb{C}^{m\times n}$ of rank-r matrices has strong curvature. That is, if σ_r is the rth singular value of $X \in \mathcal{M}_r$, then the Lipschitz constant of the projection $P(X)$ onto the tangent space $T_X\mathcal{M}_r$ of $\mathcal{M}_r$ at X is proportional to σ_r^{-1}. This means that standard time-stepping schemes for the dynamical low-rank approximation

$$\dot{Y}(t) = P(Y)F(t, Y(t)), \qquad Y(0) = Y_0 \approx A(0)$$

will break down in the presence of small singular values. The scheme of [2, 3], on the other hand, is robust in this case.

With the decomposition $Y = USV^*$, where $S \in \mathbb{C}^{r\times r}$ and U, V have orthonormal columns, the projection onto the tangent space has the representation

$$P(Y)Z = ZVV^* - UU^*ZVV^* + UU^*Z \qquad \text{for } Z \in \mathbb{C}^{m\times n}.$$

The method of [2, 3] uses this decomposition of the projection to construct a splitting scheme. For matrices, given $Y_0 = U_0S_0V_0^*$, the scheme reads:

- Solve $\dot{K}(t) = F(t, K(t)V_0^*), \quad K_0 = U_0S_0$.
- Make a QR-decomposition $[U_1, \widehat{S}_1] = \mathrm{qr}\,(K(h))$.
- Solve $\dot{S}(t) = -U_1^*F(t, U_1S(t)V_0^*)V_0, \quad S(0) = \widehat{S}_1$, and let $\widetilde{S}_0 = S(h)$.
- Solve $\dot{L}(t) = F(t, UL(t)^*)^*U_1, \quad L(0) = V_0\widetilde{S}_0^*$.
- Make a QR-decomposition $[V_1, S_1^*] = \mathrm{qr}\,(L(h))$.

Then, $Y_1 = U_1S_1V_1^*$ is a consistent approximation of $Y(h)$. For many problems F can be evaluated without forming the full $m \times n$ matrix. In such cases the scheme is very efficient, as it only works with much smaller matrices.

In [1] we prove that if $F(t, Y)$ is Lipschitz continuous in its second argument, and if it up to an ε-perturbation maps onto $T_Y\mathcal{M}_r$, then the error of the splitting scheme can be bounded in terms of ε and the time step h, independently of the singular values. The proof is based on two important properties of the scheme:

- If $F(t, A) = F(t)$, i.e., the right-hand side does not explicitly depend on A, and if $A(t) \in \mathcal{M}_r$ for all t, then the splitting scheme is exact for any time step h. This result was proven in [2].
- The matrices U and V stay constant during some of the substeps. Furthermore, the perturbation from the exact flow of FVV^* arising in the first substep is invariant to projection with VV^*, and similarly in substeps two and three with the relevant projections.

To prove the result, we construct a path $X(t)$ on $\mathcal{M}_r$ close to $A(t)$. By the assumptions on F, such a path exists. By the exactness result, the splitting schemed applied to $\dot{A}(t) = \dot{X}(t)$ would give $A(h) = X(h)$. Using the Gröbner–Alekseev lemma we estimate how much we, in each substep, deviate from the scheme applied to $\dot{X}(t)$. As $X(t)$ and $Y(t)$ are different paths on the manifold, the Lipschitz constant of F will here enter in the estimate. Using the preservation of U and V in the relevant substeps we can bound the effect of these deviations independently of the singular values. For the details we refer to [1].

As the error estimate depends on the Lipschitz constant of F, it is not valid for (spatial discretisations of) PDEs. Extending the error analysis to cover also this case remains an open problem. Numerically we get much better results for PDEs than what is explained by the present analysis.

References

[1] E. Kieri, Ch. Lubich and H. Walach, *Discretized dynamical low-rank approximation in the presence of small singular values*, SIAM J. Numer. Anal. **54** (2016), 1020–1038.
[2] Ch. Lubich and I. V. Oseledets, *A projector-splitting integrator for dynamical low-rank approximation*, BIT **54** (2014), 171–188.
[3] Ch. Lubich, I. V. Oseledets and B. Vandereycken, *Time integration of tensor trains*, SIAM J. Numer. Anal. **53** (2015), 917–941.
[4] H.-D. Meyer, U. Manthe and L. S. Cederbaum, *The multi-configurational time-dependent Hartree approach*, Chem. Phys. Lett. **165** (1990), 73–78.
[5] I. V. Oseledets, *Tensor-train decomposition*, SIAM J. Sci. Comput. **33** (2011), 2295–2317.

Dedicated Symplectic integrators for the rigid body motion.

Jacques Laskar
(joint work with Timothé Vaillant)

The free rotation of a rigid body is an integrable problem but its exact integration is costly. This is not a problem if the output is only needed over long time, but most often, the rotation is coupled with a perturbing potential, and in this case, the output is needed at each step.

It is then useful to devised splitting methods that are approximate, but of very low cost. The new integrators that are presented here are based on two ideas

- Use the algebra of the angular momentum to reduce the number of condition equations that are needed to be satisfied.
- Obtain dedicated symplectic spitting methods that are spitting methods for which the splitting coefficients depend on the problem. Here the coefficients will depend on the momenta of inertia of the rigid body.

Examples are given for the extreme cases of the spherical top and for the H2O molecule.

A two-point boundary value problem for DAEs with advances and delays arising in the differential geometry of touching tubes

John Maddocks

Filaments, or long slender tubular structures, arise in many applications in mechanics, physics and biology. Intertwined filaments in which two flexible tubes wrap around each other also frequently arise, with the most commonly encountered example probably being the X-like structure that you form in the first step of tying your shoelaces. I will show some solutions to the differential algebraic system that describes the differential geometry of such balanced intertwined structures. The system is nonstandard because it is a two-point boundary value problem for DAEs with an unknown functional deviation f(s), which can correspond to both advances and delays in the independent variable. Surprisingly the computations suggest that two slender intertwined tubes with circular cross-sections do not touch each other along a single contact curve, but rather along a double contact curve with singularities. The numerical solutions are found by an iterative procedure which appears trustworthy, but a faster and more reliable numerical solution technique would certainly be of interest, as would existence and local uniqueness results for the system of governing equations.

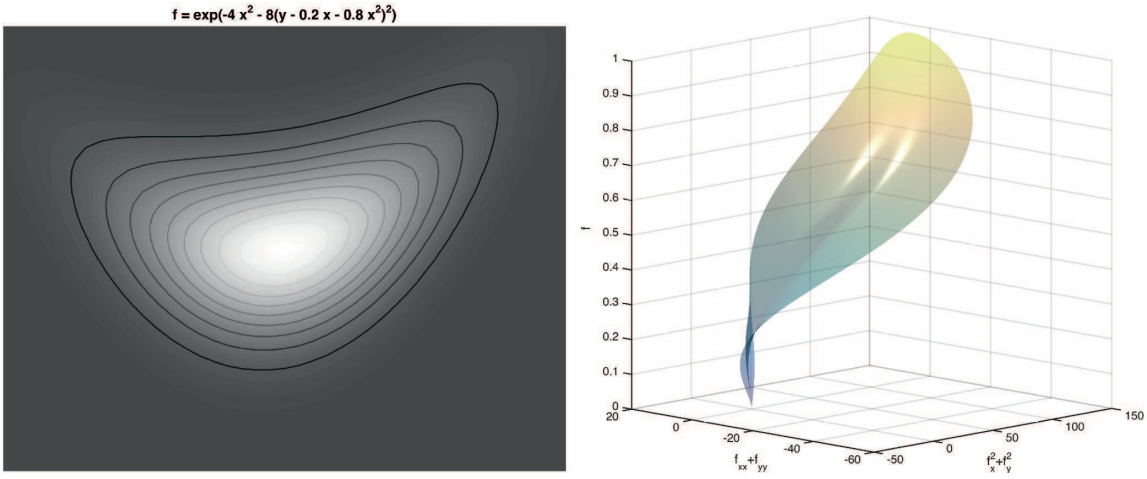
Differential invariant signatures (after Olver) for images

Robert I McLachlan
(joint work with Richard G Brown, Stephen R Marsland)

Lie group methods play a fundamental role in many aspects of computer vision and image processing. We consider the setting in which a Lie group G acts on a space M of objects such as points, curves, or images, and convenient methods of working in M/G are sought. One such method is based on the theory of invariants, i.e., on the theory of G-invariant functions on M, which has been extensively developed from mathematical, computer science, and engineering points of view.

We work in the school of invariant signatures, developed by (amongst others) Olver and Shakiban [5], and used for Euclidean object recognition (see, e.g., [1]). These references principally concern invariants of plane curves $\phi\colon S^1 \to \mathbb{R}^2$ under planar transformations $g\colon \mathbb{R}^2 \to \mathbb{R}^2$; the group action is $g \cdot \phi := g \circ \phi$. In constrast, in the present work [4] the objects are k-color images $f\colon \mathbb{R}^2 \to \mathbb{R}^k$ on which the transformations act by $g \cdot f := f \circ g^{-1}$. This is an instance of the Cartan classification problem in which the graph $(x, f(x)) \subset \mathbb{R}^{k+2}$ of the image is mapped to $(g(x), f(x))$; the problem is to to determine when two such graphs are related by a group transformation. Note that the action here is intransitive.

There are many methods of constructing differential invariants. The moving frame method provides an algorithm to generate them. For some actions a "first fundamental theorem" is known which provides a complete set of polynomial invariants. Other cases are related to instance studied in classical invariant theory.



Each approach has advantages and disadvantages. In practice we use a combination of each of the methods. Also note that even if all invariants are found, they may not separate group orbits as is desired in the classification problem.

Example 1. Let $f\colon \mathbb{R}^2 \to \mathbb{R}$ be a 1-colour image and let $G = E(2)$. The set

$$\left\{\left(f, \|\nabla f\|^2, \nabla^2 f\right)(x,y)\colon (x,y) \in \mathbb{R}^2\right\}$$

is a differential invariant of f. At generic points it is a locally embedded 2-dimensional submanifold of $\mathbb{R}^3$. A sample image and its signature are shown in the figure. This invariant comes from the invariant tensor theorem for $O(n)$, which says that all polynomial invariants for $O(n)$ acting on $f\colon \mathbb{R}^n \to R$ are given by the contractions

$$f, \quad f_i f_i, \quad f_{ii}, \quad f_{ij} f_i f_j, \quad f_{ij} f_{ij}, \quad f_{ijk} f_{ijk}, \ldots$$

of the partial derivatives of f. Clearly, at least 3 invariants (one of which is the image f itself) are needed. But is this enough to distinguish generic images? The answer is no. If the invariant signature is given as the surface

$$\nabla^2 f = H(f, \|\nabla f\|^2)$$

this does not determine f up to $E(2)$, because the solution to this nonlinear Poisson equation depends on the boundary conditions. However, it can be shown that the 4-dimensional signature $(f, f_i f_i, f_{ii}, f_{ij} f_i f_j)$ does locally determine f up to Euclidean motions.

Example 2. Let f be a 1-colour image and let $G = SA(2)$. The transformations are $x \mapsto Ax + b$, $\det A = 1$. The prolonged action is $f \mapsto f$, $f_i \mapsto A_{ij} f_j$, $f_{ij} \mapsto A_{ik} A_{il} f_{kl}, \ldots$. This is the same as the simultaneous action of $SL(2)$ on linear forms, binary forms, ternary forms, etc., studied in classical invariant theory. A generating set of polynomial invariants was found by Alexander Bessel in 1869 [2]: There are no invariants depending on first derivatives of f. There are two invariants depending on 2nd derivatives, $\det f_{ij}$ and $f_{yy} f_x^2 + f_{xx} f_y^2 - 2 f_{xy} f_x f_y$. There are 15 independent polynomial invariants depending on 3rd derivatives; the cubic ones are $f_y f_{yy} f_{xxx} - 2 f_y f_{xy} f_{xxy} - f_x f_{yy} f_{xxy} + f_y f_{xx} f_{xyy} + 2 f_x f_{xy} f_{xyy} -$

$f_x f_{xx} f_{yyy}$ and $f_{yy} f_{xy}^2 + f_{xx} f_{xyy}^2 + f_{xy} f_{xxx} f_{yyy} - f_{yy} f_{xxx} f_{xyy} - f_{xy} f_{xxy} f_{xyy} - f_{xx} f_{xxy} f_{yyy}$.

The strength of the method is that it is algorithmic; it works for any transformation group, including infinite-dimensional groups; it yields local invariants, so it can be applied to occluded images. The weakness is that it unavoidably depends on derivatives of the image. (For some groups (e.g. $E(2)$), but probably not for all, there are global invariants defined using Fourier transforms.) Thus, the number of derivatives required for a signature becomes an important invariant in its own right. For the two examples above, 2 derivatives are needed.

We study this problem for $SE(2)$, $E(2)$, $\mathrm{Sim}(2)$, $SA(2)$, $A(2)$, $\mathrm{PSL}(2,\mathbb{C})$ (the Möbius group), $\mathrm{PSL}(3,\mathbb{R})$ (the projective group), $\mathrm{Diff}_{\mathrm{vol}}$ (the volume preserving group), $\mathrm{Diff}_{\mathrm{con}}$ (the conformal maps), and Diff (all diffeomorphisms).

As the number of colours increases, one expects to need fewer derivatives. However, in some cases obstructions appear.

Example 3. For $SA(2)$ on k-colour images $f^1, \ldots, f^k$, the Poisson brackets

$$\{f^i, f^j\} := f^i_x f^j_y - f^i_y f^j_x, \quad 1 \le i, j \le k$$

are all invariant. There seems to be an ample supply ($k(k-1)/2$) of invariants that use only 1 derivative. However, these are *also* invariant under the bigger group $\mathrm{Diff}_{\mathrm{vol}}(\mathbb{R}^2)$, so they can never be a complete invariant for $SA(2)$ – a hidden symmetry. In fact, for $SA(2)$, 2 derivatives are needed for all $k \ge 1$.

The most extreme case we have covered is the Möbius group. Because it is a subgroup of the conformal maps, it needs 3 derivatives for all $k \ge 1$.

Having constructed a complete or partial invariant signature, to solve the classification problem requires being able to robustly compare two signatures. These are (locally) unparameterised submanifolds of some fixed manifold, usually Euclidean space. In work in progress with James Benn, Klas Modin, and Olivier Verdier [3], we compare signatures using a finite element discretization of *currents*, the integrals of differential forms over the submanifold. Crucially, such integrals do not depend on the parameterisation of the submanifold. A finite element space (e.g. piecewise linear) of forms is chosen and the operator norm restricted to this space provides a reliable and extremely cheap way to compare submanifolds without requiring any registration or optimisation.

References

[1] Reza Aghayan, Tim Ellis, and Jamshid Dehmeshki. Planar numerical signature theory applied to object recognition. *Journal of mathematical imaging and vision*, 48(3):583–605, 2014.

[2] A. Bessel, Ueber die Invarianten der einfachsten Systeme simultaner binärer Formen, Math. Ann. 1 (1869) 173–194.

[3] James Benn, Stephen Marsland, Robert I McLachlan, Klas Modin, and Olivier Verdier, Currents and finite elements as a tool for shape space, in preparation.

[4] Richard G Brown, Stephen Marsland, and Robert I McLachlan, Differential invariant signatures for images, in preparation.

[5] Eugenio Calabi, Peter J Olver, Chehrzad Shakiban, Allen Tannenbaum, and Steven Haker. Differential and numerically invariant signature curves applied to object recognition. *International Journal of Computer Vision*, 26(2):107–135, 1998.

The construction of parallel energy-preserving methods for Hamiltonian systems

Yuto Miyatake

(joint work with John C. Butcher)

We consider the numerical integration of Hamiltonian systems of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}y = f(y), \qquad y(t_0) = y_0 \in \mathbb{R}^N,$$

where $f(y) = S\nabla H(y)$ with a non-singular skew-symmetric constant matrix S and sufficiently differentiable Hamiltonian $H : \mathbb{R}^N \to \mathbb{R}$. Focusing on the energy-preservation property, i.e. $\frac{\mathrm{d}}{\mathrm{d}t}H(y) = 0$, we consider the construction of energy-preserving methods. Among existing energy-preserving methods, the average vector field (AVF) method [4] and its extensions, such as the AVF collocation method [3] (see also, the Hamiltonian boundary value method [1]), are prominent in terms of the long-time behaviour. However, they are implicit methods: roughly speaking, the computational cost of the AVF collocation method is almost the same as the same order Gauss Runge–Kutta method. In this talk, we construct a more efficient energy-preserving method than exists at present. Our method is constructed based on so called continuous stage Runge–Kutta (CSRK) methods.

Definition. Let $A_{\tau,\zeta}$ be a polynomial in τ and ζ. Assume that $A_{0,\zeta} = 0$. We denote by s the polynomial degree of $A_{\tau,\zeta}$ in τ. Let B_ζ be defined by $B_\zeta = A_{1,\zeta}$. We search for an s-degree polynomial Y_τ ($\tau \in [0,1]$) and y_1 such that they satisfy

$$Y_\tau = y_0 + h\int_0^1 A_{\tau,\zeta} f(Y_\zeta)\,\mathrm{d}\zeta,$$
$$y_1 = y_0 + h\int_0^1 B_\tau f(Y_\tau)\,\mathrm{d}\tau.$$

A one-step method $y_0 \mapsto y_1$ is called an s-degree continuous stage Runge–Kutta (CSRK) method.

To construct intended integrators, we need to characterize (i) an energy preserving condition, (ii) order conditions and (iii) criteria for parallel implementation using real arithmetic, in terms of $A_{\tau,\zeta}$. To simplify the notation, we denote $A_{\tau,\zeta}$ by using a matrix $M \in \mathbb{R}^{s\times s}$: $A_{\tau,\zeta} = [\tau, \frac{\tau^2}{2}, \ldots, \frac{\tau^s}{s}]M[1, \zeta, \ldots, \zeta^{s-1}]^\top$.

Then, one can prove the following properties.

Theorem 1. A CSRK method is energy-preserving, if the matrix M is symmetric.

A straightforward calculation proves this theorem. The necessity can also be proved under a certain assumption by using a technique used in [2].

Theorem 2. A CSRK method is energy-preserving and of order at least $p = 2\eta$, if the symmetric matrix M satisfies

$$\left[\frac{1}{k}, \frac{1}{k+1}, \ldots, \frac{1}{k+s-1}\right] M = i_k^\top, \qquad k = 1, \ldots, \eta,$$

where all components of $i_k \in \mathbb{R}^s$ are zero except for the k-th component which is 1.

The proof is based on the simplifying assumptions.

It is known that the computational cost of solving implicit RK methods can be reduced in a parallel computer, if a RK matrix A has only real, distinct eigenvalues. A similar discussion can also be done for CSRK methods. One can show that if

$$\begin{bmatrix} 1 & & & \\ & \frac{1}{2} & & \\ & & \ddots & \\ & & & \frac{1}{s} \end{bmatrix} M \begin{bmatrix} \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{s+1} \\ \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{s+2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{s+1} & \frac{1}{s+2} & \cdots & \frac{1}{2s} \end{bmatrix} \tag{1}$$

has only real, distinct eigenvalues, the corresponding CSRK method can be computed efficiently.

By using the above properties, one can construct efficient high order integrators. As an example, we derive fourth order integrators below. We set $s = 3$ and assume that M is given, with a parameter α, by

$$\begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \alpha \end{bmatrix} M = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}.$$

The energy-preserving and order conditions are already satisfied. For the parameter α, one can show that (1) has only real, distinct eigenvalues, if

$$-\frac{\alpha_1}{300} > \frac{1}{6}2^{2/3} + \frac{5}{24}2^{1/3} + \frac{1}{4} \approx 0.7770503941, \qquad \alpha_1 = \frac{1}{36\alpha - 7}.$$

If α satisfies this inequality, the corresponding integrators can be implemented with almost the same computational cost as the second order AVF method in parallel architecture.

In addition to the above integrators, sixth order integrators have been derived. However, the evaluation of eigenvalues becomes difficult when we consider higher order integrators. We are currently trying to give a more systematic approach to deriving higher order efficient energy-preserving integrators.

References

[1] L. Brugnano, F. Iavernaro, and D. Trigiante, *Hamiltonian boundary value methods (energy preserving discrete line integral methods)*, J. Numer. Anal. Ind. Appl. Math., 5 (2010), pp. 17–37.

[2] E. Celledoni, B. Owren and Y. Sun, *The minimal stage, energy preserving Runge–Kutta method for polynomial Hamiltonian systems is the averaged vector field method*, Math. Comp., 83 (2014), pp. 1689–1700.
[3] E. Hairer, *Energy-preserving variant of collocation methods*, J. Numer. Anal. Ind. Appl. Math., 5 (2010) pp. 73–84.
[4] G. R. W. Quispel and D. I. McLaren, *A new class of energy-preserving numerical integration methods*, J. Phys. A, 41 (2008), 045206.

Diffeomorphic density transport – a numerical challenge

Klas Modin
(joint work with Martin Bauer and Sarang Joshi)

On a manifold M with reference volume form μ, let ρ_0 and ρ_1 be smooth densities (everywhere positive functions) of the same total mass

$$\int_M \rho_0\mu = \int_M \rho_1\mu = 1. \tag{1}$$

The *density transport problem* (in the smooth category) is to find a diffeomorphism $\eta \in \mathrm{Diff}(M)$ such that

$$|D\eta^{-1}|\rho_0 \circ \eta^{-1} = \rho_1. \tag{2}$$

The left hand side is the *density action* of η on ρ_0 (geometrically, the pushforward by η of the volume form $\rho_0\mu$). Our theme here is: how can one solve the density transport problem numerically in an efficient way? For simplicity, we take $M = \mathbb{T}^n$ (the flat n-torus).

First, notice that there is no unique solution to (2). Indeed, if η is a solution, then $\eta \circ \psi$ for any diffeomorphism ψ that preserves the volume form $\rho_0\mu$ is also a solution. The standard regularization, originating from the work of Monge [1], consists in *optimal mass transport* (OMT)[1]

$$\text{minimize} \quad M(\eta) = \int_{\mathbb{T}^n} |\eta(x) - x|^2 \, \rho_0(x)\mathrm{d}x \quad \text{under the constraint (2).} \tag{3}$$

There are two main threads of numerical methods for OMT:

- To use the *dynamic reformulation*[2] of Benamou and Brenier [3], where one seeks a time-dependent density $\rho(t, x)$ and vector field $v(t, x)$ minimizing

$$\int_0^1 \int_{\mathbb{T}^n} |v(t, x)|^2 \rho(t, x)\mathrm{d}x\,\mathrm{d}t$$

under the constraints

$$\partial_t\rho + \nabla \cdot (\rho v) = 0 \quad \text{and} \quad \rho(0, \cdot) = \rho_0,\ \rho(1, \cdot) = \rho_1.$$

Based on this reformulation and a convexity result, the first approach is to construct gradient descent type methods on a space-time grid.

[1] We use here the L^2 setting. Monge originally considered L^1.
[2] The dynamic formulation of OMT is directly related to the infinite-dimensional Riemannian point-of-view advocated by Otto [2].

- To use the polar factorization of maps by Brenier [4], which states that a diffeomorphism η that fulfills (2) can be factorized as $\eta = \nabla\phi \circ \psi$, where ψ preserves $\rho_0 \mathrm{d}x$ and ϕ is a strictly convex function such that $\nabla\phi$ solves the OMT problem (3). The requirement that $\nabla\phi$ should fulfill the constraints (2) implies the Monge–Ampere equation

$$|\nabla^2\phi(x)|\rho_1(\nabla\phi(x)) = \rho_0(x).$$

  The second approach is to construct numerical methods for this equation.

In the first approach, the computational complexity is a problem (iteration on a full space-time grid is required). In the second approach, the severe nonlinearity of the Monge–Ampere equation is a problem.

It seems to us that in many applications where OMT is used *the particular choice of regularization* (3) *is not essential*. For example, in medical image registration and moving mesh adaptivity – two fields where OMT is used – there is no intrinsic reason to choose the OMT regularization. Thus, one may consider other optimality conditions that simplify the numerical discretization problem.

One possibility, that also have an appealing infinite-dimensional geometric interpretation, is the framework of *optimal information transport* (OIT) [5]. This is another dynamical formulation, where we seek a time dependent vector field $v(t, x)$ that minimize

$$I(v) = \int_0^1 \int_{\mathbb{T}^n} v(\Delta v)\,\mathrm{d}x\,\mathrm{d}t$$

under the conditions

$$\partial_t\gamma(t, x) = v(t, \gamma(t, x)), \quad \gamma(0, x) = x, \quad \gamma(1, \cdot)^*(\rho_1 \mathrm{d}x) = \rho_0.$$

This formulation might look arbitrary, but it has a straightforward geometric interpretation: of all possible solutions to the transport problem, find the solution that minimizes the distance to the identity with respect to the right-invariant Riemannian metric G on $\mathrm{Diff}(\mathbb{T}^n)$ defined by

$$G_\eta(u \circ \eta, v \circ \eta) = \int_{\mathbb{T}^n} u(\Delta v)\mathrm{d}x. \tag{4}$$

Well-posedness of the geodesic equation for this metric, as well as existence and uniqueness of the OIT problem, is given in [5].

The key to obtain efficient numerical methods for OIT is that the metric (4) has some special geometric properties, namely it induces the *Fisher–Rao metric* on the space of probability densities, principal in the field of *information geometry* [6].[3] Explicitly, the map

$$\eta \mapsto |D\eta|$$

is a Riemannian submersion (in a strict sense) between the space of diffeomorphisms $\mathrm{Diff}(\mathbb{T}^n)$ equipped with the metric (4) and the space of smooth probability densities

$$\mathrm{Dens}(\mathbb{T}^n) = \left\{ \rho \in C^\infty(\mathbb{T}^n) \middle| \rho > 0, \int_{\mathbb{T}^n} \rho\,\mathrm{d}x = 1 \right\},$$

[3]Thereby the name optimal 'information' transport.

equipped with the Fisher–Rao metric

$$F_\rho(\dot\rho,\dot\rho)=\frac{1}{4}\int_{\mathbb{T}^n}\frac{\dot\rho^2}{\rho}\,\mathrm{d}x.$$

From standard results in Riemannian geometry, it therefore follows that the minimizing path $v(t,x)$ for the OIT problem with either $\rho_0=1$ or $\rho_1=1$ must correspond to a *horizontal geodesic*: if $\gamma(t,\cdot)$ is the curve of diffeomorphisms generated by $v(t,\cdot)$, then $\gamma(t,\cdot)^*\mathrm{d}x$ is a Fisher–Rao geodesic connecting ρ_0 and ρ_1.

The same type of geometric interpretation exists for OMT, but with Fisher–Rao replaced by the Wasserstein metric. However, there is a major difference: *the Fisher–Rao geodesics are explicitly computable*. Indeed, by a change of variables they correspond to great circles on a convex portion of an infinite-dimensional sphere. Thus, we can solve the OIT problem as follows:

(1) Compute the Fisher–Rao geodesic $\rho(t)$ between ρ_0 and ρ_1; this is just an explicit expression.
(2) Lift the curve $\rho(t)$ to its corresponding horizontal geodesic curve on $\mathrm{Diff}(\mathbb{T}^n)$; this amounts to solving the *lifting equations*

$$\begin{aligned}\Delta f(t)&=\frac{\partial_t\rho(t)}{\rho(t)}\circ\gamma(t)^{-1}\\ \partial_t\gamma(t)&=\nabla f(t)\circ\gamma(t).\end{aligned}$$

A numerical algorithm for the lifting equations is obtained by equidistant time-stepping in the interval $[0,1]$, where in each time-step we need to solve a Poisson equation on a regular mesh and update the diffeomorphism $\gamma(t_k)$, which is numerically represented as a deformation of the regular mesh. By a modification, the same approach can be used also when both ρ_0 and ρ_1 are different from one and allowed to be zero. Such numerical methods are developed in [7], mainly for the purpose of medical image registration, although other applications are indicated.

Open questions: (i) Convergence analysis of the methods in [7]. (ii) Applications to r-adaptivity [8], replacing OMT by OIT. (iii) Are there other applications where OMT readily can be replaced by OIT?

References

[1] G. Monge. Mémoire sur la théorie des déblais et de remblais, 1781.
[2] F. Otto. The geometry of dissipative evolution equations: the porous medium equation. *Comm. Partial Differential Equations*, 26(1-2):101–174, 2001.
[3] J.-D. Benamou and Y. Brenier. A computational fluid mechanics solution to the Monge–Kantorovich mass transfer problem. *Numerische Mathematik*, 84(3):375–393, 2000.
[4] Y. Brenier. Polar factorization and monotone rearrangement of vector-valued functions. *Comm. Pure Appl. Math.*, 44(4):375–417, 1991.
[5] K. Modin. Generalized Hunter–Saxton equations, optimal information transport, and factorization of diffeomorphisms. *J. Geom. Anal.*, 25(2):1306–1334, 2015.
[6] S. Amari and H. Nagaoka. *Methods of information geometry*, American Mathematical Society, Providence, RI, 2000.

[7] M. Bauer, S. Joshi, and K. Modin. Diffeomorphic density matching by optimal information transport. *SIAM Journal on Imaging Sciences*, 8(3):1718–1751, 2015.
[8] C. J. Budd, W. Huang, and R. D. Russell. Adaptivity with moving grids. *Acta Numerica*, 18:111–241, 2009.

Lie-Butcher series and differential geometry. The case of symmetric spaces.

Hans Munthe-Kaas

Symmetric spaces are central objects in differential geometry, characterised by having a constant Riemannian curvature. Examples are spheres, grassman manifolds ans more generally quotients of Lie groups. Symmetric spaces appear in many applications in computational mechanics, control theory and differential geometry. In this talk we present new results on B-series type expansions for flows evolving on symmetric spaces and the algebraic structures behind such series. We also discuss new classes of numerical integration algorithms on symmetric spaces.

Structure preserving model reduction on Lie groups

Brynjulf Owren
(joint work with Elena Celledoni, Helen Parks)

The starting point for this work was an idea by Helen Parks to extend the work of Lall et al. [1] to time integrators for mechanical systems on manifolds. In large systems of ODEs one may have the situation that the flow evolves approxmately on a subspace of very small dimension. If such a subspace can be identified, one may project the full model onto this reduced space, integrate the smaller system and reconstruct the approxmate solution in large space. A common way to implement this procedure is by using the snapshot method. This means that the full system $y' = f(y)$ is integrated over a few steps from a given initial value. The solution vectors are collected to form the columns of a matrix $Y = [y_1, y_2, \ldots]$, and an approximate singular value decomposition, $Y = U\Sigma V^T$ in reduced form ($U \in \mathbb{R}^{N\times n}$), then yields a basis contained in the columns of U for the subspace to be used. The projected system in $\mathbb{R}^n$ is

$$\dot{z} = U^T f(Uz) \tag{1}$$

For mechanical systems of dimension $n = 2m$, one may start with a Lagrangian $L(q, \dot{q})$ and in this case it suffices to carry out the reduction on the q-part only of the snapshots, i.e. $Q = [q_1, q_2, \ldots] = \bar{U}\bar{\Sigma}\bar{V}^\top$. Now, setting $q = \bar{U}\bar{z}$, one obtains $\dot{q} = \bar{U}\dot{\bar{z}}$. For mechanical Lagrangians of the form $L(q, \dot{q}) = \frac{1}{2}\langle M\dot{q}, \dot{q}\rangle - V(q)$, the Euler–Lagrange equations and Legendre transformation take the form

$$M\ddot{q} = -\frac{\partial V}{\partial Q}, \qquad p = M\dot{q}$$

We can now define a *reduced* Lagrangian L_r by setting

$$L_r(\bar{z}, \dot{\bar{z}}) = \frac{1}{2}\langle M\bar{U}\dot{\bar{z}}, \bar{U}\dot{\bar{z}}\rangle - V(\bar{U}\bar{z})$$

with corresponding reduced Euler-Lagrange equations

$$\bar{U}^T M\bar{U}\ddot{\bar{z}} = -\bar{U}^T DV(\bar{U}\bar{z})$$

The Legendre transformation is $\pi = \bar{U}^T M\bar{U}\dot{\bar{z}} =: M_r\dot{\bar{z}}$ and we obtained the reduced Hamiltonian

$$H_r(z, \pi) = \frac{1}{2}\langle \pi, M_r^{-1}\pi\rangle + V(\bar{U}z)$$

Not surprisingly, numerical experiments show that the latter approach has better long time behaviour than what is obtained by using (1).

The next step is to generalise the approach to Lie groups. This is challenging because many of the ingredients in this snapshot method are based on operations in linear spaces, such as the singular value decomposition. Looking at the literature for Lie group integrators, one can see that they are predominantly based on either of the two principles

(1) Local coordinates on the group, or
(2) a global embedding of the group into a Euclidean model space

Both of these approaches have difficulties. The idea of model reduction is to create a low dimensional subspace by sampling (large) portions of the phase space. In the first approach, this requires a way to switch between charts. For example, if the phase space is formed from N copies of a Lie group, and each Lie group needs K charts, one needs in principle to keep track of representations of the solution in K^N charts. In a presented case of water molecules given in [2], we had such a situation with $K = 4$ and N in the range 50–100.

On the other hand, global embeddings are also challenging since the reduction procedure will not respect the constraints. This approach was however suggested in [1], where the following algorithm was devised

- Given a configuration manifold Q, embed it into some linear space V.
- Apply reduction to a problem in V and obtain a reduced linear space $V_r \subset V$
- Construct the reduced manifold $Q_r := V_r \cap Q$

By considering the dimensions of these spaces, one has $\dim V_r = \dim Q_r + (\dim V - \dim Q)$. For scalable problems, one may have the situation that the difference in parentheses grows rapidly as the dimension of Q grows, so that the size of the reduced linear space V_r must be chosen too large to be a viable alternative.

So far we have therefore used the first alternative above and derived locally valid representations of the full and reduced system, but with the disadvantage that the reduction can only be achieved in one chart at a time, when the solution leaves a chart, the algorithm must be restarted. Yet, the numerical experiments we have carried out are promising.

References

[1] S. Lall, P. Krysl, J. E. Marsden *Structure-preserving model reduction for mechanical systems*, Physica D **184** (2003), 304–318.

[2] A. Dullweber, B. Leimkuhler, and R. McLachlan, *Symplectic splitting methods for rigid body molecular dynamics*, J. Chem. Phys., **107** (1997), 5840–5851.

Kahan's method and its generalization

G R W Quispel

(joint work with E Celledoni, R I McLachlan, D I McLaren, B Owren)

In 1993 Kahan introduced a novel discretization of quadratic vector fields [1], and wrote:

"I have used these methods for 24 years without quite understanding why they work so well as they do, when they work."

In recent years, various authors (see below) have proved a large number of results, which are starting to give us an understanding of some of the miraculous properties of Kahan's method.

Kahan's (bilinear) discretization of the arbitrary quadratic ODE in $\mathbb{R}^n$:

$$\frac{dx_i}{dt} = a_{ijk}x_jx_k + b_{ij}x_j + c_i$$

(with summation over repeated indices implied), is defined by:

$$\frac{x_i(n+1) - x_i(n)}{h} = a_{ijk}\frac{x_j(n+1)x_k(n) + x_j(n)x_k(n+1)}{2} + b_{ij}\frac{x_j(n) + x_j(n+1)}{2} + c_i,$$

where h denotes the timestep, and $x_i(n)$ is short for $x_i(nh)$.

Note that this method (which Kahan called an "unconventional method") is linearly implicit.

After early works by Sanz-Serna [3] and by Hirota and Kimura [2], in a series of papers Suris and collaborators showed that Kahan's method preserves integrability for a large number of integrable quadratic vector fields (see e.g. refs [4] and [5] and references therein).

In reference [6] our team showed that Kahan's method is the restriction of the Runge-Kutta method

$$\frac{x_{n+1} - x_n}{h} = 2f\left(\frac{x_n + x_{n+1}}{2}\right) - \frac{1}{2}f(x_n) - \frac{1}{2}f(x_{n+1})$$

to quadratic vector fields. (Here $x_n := x(n)$, etc).

In the same paper we also showed that Kahan's method exactly preserves a modified Hamiltonian and a modified measure for Hamiltonian systems in $\mathbb{R}^n$ (whether integrable or not).

Generalizing Kahan's method, in reference [7] we introduced new (multilinear) k-step discretization methods using polarization. These methods exactly preserve a modified measure as well as k independent "modified Hamiltonian" k-integrals [8], when applied to homogeneous degree $k+1$ Hamiltonian vector fields in $\mathbb{R}^n$. (The case $k=2$ corresponds to Kahan's method).

Finally, in refs [6], [9], [10], [11], resp. [7], we showed how Kahan's method resp. more general polarization methods, preserve integrability for several integrable vector fields of degree 2 resp. 3.

References

[1] W Kahan, Unconventional numerical methods for trajectory calculations, Unpublished lecture notes, 1993.

[2] K Kimura and R Hirota, Discretization of the Lagrange top, J. Phys. Soc. Jap. **69** (2000), 3193–3199.

[3] J M Sanz-Serna, An unconventional integrator of W. Kahan, App. Num. **16** (1994), 245–250.

[4] A N W Hone and M Petrera, Three-dimensional discrete systems of Hirota-Kimura type and deformed Lie-Poisson algebras, J. Geom. Mech. **1** (2009), 55–85. (doi:10.3934/jgm.2009.1.55)

[5] M Petrera, A Pfadler and Y B Suris, On integrability of Hirota-Kimura type discretizations, Regular and Chaotic Dynamics **16** (2011), 245–289.

[6] E Celledoni, R I McLachlan, B Owren and G R W Quispel, Geometric properties of Kahan's method, J Phys. A **46** (2013), 025001.

[7] E Celledoni, R I McLachlan, D I McLaren, B Owren and G R W Quispel, Discretization of polynomial vector fields by polarization, Proc. Roy. Soc. **A471** (2015) 20150390, 10pp.

[8] F A Haggar, G B Byrnes, G R W Quispel and H W Capel, k-integrals and k-Lie symmetries in discrete dynamical systems, Physica A **233** (1996), 379–394.

[9] E Celledoni, R I McLachlan, D I McLaren, B Owren and G R W Quispel, Integrability properties of Kahan's method, J. Phys. A **47** (2014), 365202.

[10] P H van der Kamp, T E Kouloukas, G R W Quispel and P Vanhaecke, Integrable and superintegrable systems associated with multisums of products, Proc. Roy. Soc. A (2014) **470**, 20140481.

[11] T E Kouloukas, G R W Quispel and P Vanhaecke, Liouville integrability and superintegrability of a generalized Lotka-Volterra system and its Kahan discretization, arXiv: 1601.05006.

Landau damping for the Vlasov HMF equation: analysis and time discretization

Frédéric Rousset

(joint work with E. Faou, R. Horsin)

The Vlasov HMF model is the simplest Vlasov type equation. This model has received much interest in the physics literature for many reasons: It is a simple ideal toy model that keeps several features of the long range interactions, it is a simplification of physical systems like charged or gravitational sheet models and it is rather easy to make numerical simulations on it. We refer for example to [1], [11], [2], [5], [6] for more details.

The Vlasov-HMF model reads

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = \partial_x\Big(\int_{\mathbb{R}\times\mathbb{T}} P(x-y) f(t,y,u)\mathrm{d}u\mathrm{d}y\Big)\partial_v f(t,x,v), \tag{1}$$

where $(x,v) \in \mathcal{T} \times \mathbb{R}$ and the kernel $P(x)$ is given by $P(x) = \cos(x)$. Note that the main difference with other nonlinear Vlasov equations like the Vlasov-Poisson equation is the regularity of the kernel: in this latter case, $P(x) = \sum_{k\geq 0} k^{-2}\cos(kx)$ is the kernel associated with the inverse of the Laplace operator. The HMF model is thus the simplest nonlinear model with the structure (1). We consider initial data under the form $f_0(x,v) = \varepsilon r_0(x,v)$ where ε is a small parameter and r_0 is of size one (in a suitable functional space).

$$f(t,x,v) = \varepsilon r(t,x,v).$$

Our aim is to describe the large time behavior of f (or r) for ε sufficiently small. To achieve that, it is convenient to first filter out the effect of the free transport and to study "the profile" of the solution as it also widely done in the study of dispersive equations. We thus set $g(t,x,v) = r(t,x+tv,v)$, so that g solves

$$\partial_t g = \varepsilon\{\phi(t,g), g\}.$$

where

$$\phi(t,g)(x,v) = \int_{\mathbb{R}\times\mathbb{T}} (\cos(x-y+t(v-u)))g(t,y,u)\mathrm{d}u\mathrm{d}y$$

and $\{f,g\} = \partial_x f \partial_v g - \partial_v f \partial_x g$ is the usual microcanonical Poisson bracket. We shall usually write $\phi(t)$ when the dependence in g is clear.

Let us also define the weighted Sobolev norm

$$\|f\|^2_{\mathcal{H}^n} = \sum_{|p|+|q|\leqslant n} \int_{\mathcal{T}\times\mathbb{R}} (1+|v|^2)^{m_0} |\partial_x^p \partial_v^q f|^2 \mathrm{d}x\mathrm{d}v,$$

and denote by $\mathcal{H}^n$ the corresponding function space. Let us finally define for every $s \geq 4$ and $T \geq 0$ the weighted norm

$$Q_{T,s}(g) = \sup_{t\in[0,T]} \frac{\|g(t)\|_{\mathcal{H}^s}}{\langle t\rangle^3} + \sup_{t\in[0,T]} \sup_{k\in\{\pm 1\}} \langle t\rangle^{s-1} |\zeta_k(t)| + \sup_{t\in[0,T]} \|g(t)\|_{\mathcal{H}^{s-4}}$$

where

$$\zeta_k(t) = \hat{g}_k(t,kt), \quad k \in \{\pm 1\}.$$

The result obtained in [8] is that

Theorem 7. *Let us fix $s \geq 7$ and $R_0 > 0$ such that $Q_{0,s}(g) \leq R_0$. Then there exists $R > 0$ and $\varepsilon_0 > 0$ such that for every $\varepsilon \in (0,\varepsilon_0]$ and for every $T \geq 0$, we have the estimate*

$$Q_{T,s}(g) \leq R.$$

As a consequence of this result, we easily obtain that there exists $g^\infty(x,v) \in \mathcal{H}^{s-4}$ such that for all $r \leq s-4$ and $r \geq 1$,

$$\forall\, t \geq 0, \quad \|g(t,x,v) - g^\infty(x,v)\|_{\mathcal{H}^r} \leq \frac{C}{\langle t\rangle^{s-r-3}}.$$

Going back to the original coordinates, we also easily deduce that f converges weakly when t tends to $+\infty$ to

$$\eta^\infty(v) := \frac{\varepsilon}{2\pi} \int_{\mathcal{T}} g^\infty(x,v)\mathrm{d}x.$$

It is actually shown in [8] that the same result actually holds true in the vicinity of any homogeneous stationary solution $\eta(v)$ that satisfies a stability condition (the well-known Penrose stability condition in plasmas physics).

Analogous results for the Vlasov Poisson system were previously obtained by Mouhot and Villani [10] and by Bedrossian-Masmoudi-Mouhot [4]. Nevertheless, for the Vlasov Poisson system, the results require analytic or Gevrey regularity of the data. It was shown by Lin and Zeng [9] that Landau damping cannot hold with too rough regularity (H^s for $s < 3/2$ for example). Their construction is valid for both Vlasov-Poisson and Vlasov-HMF. It is still not known if Landau damping would hold for Vlasov-Poisson at higher Sobolev regularity (though some formal computations in [10] suggests that the Gevrey-3 regularity could be optimal). The main feature of the Vlasov-HMF model in this analysis is that the nonlinearity turns out to be non resonant.

In order to design numerical schemes that captures the long time behavior of the Vlasov equation, it is then natural to ask that the solution of the scheme also satisfies some kind of Landau damping. In [7], we have studied the time discretization of (1) by splitting methods. We split the equation between the free part

$$\partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0, \quad f(0,x,v) = f^0(x,v),$$

whose solution is given explicitely by $\varphi_T^t(f^0)(x,v) := f^0(x - tv, v)$, and the potential part

$$\partial_t f(t,x,v) = \partial_x \Big(\int_{\mathbb{R}\times\mathbb{T}} P(x-y) f(t,y,u) \mathrm{d}u\mathrm{d}y \Big) \partial_v f(t,x,v), \quad f(0,x,v) = f^0(x,v),$$

whose solution is explicitely given by

$$\varphi_P^t(f^0) = f^0(x, v + tE(f^0,x)),$$

where $E(f,x) = \partial_x \Big(\int_{\mathbb{R}\times\mathbb{T}} P(x-y) f(y,u) \mathrm{d}u\mathrm{d}y \Big)$ is indeed constant in time.

The Lie splittings is for example given by the formula

$$f^{n+1} = \varphi_P^h \circ \varphi_T^h(f^n),$$

and the Strang splitting by the formula

$$f^{n+1} = \varphi_T^{h/2} \circ \varphi_P^h \circ \varphi_T^{h/2}(f^n)$$

where $h > 0$ is the time step. The same results hold for the symmetric splittings where the roles of T and P are swapped.

We can then define the sequence of function $r^n(x,v)$ by the formula

$$f^n(x,v) = \varepsilon r^n(x,v), \quad g^n(x,v) = r^n(x + nhv, v).$$

In [7], we have proven the Landau damping for these splitting schemes, in the sense that there exists $g_h^\infty(x,v)$ such that if ε and h are sufficiently small, there exists $C > 0$ such that

$$\forall\, n \geq 0, \quad \|g^n(x,v) - g_h^\infty(x,v)\|_{\mathcal{H}^r} \leq \frac{C}{\langle nh \rangle^{s-r-3}}.$$

This allows to prove that for example for the Strang splitting, the scheme is of order two globally in time: we have that for h and ε sufficiently small, there exists $C > 0$ such that

$$\|g^n(x,v) - g(nh,x,v)\|_{\mathcal{H}^r} \leq Ch^2 \quad \forall n \in \mathbb{N}.$$

References

[1] J. Barré, F. Bouchet, T. Dauxois, S. Ruffo and Y. Yamaguchi, *The Vlasov equation and the Hamiltonian Mean-Field model*, Physica A 365, 177, 2005;

[2] J. Barré, A. Olivetti and Y.Y. Yamaguchi, *Algebraic damping in the one-dimensional Vlasov equation*, J. Phys. A 44, 405502 (2011)

[3] J. Barré, Y. Y Yamaguchi, *On the neighborhood of an inhomogeneous stable stationary solution of the Vlasov equation - Case of the Hamiltonian mean-field model*, preprint, 2013.arXiv:1311.3182

[4] J. Bedrossian, N. Masmoudi and C. Mouhot, *Landau damping: paraproducts and Gevrey regularity*, preprint 2013, arXiv:1311.2870;

[5] E. Caglioti, F. Rousset, *Long time estimates in the mean field limit.* Arch. Ration. Mech. Anal. 190 (2008), no. 3, 517–547;

[6] E. Caglioti, F. Rousset, *Quasi-stationary states for particle systems in the mean-field limit.* J. Stat. Phys. 129 (2007), no. 2, 241–263;

[7] On numerical Landau damping for splitting methods applied to the Vlasov-HMF model, http://arxiv.org/abs/1510.06555;

[8] E. Faou, F. Rousset, *Landau damping in Sobolev spaces for the Vlasov HMF model* Arch. Ration. Mech. Anal. 219 (2016), no. 2, 887–902;

[9] Zhiwu Lin and Chongchun Zeng, *Small BGK waves and nonlinear Landau damping,* Comm. Math. Phys., 306, 291-331 (2011).

[10] C. Mouhot, C. Villani, *On Landau damping.* Acta Math. 207 (2011), no. 1, 29–201;

[11] Y. Yamaguchi, J. Barré, F. Bouchet, T. Dauxois and S. Ruffo, *Stability criteria of the Vlasov equation and quasi stationary states of the HMF model*, Physica A 337, 36, 2004;

Word-series analysis of splitting stochastic integrators

J.M. Sanz-Serna

(joint work with A. Álamo)

The importance of splitting integrators has been increasing steadily in the recent decades. Their flexibility in treating the different terms (diffusion, reaction, advection, ...) that may be present in a partial differential equation and their capability of keeping geometric properties are among the reasons for their popularity. Typically splitting algorithms are analysed in a way that is different from that used for standard integrators like Runge-Kutta schemes. In fact, the common approach starts by writing each flow being composed as the exponential of an operator; then the various exponentials are combined into a single one by means of the Baker-Campbell-Hausdorff (BCH) formula. In this way one really obtains the expansion in powers of the step-size Δt of the *modified equation*, which is different from the situation for standard integrators, where one expands the *map* $\psi_{\Delta t}$ that sends the approximation x_n at the current step into the next: $x_{n+1} = \psi_{\Delta t}(x_n)$. In (1999), A. Murua and myself [1] suggested a B-series technique to expand the map $\psi_{\Delta t}$; that approach does not invoke the BCH formula, whose combinatorial intricacies

are known to be very high. Recently *word series* [2] have been put forward as an alternative to B-series. The scope of applicability of word series is much narrower than that of B-series [3]; however, when applicable, word series are more easily handled than B-series. Word series, as B-series, have an application range that exceeds numerical mathematics; they may be used to perform averaging, to reduce discrete or dynamical systems to normal form, etc. The interested reader is referred to my web page `http://www.sanzserna.org/` for relevant publications.

In the talk I reported work in progress by Alfonso Álamo (Ph.D. student at Valladolid) and myself on the use of word series to analyse splitting integrators for stochastic differential equations. While both the Ito and Stratonovich interpretation have been treated by us, my oral presentation focused on the simpler Stratonovich case and considered strong and weak local errors. I showed the power of the new approach by analysing in detail two integrators for the Langevin dynamics that, while possessing very similar formulations, show widely different practical performances. The new technique may also be applied advantageously to derive modified equations, to find invariant densities, etc.

References

[1] A. Murua and J.M. Sanz-Serna, *Order conditions for numerical integrators obtained by composing simpler integrators*, Phil. Trans. R. Soc. Lond. A **357** (1999), 1079–1100.

[2] A. Murua and J.M. Sanz-Serna, *Word series for dynamical systems and their numerical integrators* (arXiv:1502.05528), Foundations of Computational Mathematics, to appear, DOI 10.1007/s10208-015-9295-3

[3] J.M. Sanz-Serna and A. Murua, *Formal series and numerical integrators: some history and some new techniques* (arXiv: 1503.06976), in Proceedings of the 8th International Congress on Industrial and Applied Mathematics (ICIAM 2015), Lei Guo and Zhi-Ming eds., Higher Education, Press, Beijing, 2015, 311-331.

Derivation of a low regularity exponential-type integrator for semilinear Schrödinger equations with polynomial nonlinearities

Katharina Schratz

(joint work with Alexander Ostermann)

Splitting methods as well as classical exponential integration schemes for semilinear Schrödinger equations of type

$$i\partial_t u(t,\mathbf{x}) = -\Delta u(t,\mathbf{x}) + \mu\,|u(t,\mathbf{x})|^{2p}\,u(t,\mathbf{x}), \quad (t,\mathbf{x}) \in \mathbb{R}\times\mathbb{T}^d, \quad p\in\mathbb{N}, \quad \mu\in\mathbb{R}$$

are extensively studied in the literature. As part of the construction of these numerical methods the *stiff part* (i.e., the terms involving the differential operator $i\Delta$) is differently approximated. However, for both method classes first-order convergence in H^s requires solutions in H^{s+2}, see for instance [1, 2]. Recently, the low regularity exponential-type integrator

$$u^{n+1} = \mathrm{e}^{i\tau\Delta}\left[u^n - i\mu\tau\big(u^n\big)^{p+1}\,\varphi_1(-2i\tau\Delta)\big(\big(\overline{u^n}\big)^p\big)\right] \tag{1}$$

was introduced in [3]. Here u^n is an approximation to the exact solution u at time $t_n = n\tau$, and φ_1 denotes the entire function

$$\varphi_1(z) = \frac{\mathrm{e}^z - 1}{z}.$$

Compared to classical splitting and exponential integration schemes this exponential-type integrator allows less regular solutions. More precisely, its first-order convergence holds in H^s for solutions in H^{s+1} for $s > d/2$.

In [3] the exponential-type integrator (1) was only explicitly derived for cubic nonlinearities ($p = 1$). Here we give a detailed derivation for general nonlinearities $p \in \mathbb{N}$. Henceforth, we will use the notation

$$\begin{aligned} K = (\mathbf{k}_1, \ldots, \mathbf{k}_{p+1}), \quad \mathbf{k}_j = (k_{j1}, \ldots, k_{jd}) \in \mathbb{Z}^d, \\ L = (\boldsymbol{\ell}_1, \ldots, \boldsymbol{\ell}_p), \quad \boldsymbol{\ell}_j = (\ell_{j1}, \ldots, \ell_{jd}) \in \mathbb{Z}^d, \\ \mathbf{k} \cdot \mathbf{x} = k_1 x_1 + \ldots + k_d x_d, \quad \mathbf{k}^2 = \mathbf{k} \cdot \mathbf{k} \quad \text{for } \mathbf{k}, \mathbf{x} \in \mathbb{R}^d. \end{aligned}$$

The construction of (1) is based on iterating Duhamel's formula in the *twisted* variable $v(t) = \mathrm{e}^{-it\Delta}u(t)$. Note that the twisted variable satisfies

$$\begin{aligned} v(t_n + \tau) &= v(t_n) \\ &\quad - i\mu \int_0^\tau \mathrm{e}^{-i(t_n+s)\Delta} \Big[\big| \mathrm{e}^{i(t_n+s)\Delta} v(t_n + s) \big|^{2p} \mathrm{e}^{i(t_n+s)\Delta} v(t_n + s) \Big] \mathrm{d}s. \end{aligned} \tag{2}$$

Thus, for $r > d/2$ the following bound holds in the H^r norm:

$$\begin{aligned} \|v(t_n + s) - v(t_n)\|_r &\le |\mu| \int_0^s \|v(t_n + \xi)\|_r^{2p+1} \mathrm{d}\xi \\ &\le s|\mu| \sup_{0 \le \xi \le s} \|v(t_n + \xi)\|_r^{2p+1}. \end{aligned}$$

In this sense we have for $|s| \le \tau$

$$v(t_n + s) \approx v(t_n) \tag{3}$$

for a small time step τ. Inserting (3) into (2) yields the approximation

$$v(t_n + \tau) \approx v(t_n) - i\mu \int_0^\tau \mathrm{e}^{-i(t_n+s)\Delta} \Big[\big| \mathrm{e}^{i(t_n+s)\Delta} v(t_n) \big|^{2p} \mathrm{e}^{i(t_n+s)\Delta} v(t_n) \Big] \mathrm{d}s \tag{4}$$

which is the basis of our numerical scheme. We are left with deriving a numerical approximation to

$$I_p^\tau(w, t_n) = \int_0^\tau \mathrm{e}^{-i(t_n+s)\Delta} \Big[\big| \mathrm{e}^{i(t_n+s)\Delta} w \big|^{2p} \mathrm{e}^{i(t_n+s)\Delta} w \Big] \mathrm{d}s.$$

With the aid of the Fourier expansion we obtain the representation

$$\begin{aligned} I_p^\tau(w, t_n) = \sum_{\substack{\mathbf{k}_1, \ldots, \mathbf{k}_{p+1} \in \mathbb{Z}^d \\ \boldsymbol{\ell}_1, \ldots, \boldsymbol{\ell}_p \in \mathbb{Z}^d}} & \hat{w}_{\mathbf{k}_1} \ldots \hat{w}_{\mathbf{k}_{p+1}} \overline{\hat{w}_{\boldsymbol{\ell}_1}} \ldots \overline{\hat{w}_{\boldsymbol{\ell}_p}} \\ & \times \mathrm{e}^{-i\left(\sum_{j=1}^{p+1} \mathbf{k}_j + \sum_{j=1}^{p} \boldsymbol{\ell}_j \right) \cdot \mathbf{x}} \int_0^\tau \mathrm{e}^{i(t_n+s)\Omega_p(K,L)} \mathrm{d}s, \end{aligned} \tag{5}$$

where we have set

$$\Omega_p(K,L) = \Big(\sum_{j=1}^{p+1} \mathbf{k}_j - \sum_{j=1}^{p} \boldsymbol{\ell}_j\Big)^2 - \sum_{j=1}^{p+1} \mathbf{k}_j^2 + \sum_{j=1}^{p} \boldsymbol{\ell}_j^2.$$

Next we split Ω_p into pure and mixed quadratic terms. Note that

$$\begin{aligned}\Omega_p(K,L) = 2\sum_{j=1}^{p} \boldsymbol{\ell}_j^2 + \sum_{\alpha=1}^{p+1} \mathbf{k}_\alpha \Big(\sum_{\nu\neq\alpha} \mathbf{k}_\nu\Big) \\ - 2\Big(\sum_{\alpha=1}^{p+1} \mathbf{k}_\alpha\Big)\Big(\sum_{\beta=1}^{p} \boldsymbol{\ell}_\beta\Big) + \sum_{\beta=1}^{p} \boldsymbol{\ell}_\beta \Big(\sum_{\nu\neq\beta} \boldsymbol{\ell}_\nu\Big).\end{aligned}$$

Furthermore,

$$\sum_{j=1}^{p} \boldsymbol{\ell}_j^2 = \Big(\sum_{j=1}^{p} \boldsymbol{\ell}_j\Big)^2 - \sum_{\beta=1}^{p} \boldsymbol{\ell}_\beta \Big(\sum_{\nu\neq\beta} \boldsymbol{\ell}_\nu\Big).$$

This yields that

$$\Omega_p(K,L) = 2\Big(\sum_{j=1}^{p} \boldsymbol{\ell}_j\Big)^2 + R_p(K,L)$$

with the remainder term

$$\begin{aligned}R_p(K,L) = \sum_{\alpha=1}^{p+1} \mathbf{k}_\alpha \Big(\sum_{\nu\neq\alpha} \mathbf{k}_\nu\Big) - 2\Big(\sum_{\alpha=1}^{p+1} \mathbf{k}_\alpha\Big)\Big(\sum_{\beta=1}^{p} \boldsymbol{\ell}_\beta\Big) \\ - \sum_{\beta=1}^{p} \boldsymbol{\ell}_\beta \Big(\sum_{\nu\neq\beta} \boldsymbol{\ell}_\nu\Big)\end{aligned}$$

consisting of mixed quadratic terms only. In order to obtain an *efficient and practical* low regularity implementation we only

$$\text{treat the } \textit{dominant} \text{ quadratic term } 2\Big(\sum_{j=1}^{p} \boldsymbol{\ell}_j\Big)^2 \text{ in } \Omega_p \text{ exactly.}$$

This yields for $0 \le \gamma \le 1$ the approximation

$$\begin{aligned}&\int_0^\tau \mathrm{e}^{i(t_n+s)\Omega_p(K,L)}\mathrm{d}s \\ &\quad= \mathrm{e}^{it_n\Omega_p(K,L)} \int_0^\tau \mathrm{e}^{2is\left(\sum_{j=1}^{p} \boldsymbol{\ell}_j\right)^2}\Big(1 + \mathcal{O}(s^\gamma R_p(K,L)^\gamma)\Big)\mathrm{d}s \\ &\quad= \mathrm{e}^{it_n\Omega_p(K,L)}\ \varphi_1\Big(2i\tau\Big(\sum_{j=1}^{p} \boldsymbol{\ell}_j\Big)^2\Big) + \mathcal{O}(\tau^{1+\gamma} R_p(K,L)^\gamma).\end{aligned} \tag{6}$$

Plugging (6) into (5) shows that

$$I_p^\tau(w,t_n) = \Psi_p^\tau(w,t_n) + \mathcal{R}_p^\tau(w,t_n),$$

where

$$\Psi_p^\tau(w,t_n) = \tau \mathrm{e}^{-it_n\Delta}\Big[\big(\mathrm{e}^{it_n\Delta}w\big)^{p+1}\ \varphi_1(-2\tau i\Delta)\big((\mathrm{e}^{-it_n\Delta}\overline{w})^p\big)\Big]$$

is the sought-after approximation. The remainder $\mathcal{R}_p^\tau$ satisfies the bound

$$\|\mathcal{R}_p^\tau(w,t_n)\|_r \le c\tau^{1+\gamma}\|w\|_{r+\gamma}^{2p+1} \quad \text{for} \quad 0 \le \gamma \le 1, \quad r > d/2.$$

Inserting the approximation $\Psi_p^\tau(v^n,t_n)$ into (4) with $v(t_n)$ replaced by v^n, and twisting the solution back again, i.e., setting

$$u^n = \mathrm{e}^{it_n\Delta}v^n$$

finally yields the scheme (1). For a rigorous error analysis of that scheme in dimensions $d \ge 1$ we refer to [3].

References

[1] M. Hochbruck, A. Ostermann, *Exponential integrators*, Acta Numer. **19** (2010), 209–286.
[2] C. Lubich, *On splitting methods for Schrödinger–Poisson and cubic nonlinear Schrödinger equations*, Math. Comp. **77** (2008), 2141–2153.
[3] A. Ostermann, K. Schratz, *Low regularity exponential-type integrators for semilinear Schrödinger equations in the energy space*, Preprint, http://arxiv.org/abs/1603.07746 (2016)

Geometric asymptotic reduction: the gyrokinetic model for magnetic fusion plasmas

Eric Sonnendrücker

Magnetic confinement thermonuclear fusion research investigates the possibility of gaining energy by confining a Deuterium and Tritium plasma (*i.e.* gas of charged particles) at a high temperature and density for a long enough time, such that energy produced by fusion reactions positively balances the initial energy input. One of the major obstacles is the turbulent transport of particles and energy out of the plasma that needs to be reduced. The adequate model for studying this process would be the Vlasov-Maxwell system. However due to the large confining magnetic field this model can be further reduced into the so-called gyrokinetic model.

The gyrokinetic reduction of the Vlasov-Maxwell equations consists in a sequence of changes of variables aiming at removing the fast angular variable representing the rotation of the particles around the magnetic field lines. This has the advantage for numerical simulations of reducing the phase space dimension by one variable and also of removing the fast gyration time scale. There are two natural formulations: one called the symplectic formulation is based on the parallel velocity and the other is based on the canonical parallel momentum and called hamiltonian [1]. Both have major drawbacks for a numerical Particle In Cell simulations, which are enhanced for MHD modes. The symplectic formulation contains $\partial_t A$ terms in the equations of motion of the gyrocenters, which necessitates an implicit discretisation for stability and the hamiltonian formulation introduces a large skin term in the parallel Ampere equation, which cancels with the large adiabatic part of the current computed as a Monte Carlo estimate, which is noisy. This needs a very well tuned control variate for a sufficiently accurate computation [2]. An alternative approach, based on a new variable intermediate between the canonical parallel momentum and velocity has been introduced recently in [3, 4]. This can be interpreted as a integrating factor method, for the integration of the gyrocenter equations of motion of either the symplectic or the hamiltonian formulation and enables to get rid of the numerical issues of either of the original formulations. This simple algorithm enables to take a much larger time step in all cases and larger by more than an order of magnitude for MHD modes [5]. The so-called mixed formulation can be directly derived from the original electromagnetic particle Lagrangian using Lie transforms as the original gyrokinetic equations and cast

in a field theoretic Lagrangian of the same form as the one obtained in [6]. This enables in particular to derive an exact conserved energy and total canonical angular momentum using a Noether theorem. Moreover by directly discretising the field theoretic Lagrangian using a Monte-Carlo approach for the Vlasov term and a Finite Element approach for the field terms, we get a discrete Lagrangian, be it with a large number of degrees of freedom, which itself generates exact conserved quantities at the semi-discrete level. The corresponding Euler-Lagrangian equations have a Poisson structure, which can be used for the following time discretisation.

References

[1] A.J. Brizard, T.S. Hahm, *Foundations of nonlinear gyrokinetic theory*, Reviews of modern physics **79**, 421 (2007)

[2] R. Hatzky, A. Könies, A. Mishchenko, *Electromagnetic gyrokinetic PIC simulation with an adjustable control variates method*, J. Comput. Phys. **225**, 568 (2007)

[3] A. Mishchenko, M. Cole, R. Kleiber, A. Könies, *New variables for gyrokinetic electromagnetic simulations*, Phys. Plasmas **21** (5), 052113 (2014)

[4] A. Mishchenko, A. Könies, R. Kleiber, M. Cole, *Pullback transformation in gyrokinetic electromagnetic simulations*, Phys. Plasmas **21** (5), 092110 (2014)

[5] R. Kleiber, R. Hatzky, A. Könies, A. Mishchenko, and E. Sonnendrücker, *An explicit large time step particle-in-cell scheme for nonlinear gyrokinetic simulations in the electromagnetic regime*, Physics of Plasma, to appear (2016)

[6] H. Sugama, *Gyrokinetic field theory*, Phys. Plasmas **7**, 466 (2000)

What is integrability of (discrete) variational systems?

Yuri B. Suris

We propose a notion of a pluri-Lagrangian problem [3, 2, 7], which should be understood as an analog of multi-dimensional consistency [1] for variational systems. This is a development along the line of research of discrete integrable Lagrangian systems initiated Lobb and Nijhoff [5], however having its more remote roots in the theory of pluriharmonic functions, in the Z-invariant models of statistical mechanics and their quasiclassical limit, as well as in the theory of variational symmetries going back to Noether. A d-dimensional pluri-Lagrangian problem can be described as follows:

Given a d-form $\mathcal{L}$ on an m-dimensional space $\mathbb{R}^m$ or $\mathbb{Z}^m$ (called multi-time, with $m > d$), whose coefficients depend on a function x of m independent variables (called field), find those fields x which deliver critical points to the action functionals $S_\Sigma = \int_\Sigma \mathcal{L}$ for any *d-dimensional manifold Σ in the multi-time.*

Let us illustrate this definition by the case of discrete-time Lagrangian mechanics, $d = 1$ (cf. [6]). Consider a 1-parameter family of pairwise commuting symplectic maps $F_\lambda : T^*M \to T^*M$, $F_\lambda(q,p) = (\widetilde{q},\widetilde{p})$, possessing generating (Lagrange) functions $L(q,\widetilde{q};\lambda)$, so that

$$F_\lambda : \; p = -\frac{\partial L\,(q,\widetilde{q};\lambda)}{\partial q}, \quad \widetilde{p} = \frac{\partial L\,(q,\widetilde{q};\lambda)}{\partial \widetilde{q}}.$$

The commutativity of the corresponding m maps allows us to define, for any $(q_0, p_0) \in T^*M$, the function $(q, p) : \mathbb{Z}^m \to T^*M$ by setting

$$(q(n + e_i), p(n + e_i)) = F_{\lambda_i}\big(q(n), p(n)\big), \quad n \in \mathbb{Z}^m, \quad 1 \le i \le m.$$

We will abbreviate $(q, p) = (q(n), p(n))$, $(q_i, p_i) = (q(n + e_i), p(n + e_i))$, and $(q_{-i}, p_{-i}) = (q(n - e_i), p(n - e_i))$ for a general $n \in \mathbb{Z}^m$ and for any $1 \le i \le m$. The following *2D corner equations* hold true everywhere on $\mathbb{Z}^m$:

$$\frac{\partial L(q, q_i; \lambda_i)}{\partial q} - \frac{\partial L(q, q_j; \lambda_j)}{\partial q} = 0, \quad \frac{\partial L(q_{-i}, q; \lambda_i)}{\partial q} + \frac{\partial L(q, q_j; \lambda_j)}{\partial q} = 0,$$

$$\frac{\partial L(q_{-i}, q; \lambda_i)}{\partial q} - \frac{\partial L(q_{-j}, q; \lambda_j)}{\partial q} = 0.$$

Introduce a *discrete 1-form* $\mathcal{L}$ on $\mathbb{Z}^m$ by setting $\mathcal{L}(n, n + e_i) = L(q, q_i; \lambda_i)$. Then the 2D corner equations tell us that any solution $q : \mathbb{Z}^m \to M$ delivers a critical point to the action functional

$$S_\Gamma = \sum_{\mathfrak{e} \in \Gamma} \mathcal{L}(\mathfrak{e})$$

for any directed path Γ in $\mathbb{Z}^m$ (concatenation of directed edges $\mathfrak{e}$) under variations that fix the fields at the endpoints of the path Γ. In other words, the field $q : \mathbb{Z}^m \to M$ solves the *pluri-Lagrangian problem* for the Lagrangian 1-form $\mathcal{L}$.

Theorem. *The value of the exterior derivative* $d\mathcal{L}$ *on any elementary square* $\sigma_{ij} := (n, n + e_i, n + e_i + e_j, n + e_j)$ *is constant on solutions of the system of 2D corner equations:*

$$d\mathcal{L}(\sigma_{ij}) := L(q, q_i; \lambda_i) + L(q_i, q_{ij}; \lambda_j) - L(q_j, q_{ij}; \lambda_i) - L(q, q_j; \lambda_j) = c(\lambda_i, \lambda_j).$$

Theorem. *The pluri-Lagrangian 1-form* $\mathcal{L}$ *is closed on solutions,* $d\mathcal{L} = c(\lambda, \mu) = 0$*, if and only if* $\partial L(q, \widetilde{q}; \lambda)/\partial\lambda$ *is a common integral of motion for all* F_μ*.*

The latter theorem clarifies the meaning of the mysterious "spectrality property" discovered by Kuznetsov and Sklyanin [4] for Bäcklund transformations.

Similarly, in the case $d = 2$, one starts with a discrete 2-form, that is, a real-valued function $\mathcal{L}$ of oriented elementary squares $\sigma_{ij} = (n, n+e_i, n+e_i+e_j, n+e_j)$ of $\mathbb{Z}^m$, such that $\mathcal{L}(\sigma_{ij}) = -\mathcal{L}(\sigma_{ji})$. We will assume that $\mathcal{L}$ depends on some field $x : \mathbb{Z}^m \to \mathcal{X}$ ($\mathcal{X}$ being some vector space), more precisely, $\mathcal{L}(\sigma_{ij}) = L(x, x_i, x_j, x_{ij})$ depends on the values of x at the four vertices of σ_{ij}. To an arbitrary oriented quad-surface Σ in $\mathbb{Z}^m$, there corresponds the *action functional*

$$S_\Sigma = \sum_{\sigma \in \Sigma} \mathcal{L}(\sigma).$$

We derive the main building blocks of the multi-time Euler-Lagrange equations for a discrete pluri-Lagrangian problem with $d = 2$, the so called 3D corner equations. These are discrete Euler-Lagrange equations for all possible 3D corners in $\mathbb{Z}^m$, which are quad-surfaces consisting of three elementary squares adjacent to a vertex

of valence 3. Denote the discrete exterior derivative $d\mathcal{L}$ evaluated on an oriented elementary cube σ_{ijk} of the coordinate directions i, j, k by

$$S^{ijk} = d\mathcal{L}(\sigma_{ijk}) = \Delta_k \mathcal{L}(\sigma_{ij}) + \Delta_i \mathcal{L}(\sigma_{jk}) + \Delta_j \mathcal{L}(\sigma_{ki}).$$

The system of 3D corner equations consists of the equations

$$\frac{\partial S^{ijk}}{\partial x} = 0, \quad \frac{\partial S^{ijk}}{\partial x_i} = 0, \quad \frac{\partial S^{ijk}}{\partial x_j} = 0, \quad \frac{\partial S^{ijk}}{\partial x_k} = 0,$$

$$\frac{\partial S^{ijk}}{\partial x_{ij}} = 0, \quad \frac{\partial S^{ijk}}{\partial x_{jk}} = 0, \quad \frac{\partial S^{ijk}}{\partial x_{ik}} = 0, \quad \frac{\partial S^{ijk}}{\partial x_{ijk}} = 0,$$

for each triple i, j, k. Symbolically, $\delta(d\mathcal{L}) = 0$, where δ stands for the "vertical" differential (differential with respect to the dependent field variables x).

The system of 3D corner equations encompasses all possible discrete Euler-Lagrange equations for all possible quad-surfaces. This is a direct consequence of the following fundamental geometric fact: *the vertex star of any interior vertex of an oriented quad-surface in $\mathbb{Z}^m$ can be represented as a sum of (oriented) 3D corners in $\mathbb{Z}^{m+1}$*. Observe that the "almost closedness" of the 2-form $\mathcal{L}$ on solutions of the system of 3D corner equations is built-in from the outset.

Theorem. *For any triple of the coordinate directions i, j, k, the exterior derivative of $\mathcal{L}$ over an elementary cube of these coordinate directions is constant on solutions of the system of 3D corner equations:*

$$d\mathcal{L}(\sigma_{ijk}) = c^{ijk} = \text{const} \quad (\text{mod } \partial S^{ijk}/\partial x = 0, \ \ldots, \ \partial S^{ijk}/\partial x_{ijk} = 0).$$

We analyze the system of 3D corner equations for a special class of *three-point 2-forms*, corresponding to integrable quad-equations of the ABS list [1]:

$$\mathcal{L}(\sigma_{ij}) = L(x, x_i; \alpha_i) - L(x, x_j; \alpha_j) - \Lambda(x_i, x_j; \alpha_i, \alpha_j).$$

Of course, the function Λ should satisfy $\Lambda(x, y; \alpha, \beta) = -\Lambda(y, x; \beta, \alpha)$ to ensure the skew-symmetry property $\mathcal{L}(\sigma_{ji}) = -\mathcal{L}(\sigma_{ij})$. The system of 3D corner equations for such a 2-form $\mathcal{L}$ consists of six equations for each elementary cube: for the vertices x and x_{ijk} there are no equations, while for the vertices x_i, resp. x_{ij} we have the following *four-leg, five-point equations*:

$$\psi(x_i, x_{ij}; \alpha_j) - \psi(x_i, x_{ik}; \alpha_k) - \phi(x_i, x_k; \alpha_i, \alpha_k) + \phi(x_i, x_j; \alpha_i, \alpha_j) = 0,$$
$$\psi(x_{ij}, x_i; \alpha_j) - \psi(x_{ij}, x_j; \alpha_i) - \phi(x_{ij}, x_{ik}; \alpha_j, \alpha_k) + \phi(x_{ij}, x_{jk}; \alpha_i, \alpha_k) = 0.$$

Here, we introduced the notation

$$\psi(x, y; \alpha) = \partial L(x, y; \alpha)/\partial x, \quad \phi(x, y; \alpha, \beta) = \partial \Lambda(x, y; \alpha, \beta)/\partial x.$$

Theorem. *For the discrete 2-forms $\mathcal{L}$ for quad-equations of the ABS list, the corresponding systems of 3D corner equations are consistent, as well. Moreover, the 2-form $\mathcal{L}$ is closed on solutions of the 3D corner equations.*

This closes a conceptual gap left in the work [5] by showing that the corresponding 2-forms are closed not only on solutions of (non-variational) quad-equations, but also on general solutions of the corresponding Euler-Lagrange equations.

Theorem. *If the three-point discrete 2-form $\mathcal{L}$ is closed on solutions of the system of 3D corner equations, then the latter system admits the parameter dependent family of conservation laws*

$$\Delta_j P_{ik} = \Delta_k P_{ij},$$

with the densities

$$P_{ij} = \frac{\partial L(x, x_i; \alpha_i)}{\partial \alpha_i} - \frac{\partial \Lambda(x_i, x_{ij}; \alpha_i, \alpha_j)}{\partial \alpha_i}.$$

References

[1] V.E. Adler, A.I. Bobenko, and Yu.B. Suris, *Classification of integrable equations on quad-graphs. The consistency approach*, Comm. Math. Phys., **233** (2003), 513–543.

[2] A.I. Bobenko, Yu.B. Suris. *Discrete pluriharmonic functions as solutions of linear pluri-Lagrangian systems*, Commun. Math. Phys. **336** (2015) 199–215.

[3] R. Boll, M. Petrera, Yu.B. Suris. *What is integrability of discrete variational systems?* Proc. Royal Soc. A, **470** (2014), No. 2162, 20130550, 15 pp.

[4] V.B. Kuznetsov, E.K. Sklyanin, *On Bäcklund transformations for many-body systems*, J. Phys. A: Math. Gen. **31** (1998), 2241–2251.

[5] S. Lobb, F.W. Nijhoff, *Lagrangian multiforms and multidimensional consistency*, J. Phys. A: Math. Theor., **42** (2009), no. 454013.

[6] Yu.B. Suris. *Variational formulation of commuting Hamiltonian flows: multi-time Lagrangian 1-forms*, J. Geom. Mechanics, **5** (2013) 365–379.

[7] Yu.B. Suris, M. Vermeeren. *On the Lagrangian structure of integrable hierarchies*, `arXiv:1510.03724 [math-ph]`.

Parareal-like multiscale coupling schemes

Richard Tsai

In multiscale computations, one typically is interested in computing efficiently an effective system that can be derived from the given full system whose solutions have a wide range of length scales. The need for doing so comes from the daunting computational complexity for resolving the length scales that are very small compared to the required size of computational domain. For systems that have sufficiently wide separation of scales, the effective systems may be computed by appropriately averaging the operators and the solutions of the full systems. This is the typical setup for numerical homogenizations.

As multiscale computations for more classical settings have reached a mature stage, it is now necessary to develop new strategies addressing some of the core problems of scientific computing for the coming era that require leaving the contexts considered previously. We would like to tackle problems in which ***(i) wide range of scales are present in the entire time domain of interest; or (ii) intermittencies occur in the system at times which cannot be determined a priori.***

While an effective macroscopic solution for situation (i) may exist globally, the macroscopic model for (ii) may fail to be valid at localized regions (in space and in time), depending on the states being computed. Both situations require more extensive microscopic simulations in order to compute the effective solutions accurately. The need to deal with intermittency shows up in many challenging problems, ranging from more simple dynamical systems having some oscillatory modes going through resonances, to fluid flows transitioning in and out of turbulence in localized regions. The intermittent features could take place in longer time scales than those typically considered in the more classical setups. In order to compute the non-trivial effective behavior of such systems, it is necessary to consider more extensive and systematic sampling of the dynamical system's phase space. However, computing microscopic simulation in larger domains calls for further reduction of the resulting computational complexity. Without further reduction, the resulting multiscale scheme may not be competitive with even a conventional solver. Parallelization-in-time may offer the needed reduction of computational complexity.

On the other hand, the increase in computing power in recent (and future) computer infrastructures have been relying on increasing the number of parallel processors rather than the clock speed. Computations of the class of highly oscillatory dynamical systems will not benefit from the available exa-scale computing power unless parallelization-in-time can be performed. However, due to causality, parallel-in-time computations have not been as successful as parallel computations in space. Adding to the difficulty, the presence of fast oscillations in the solutions increases the sensitivity of the solvers and makes the approaches involving shooting and Newton's solvers virtually unusable. Even though there have also been active research in developing numerical algorithms that allow massive parallel-in-time computations for solving initial value problems, it is widely recognized that robust and convergent numerical computation using such parallel-in-time algorithms still remains a main challenge.

In this talk, we discuss a fixed point iteration scheme of the form

$$\begin{aligned} v_{n+1}^{k+1} &= \theta C_H v_n^{k+1} + \left(F_H v_n^k - \theta C_H v_n^k\right), \\ v_0^k &= v_0, \end{aligned} \tag{1}$$

for $k = 0, 1, 2, \cdots$, $n = 0, 1, 2, \cdots, N$. Here C_H is the solution operator of step size H for the "coarse" scale initial value problem

$$\frac{d}{dt}u = L(u, u_x, u_{xx}), \;\; u(x, t = 0) = u_0(x), \tag{2}$$

and F_H for

$$\frac{d}{dt}u^\epsilon = L_\epsilon(u^\epsilon, u^\epsilon_x, u^\epsilon_{xx}), \;\; u^\epsilon(x, t = 0) = u_0^\epsilon(x). \tag{3}$$

$F_H v_n^k$ can be computed in parallel in smaller time intervals and will sample all the scales in the full system. The scheme in (1) is derived from:

$$v_{n+1}^{k+1} = \theta C_H v_n^{k+1} + (1-\theta) C_H v_n^k + \left(F_H v_n^k - C_H v_n^k\right).$$

The size of the "corrector" term $F_H v - C_H v$ has great influence to the stability of the scheme.

By studying such type of model problems, we would like to find out: (a) whether the microscopic features in u^ϵ can be *re-introduced* into the macroscopic solutions and thus making up the deficiencies in the macroscopic model; (b) the stability and convergence properties of such coupling; (c) acceleration and improvement through the design of θ.

The focus of this talk is on the role of θ, which can be a real number, a complex number, or an operator which is called a "phase alignment operator" in [1]. We show that for dissipative systems, taking $\theta \in (0, 1)$ may improves the stability of the classical parareal scheme (corresponding to taking $\theta \equiv 1$). We show further that for systems on the complex plane that have imaginary eigenvalues, it may be necessary to take complex valued θ in order to "match" the phases of $F_H v$ and $C_H v$. We demonstrate our theory by a "de-homogenization" example. In the example, we use (1) to couple a standard equation found in parabolic homogenization to its homogenized equation. We show that fine scale details are correctly "put" back to the solutions of (1) after very few iterations in k. We discuss a few challenging highly oscillatory systems, and show that θ has to be further generalized to non-trivial operators in order to be able to match the phases of $F_H v$ and $C_H v$. These examples may be considered a warm up excercises towards the directions that we outline above.

References

[1] G. Ariel, S.-J. Kim, R. Tsai *Parareal methods for highly oscillatory ordinary differential equations*, ArXiv 1503.02094.

Long term rotation of Ceres and Vesta

Timothée Vaillant
(joint work with Jacques Laskar)

The mission of the spacecraft Dawn is to study Ceres and Vesta, the largest asteroids of the main belt. This space probe, which is at present in orbit around Ceres, should allow to test different models of ice distribution on the surface, which depend on the orbit and the rotation.

However, the orbital motion of the two asteroids is chaotic [1]. To study the phenomena, which affect them, we then develop a secular model, which consists to average the general orbital motion on the orbit and describes only the evolution of the orbit. This model allows to identify the different secular frequencies of their orbital motions

To obtain the long term rotation, we can average on the fast rotation motion of these two bodies and obtain a secular rotation model, which only describes the evolution of the angular momentum. Two secular rotation models exist: a scalar model and a vectorial model. The hamiltonian of the scalar model [2, 3, 4] allows to obtain the secular evolution of the Andoyer canonical variables, which

locates the body in the space. The long term rotation is then forced by the secular orbital motion. The hamiltonian of the vectorial model [5, 6] describes the secular evolution of the angular momentum whether or not it is forced by the general or secular orbital motion. This model can then allow to observe the interaction between the orbital and secular motions.

We observe that these two models give identical results for the long term evolution of the angular momenta of Ceres and Vesta. They also allow to observe secular resonances, which occur when the secular frequency of precession of the angular momentum is close to a secular frequency of the orbital motion. Secular resonances can then be responsible for a stronger variation of the inclination of the angular momemtum with respect to the plane of the orbital motion.

References

[1] J. Laskar, M. Gastineau, J.-B. Delisle, A. Farrés, A. Fienga, *Strong chaos induced by close encounters with Ceres and Vesta*, Astronomy and Astrophysics **532** (2011), L4.
[2] H. Kinoshita, *Theory of the rotation of the rigid earth*, Celestial Mechanics **15** (1977), 277–236.
[3] J. Laskar, P. Robutel, *The chaotic obliquity of the planets*, Nature **361** (1993), 608–612.
[4] J. Laskar, F. Joutel, P. Robutel, *Stabilization of the Earth's obliquity by the Moon*, Nature **361** (1993), 615–617.
[5] G. Boué, J. Laskar, *Precession of a planet with a satellite*, Astronomy and Astrophysics **185** (2006), 312–330.
[6] J. Laskar, A. Fienga, M. Gastineau, H. Manche, *La2010: a new orbital solution for the long-term motion of the Earth*, Astronomy and Astrophysics **532** (2011), A89.

Modified equations for variational integrators

Mats Vermeeren

It is well-known that if a symplectic integrator is applied to a Hamiltonian system, then the modified equation, whose solutions interpolate the numerical solutions, is again Hamiltonian. We investigate this property from the variational side. We present a technique to construct a Lagrangian for the modified equation from the discrete Lagrangian $L_{\mathrm{disc}}(x_{j-1}, x_j)$ of a variational integrator.

The first step of the construction consist solely of elementary analysis. Using Taylor expansion and the Euler-MacLaurin formula we find the *meshed modified Lagrangian* $\mathcal{L}_{\mathrm{mesh}}[x(t)]$, a formal power series in the step size h which satisfies

$$\int_a^b \mathcal{L}_{\mathrm{mesh}}[x(t)]\,\mathrm{d}t = \sum_j L_{\mathrm{disc}}(x(jh), x(jh+h)).$$

The meshed Lagrangian borrows its name from the unconventional variational principle that it satisfies:

Definition 1. *A* meshed variational problem *with mesh size h consist in finding smooth critical curves of some action $\int_a^b \mathcal{L}[x(t)]\,\mathrm{d}t$ in the set of piecewise smooth*

curves $\mathcal{C}^{M,h}$ whose nonsmooth points occur at times that are an integer multiple of h apart form each other,

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

A consequence of this definition is that the Euler-Lagrange equations

$$\frac{\delta \mathcal{L}}{\delta x} := \sum_j (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}t^j} \frac{\partial \mathcal{L}}{\partial x^{(j)}} = 0$$

are not sufficient for criticality. In addition, one has the necessary conditions

$$\frac{\partial \mathcal{L}}{\partial x^{(j)}} = 0 \qquad \forall j \geq 2,$$

which can be seen as a generalization of natural boundary conditions, or a version of the Weierstrass-Erdmann corner conditions where every point is a corner. We refer to them as *natural interior conditions*.

Since we are dealing with formal power series, we need to truncate them before we can do any analysis. It will be useful to consider families of curves, parameterized by the step size h, that are critical up to a truncation error:

Definition 2. *A family of curves $x_h : [a,b] \to \mathbb{R}$ is (meshed) k-*critical *for some family of actions $S_h = \int_a^b \mathcal{L}_h \,\mathrm{d}t$ if for any piecewise smooth variation δx_h of x_h, with nonsmooth points in a mesh of size h, there holds $\delta S_h = \mathcal{O}\big(h^{k+1} \,\|\delta x_h\|_1\big)$.*

A family of curves $x_h : [a,b] \to \mathbb{R}$ is k-critical if and only if

$$\frac{\delta \mathcal{L}_h}{\delta x} = \mathcal{O}(h^{k+1}) \qquad \text{and} \qquad \frac{\partial \mathcal{L}_h}{\partial x^{(j)}} = \mathcal{O}(h^{j+k+1}) \quad \forall j \geq 2.$$

By construction variations within one mesh interval do no affect the action for the meshed modified Lagrangian $\mathcal{L}_{\text{mesh}}$. This implies that any curve that satisfies the Euler-Lagrange equations also satisfies the natural interior conditions. In particular this means that the modified equation can be obtained as the Euler-Lagrange equation of $\mathcal{L}_{\text{mesh}}$. These observations allow us to define a classical modified Lagrangian, depending only on x and $\dot{x}$:

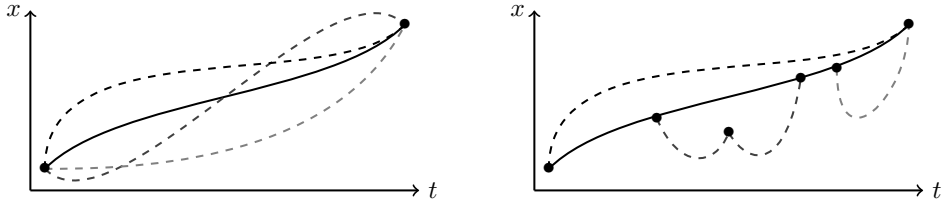


FIGURE 1. A smooth curve and a few variations for the classical (left) and meshed (right) variational problem.

Definition 3. *The* modified Lagrangian *is defined by replacing all second and higher derivatives in the meshed modified Lagrangian according to the modified equation,*

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

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

For general Lagrangians, these replacements will affect the Euler-Lagrange equations. However, due to the property that the Euler-Lagrange equations for $\mathcal{L}_{\mathrm{mesh}}$ imply the natural interior conditions, this is not the case here. It follows that the Euler-Lagrange equations for the modified Lagrangian are equivalent to the modified equation.

This construction is described in detail in [4]. Background on modified equations, especially from the Hamiltonian point of view, can be found in [1, Chapter IX] and the references therein. More on the theory of variational integrators can be found in [2] and a different approach to modified equations for variational integrators is presented in [3].

The extension of the method outlined here to some classes of degenerate Lagrangians is a work in progress. Open questions are whether it is of any use for nonholonomic systems or for PDEs.

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*. Springer, 2006.
[2] J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numerica 2001*, 10:357–514, 2001.
[3] M. Oliver and S. Vasylkevych. A new construction of modified equations for variational integrators. *Preprint*, 2012.
[4] M. Vermeeren. Modified equations for variational integrators. `arXiv:1505.05411`, 2015.

Postprocessed integrators for the high order sampling of the invariant distribution of stiff SDEs and SPDEs

Gilles Vilmart
(joint work with Charles-Edouard Bréhier)

Note: papers available at `http://www.unige.ch/~vilmart/publications.html`

J.C. Butcher's effective order is a popular methodology in the deterministic literature for the construction of efficient and accurate integrators over long times for differential equations. The idea is to introduce a kernel Φ_h of low order but cheap to compute, and a suitable processor χ_h, such that the composition $y_{n+1} = \chi_h \circ \Phi_h \circ \chi_h^{-1}(y_n)$ has a high order of accuracy for a given system of differential equation. Using a constant timestep size h, one can compute simply

$$y_n = \chi_h \circ \Phi_h^n \circ \chi_h^{-1}(y_0)$$

and achieve a high order of accuracy, where the preprocessor χ_h^{-1} and the postprocessor χ_h can be computed only once, respectively at the beginning and the end of the integration (or when the solution is needed).

Inspired by recent contributions on high order integrators based on modified equations for stochastic differential equations (SDEs), see [1, 2, 3] and references therein, we show in [5] (finite dimensional case) and in [4] (SPDE case) that this technique can be extended to the stochastic context for the construction of efficient high order integrators for the sampling of the invariant measure of ergodic stiff problems. In this context, note that only the postprocessor χ_h is needed, and the preprocessor χ_h^{-1} becomes useless, because the ergodic averages over long times are independent of the choice of the initial condition.

The approach is illustrated in [4] with a high-order modification with negligible overhead of the standard implicit Euler-Maruyama method for an abstract class of semi-linear parabolic SPDEs with additive space-time noise in a Hilbert space $\mathcal{H}$,

$$du(t) = (Au(t) + F(u(t)))\,dt + dW^Q(t), \quad u(0) = u_0. \tag{1}$$

Here, $-A : \mathcal{H} \to \mathcal{H}$ is a positive unbounded self-adjoint linear operator with compact resolvent, $F = -DV$ is a Lipchitz continuous nonlinearity deriving from a continuously differentiable potential function $V : \mathcal{H} \to \mathbb{R}$, and the initial condition $u_0 \in \mathcal{H}$ is assumed deterministic for simplicity. We further assume that $\big(W^Q(t)\big)_{t\geq 0}$ is a Q-Wiener process on $\mathcal{H}$ defined on a probability space fulfilling the usual conditions, and the covariance operator $Q : \mathcal{H} \to \mathcal{H}$ is a bounded, nonnegative self-adjoint linear operator, assumed to commute with A. We use the following trace condition on the operators A, Q,

$$\overline{s} = \sup\Big\{ s \in (0,1)\ ,\ \mathrm{Trace}\Big((-A)^{-1+s}Q\Big) < +\infty \Big\} > 0,$$

which guaranties the existence and uniqueness of a mild solution to (1) defined for all $t \geq 0$. Under standard assumptions, we obtain that (1) admits a unique invariant distribution μ_∞. This means that for all (smooth and Lipschitz) test functions $\phi : \mathcal{H} \to \mathbb{R}$, and for all initial conditions u_0, we have with probability 1,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \phi(u(t))dt = \int_{\mathcal{H}} \phi(y) d\mu_\infty(y).$$

It is a standard approach to take advantage of the above ergodicity property to approximate ergodic integrals of the form $\int_{\mathcal{H}} \phi(y)d\mu_\infty(y)$, by introducing discretization schemes for (1).

Standard implicit Euler. Considering the simplest implicit Euler-Maruyama method defined by $v_{n+1} = v_n + hAv_{n+1} + hF(v_n) + \sqrt{h}\xi_n^Q$, equivalently

$$v_{n+1} = J_1 \left(v_n + hF(v_n) + \sqrt{h}\xi_n^Q \right), \tag{2}$$

where $v_0 = u(0)$, $J_1 = (I - hA)^{-1}$ and $\xi_n^Q = h^{-1/2}\big(W^Q((n+1)h) - W^Q(nh)\big)$, yields an ergodic scheme with order $\overline{s}$ of accuracy for sampling the invariant measure,

i.e. for all $r \in (0, \overline{s})$ the following estimate holds for all time $t_n = nh$,

$$\left|\mathbb{E}(\phi(v_n)) - \int_{\mathcal{H}} \phi(y) d\mu_\infty(y)\right| \leq K(u(0), \phi) e^{-\lambda t_n} + C(\phi) h^r, \tag{3}$$

where the constants $\lambda, K, C > 0$ are independent of h, n. The low order $\overline{s}$ of the standard implicit Euler method, instead of 1 in finite dimension, is a consequence of the low regularity assumed on the space-time noise.

New postprocessed integrator. Without any additional smoothness assumption on the space-time noise, we introduce in [4] the following modification of (2) with negligible overhead,

$$\begin{aligned} u_{n+1} &= J_1\Big(u_n + hF\big(u_n + \frac{1}{2}\sqrt{h}J_2\xi_n^Q\big) + \frac{\sqrt{2}-1}{2}\sqrt{h}J_2\xi_n^Q\Big) + \frac{3-\sqrt{2}}{2}\sqrt{h}J_2\xi_n^Q, \\ \overline{u}_n &= u_n + \frac{1}{2}\sqrt{h}J_3\xi_n^Q, \end{aligned} \tag{4}$$

where the operators J_2, J_3 satisfy

$$J_2 = (I - \frac{3-\sqrt{2}}{2}hA)^{-1}, \quad J_3 Q J_3^T = (I - \frac{h}{2}A)^{-1}Q,$$

and $\overline{u}_n = \chi_h(u_n)$ corresponds to the postprocessor. We prove that the scheme (4) is again ergodic, and show in a simplified linear case (F bounded linear operator commuting with A, Q) that it achieves the improved order $\overline{s} + 1$ of accuracy, precisely (3) holds for all $r \in (0, \overline{s} + 1)$ with v_n replaced by $\overline{u}_n$. In addition, there is no discretization error is the absence of nonlinearity ($F = 0$). We also show that (4) has order 2 of accuracy for the invariant measure for nonlinear problems in finite dimension (instead of order 1 for (2)).

Numerical experiments, including the stochastic semilinear heat equation with Dirichlet boundary conditions on (0,1) with space-time white noise ($\overline{s} = 1/2$),

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) + f(u(x,t)) + \frac{\partial W}{\partial t}(x,t), \tag{5}$$

confirm the theoretical findings and suggest that the high order estimates persist in the semilinear case (f nonlinear), as shown in Figure 1.

References

[1] A. Abdulle, D. Cohen, G. Vilmart, and K. C. Zygalakis. High order weak methods for stochastic differential equations based on modified equations. *SIAM J. Sci. Comput.*, 34(3):1800–1823, 2012.

[2] A. Abdulle, G. Vilmart, and K. C. Zygalakis. High order numerical approximation of the invariant measure of ergodic SDEs. *SIAM J. Numer. Anal.*, 52(4):1600–1622, 2014.

[3] A. Abdulle, G. Vilmart, and K. C. Zygalakis. Long time accuracy of Lie-Trotter splitting methods for Langevin dynamics. *SIAM J. Numer. Anal.*, 53(1):1–16, 2015.

[4] C.-E. Bréhier and G. Vilmart. High-order integrator for sampling the invariant distribution of a class of parabolic spdes with additive space-time noise. *Preprint submitted for publication*, 2015. arXiv:1505.05061.

[5] G. Vilmart. Postprocessed integrators for the high order integration of ergodic SDEs. *SIAM J. Sci. Comput.*, 37(1):A201–A220, 2015.

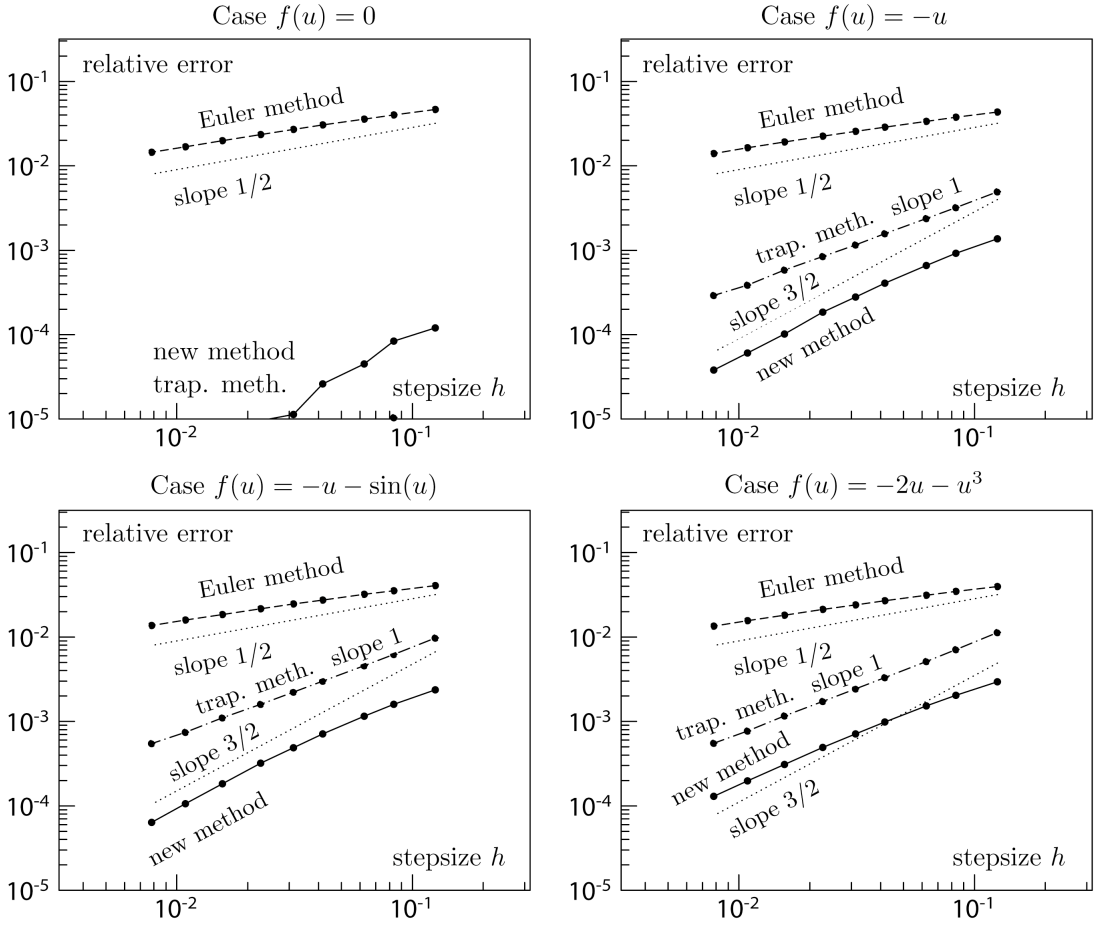


FIGURE 1. Figure from [4]. Comparison of the new method (4) (solid lines) with the standard linearized implicit Euler method (2) (dashed lines) and the trapezoidal method (dashed-dotted lines) for the stochastic heat equation (5) with nonlinearity $f(u)$ discretized in space with $N = 100$ grid points (using a standard finite difference). Errors for $\mathbb{E}(\exp(-\|u(T)\|^2))$ at final time $T = 1$ versus the stepsize h. The expectations are approximated computing the averages over 10^9 samples.

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