

RESONANCE-BASED SCHEMES FOR LOW-REGULARITY SIMULATIONS OF DISPERSIVE EQUATIONS AND BEYOND

1. INTRODUCTION AND CONTEXT

Decades of sustained and sophisticated study of numerical methods for evolution equations has resulted in the development of a toolbox of powerful techniques for the simulation of smooth dynamics, including Runge–Kutta schemes, splitting methods and exponential integrators [10, 12, 16]. With the help of those techniques, the approximation of linear problems and smooth solutions is nowadays well understood. However, a reliable description of ‘nonsmooth’ phenomena (such as for problems at low-regularity and high oscillations) remains a challenging open problem. The central objective of the ERC Starting Grant ‘LAHACODE - Low-regularity and high oscillations: numerical analysis and computation of

dispersive evolution equations’ lies in making a crucial step towards closing this gap. In this article we will survey recent progress in the study of a new class of numerical methods, so-called ‘resonance-based’ schemes, which build the cornerstone of LAHACODE. They were originally tailored to approximate low-regularity dynamics of dispersive equations

$$(1) \quad \partial_t u - i\mathcal{L}u = f(u), \quad u(0) = v,$$

($\mathcal{L}$ denoting the leading differential operator) and could be successfully extended to a much wider class of equations [4, 21, 13] (heat, Ginzburg–Landau, half-wave, wave, Navier–Stokes, etc). The inspiration of resonance-based schemes lies in controlling the underlying dynamics of (1) which are driven by the nonlinear frequency interactions between the differential operator $\mathcal{L}$ and the nonlinearity $f(u)$, and at

first order take the form (cf. (6))

$$(2) \quad e^{-i\xi\mathcal{L}} f \left(e^{i\xi\mathcal{L}} v \right),$$

where ξ is a local time variable. A key challenge from a numerical point of view lies in reproducing the nonlinear dynamics (2) on the discrete level. Classical integrators are mainly based on linearisations of frequency interactions, e.g., splitting methods and exponential integrators with

$$(3) \quad e^{-i\xi\mathcal{L}} f \left(e^{i\xi\mathcal{L}} v \right) \approx f(v),$$

$$\text{and } f \left(e^{i\xi\mathcal{L}} v \right) \approx f(v),$$

respectively. These linearisations require a lot of smoothness in the system. The central idea behind resonance based schemes lies in moving away from frequency linearisations (such as (3)) towards embedding the underlying structure of resonances (2) into the numerical discretisation. This allows us to

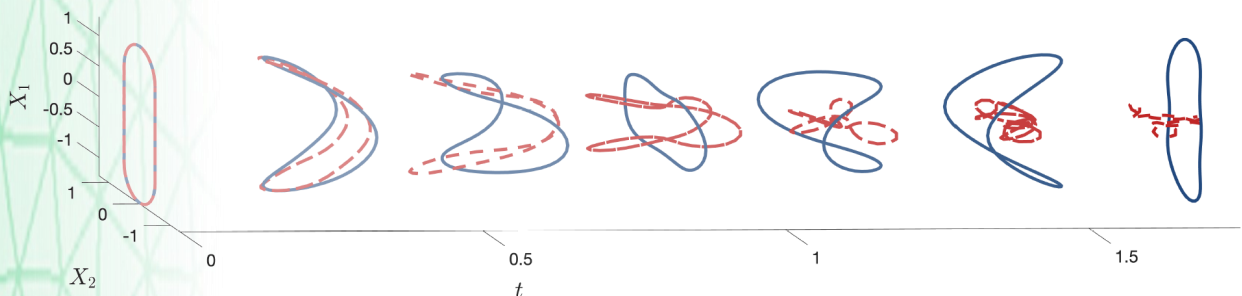


Figure 1. Evolution of low-regularity vortex filament as is shed for example by modern air purifiers. The solid blue curve shows correct dynamics obtained with resonance-based scheme [5], and the dashed red curve corresponds to break-down behaviour of a classical method based on the backward differentiation formula.

solve a larger class of equations efficiently under lower regularity assumptions (cf. Fig. 1: The evolution of a low-regularity vortex filament of piecewise constant curvature as described in section 3.1).

2. METHODOLOGY AND NOVEL CONSTRUCTIONS

The key idea of this new class of resonance based-schemes is best exhibited by considering a simple example such as the cubic Schrödinger equation (NLSE):

$$(4) \quad i\partial_t u = -\Delta u + \mu |u|^2 u,$$

for $t > 0$ over the periodic d -dimensional torus $\mathbf{x} \in \mathbb{T}^d = [-\pi, \pi]^d$ with initial condition $u(0, \mathbf{x}) = u_0(\mathbf{x})$.

A prominent technique for the NLSE is splitting [16], whereby we solve two auxiliary problems (the linear and nonlinear one) separately in each time step. The advantage of this splitting ansatz over direct approaches is that the subproblems are simpler to solve numerically, for example using spectral basis functions in $\mathcal{O}(M^d(\log M)^d)$ operations, by exploiting the fast Fourier transform (FFT). However, this comes at the prize of neglecting all nonlinear interactions between $-\Delta$ and $|u|^2 u$ based on a linearization of the form (3) which requires highly regular solutions.

More precisely, the local error in the Lie splitting method is driven by the Lie commutator of the dispersive and the nonlinear part of the

equation [14, Section 4.2]

$$\begin{aligned} \frac{1}{2}[\Delta, |u|^2](u) &= (\nabla u \cdot \nabla \bar{u})u \\ &+ \nabla(u\bar{u}) \cdot \nabla u \\ &+ \frac{1}{2}|u|^2 \Delta u + \frac{1}{2}(u\Delta \bar{u})u. \end{aligned}$$

To achieve first order convergence with the Lie splitting method in the Sobolev space H^r , $r \geq 0$, one thus has to require solutions which lie at least in H^{r+2} due to the leading error term $(u\Delta \bar{u})u$. If this regularity is not met the order of convergence drastically breaks down leading to large errors and huge computational costs (cf. Fig. 2).

The central aim of resonance based schemes is to overcome this burden as far as possible with the key idea of embedding the nonlinear frequency interactions between the differential operator and nonlinearity into the numerical discretisation. To stay close to the central dynamics the new schemes are based on iterations of Duhamel's formula (the variations of constants solution) for (4). Here we suppress the $\mathbf{x}$ -dependence of the solution and focus on the time-stepping part:

$$\begin{aligned} (5) \quad u(\tau) &= e^{i\tau\Delta} u(0) \\ &- i\mu \int_0^\tau e^{i(\tau-s)\Delta} |u(s)|^2 u(s) ds. \end{aligned}$$

Iterating Duhamel's formula (5) (i.e., using that $u(s) \approx \exp(is\Delta) u(0) + \mathcal{O}(s)$) we formally find that

$$\begin{aligned} (6) \quad u(\tau) &= e^{i\tau\Delta} u(0) \\ &- i\mu \int_0^\tau e^{i(\tau-s)\Delta} |e^{is\Delta} u(0)|^2 \\ &\quad e^{is\Delta} u(0) ds \\ &+ \mathcal{O}(\tau^2). \end{aligned}$$

In the above formula we clearly see that the dynamics of the solution are (at first order) driven by the nonlinear frequency interaction of $\pm i\Delta$ and $|u|^2 u$, i.e.,

$$(7) \quad e^{-is\Delta} |e^{is\Delta} u(0)|^2 e^{is\Delta} u(0),$$

cf. also (2).

Ideally, we would like to embed all the nonlinear frequency interactions (7) into our numerical scheme. This, however, would not lead to a computationally efficient scheme as the computations would need to be carried out fully in Fourier space (with computational efforts at order $\mathcal{O}(M^{3d})$). To achieve a low regularity approximation that is also computationally efficient we thus filter out the dominant parts of the interactions in (7) and treat them exactly within the discretisation, while only neglecting the lower order parts. In the general setting (2) this corresponds to the filtering

$$\begin{aligned} (8) \quad e^{-i\xi\mathcal{L}} f(e^{i\xi\mathcal{L}} v) \\ \approx [e^{i\xi\mathcal{L}_{\text{dom}}} f_{\text{dom}}(v)] f_{\text{low}}(v). \end{aligned}$$

Here $\mathcal{L}_{\text{dom}}$, f_{dom} represent the dominant part of these operators that can be found in a systematic way. In case of the NLSE (4) this approximation leads to the

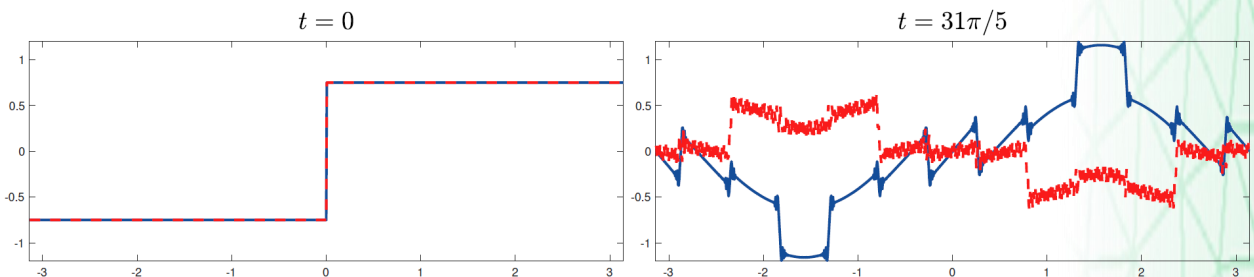


Figure 2. Simulation of the Talbot effect in the nonlinear Schrödinger equation (solid blue curve shows correct localisation effect obtained for piecewise constant initial data with resonance-based scheme, dashed red curve shows oscillatory break-down behaviour of splitting scheme with same discretisation parameters).

following scheme (cf. [20])

$$(9) \quad u^{n+1} = e^{i\tau\Delta} \left[u^n - i\mu\tau(u^n)^2 (\phi_1(-2i\tau\Delta)\overline{u^n}) \right].$$

The advantage of the above resonance-based scheme lies in the fact that firstly, like splitting methods, each time step requires just $\mathcal{O}(M^d(\log M)^d)$ operations through the application of FFTs and local multiplications, and secondly it converges under much lower regularity assumptions. More precisely it holds that:

Theorem 2.1 (See [20]). Let $T > 0$ and suppose $u \in C([0, T]; H^2(\mathbb{T}^d))$, then there exists a constant $C > 0$ and $\tau_0 > 0$ such that for all $\tau \leq \tau_0$ and all $0 \leq n \leq T/\tau$

$$\|u(n\tau) - u^n\|_{H^1} \leq \tau C.$$

The favorable error behaviour is well observed in practice, see, e.g., Fig. 3.

2.1. Dispersive nonlinear equations. The key idea (8) extends to a much wider range of problems. A general framework of resonance-based schemes for a wide class of applications was introduced in [7] based on so-called decorated tree formalism which is inspired by singular SPDEs with Regularity Structures [6, 11].

For example the terms in (6) for a spectral spatial discretization can be denoted by two trees:

The trivial tree with a single node $T_0 = 1$, corresponding to $e^{i\tau\Delta}u(0)$ and a tree with a root and three leaves

$$T_1 = \begin{array}{c} \begin{array}{ccc} k_1 & k_2 & k_3 \\ \diagdown & | & \diagup \\ \bullet & & \end{array} \end{array},$$

corresponding to the integral

$$-i\mu \int_0^\tau e^{i(\tau-s)\Delta} |e^{is\Delta}u(0)|^2 ds.$$

This tree formalism allows us to control in a systematic way higher

order iterations of nonlinear frequency interactions within high order iterations of Duhamel's formula (5) leading to resonance-based schemes up to arbitrary order. For their construction for a large class of nonlinear PDEs on general domains (i.e., without imposing periodic boundary conditions) see also [4].

A particular challenge in the error analysis of numerical schemes lies in achieving rigorous convergence results in function spaces of very low regularity, such as L^2 as classical bilinear estimates break down [2]. Indeed, to control the nonlinearities one has to exploit discrete analogues of important PDE techniques, such as Bourgain spaces and Strichartz estimates (cf. [1, 17, 19, 18]).

2.2. General evolution equations.

The above ideas extend to the approximation of low-regularity dynamics in a broad class of evolution equations of the form

$$\partial_t u - \mathcal{L}u = f(u, \bar{u}),$$

with homogeneous boundary conditions on a domain $\Omega \subset \mathbb{R}^d$,

where $\mathcal{L}$ is the generator of a strongly continuous semigroup of contractions on a Hilbert space (covering for example a large class of parabolic equations including nonlinear heat equations) [21]. If the nonlinearity f is tensorized in the form $f(v, \omega) = \mathcal{B}(F(v) \cdot G(\omega))$, the first-order low-regularity integrator takes the form

$$u^{n+1} = e^{\tau\mathcal{L}} \left(u^n + \tau \mathcal{B} \left(F(u^\ell) \cdot \varphi_1(\tau\mathcal{A}) G(\overline{u^\ell}) \right) \right)$$

where we have set $\mathcal{A} = -\mathcal{L} + \bar{\mathcal{L}}$.

This method has similarly favourable convergence properties in the low-regularity regime as the scheme (9).

2.3. Structure preservation.

Structure preserving algorithms nowadays constitute the core of computational mathematics. A revolutionary step was set by the theory of geometric numerical analysis ([10]). The natural question arises in how far resonance based (or their general form of low regularity integrators) preserve the underlying structure of the PDE (e.g., energy, momentum, mass,

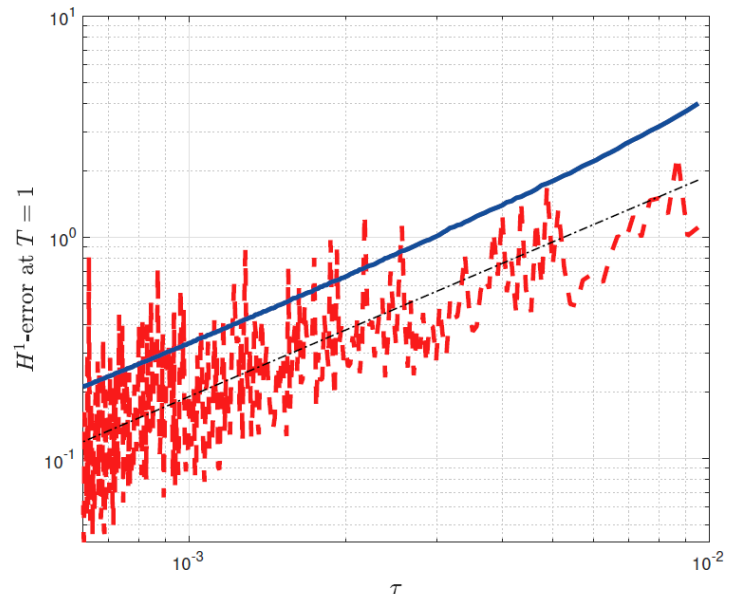


Figure 3. Convergence plot (double logarithmic): H^1 -error vs time step τ . Solid blue curve: resonance based scheme (9); dashed red curve: Lie splitting (reference line $\mathcal{O}(\tau)$); black dash-dotted).

etc.) over long times. To answer this question, let us turn back to our example of NLSE (4) for which we can express the first integral from (6) in the form

$$I_\tau = \int_0^\tau e^{i\omega s} f(s) \, ds$$

where $\omega = 2k_1^2$ is the dominant frequency, and

$$f(s) := \overline{\hat{u}_{k_1}(t_n + s)} \hat{u}_{k_2}(t_n + s) \hat{u}_{k_3}(t_n + s)$$

is the amplitude.

Highly oscillatory quadrature, and in particular the design of Filon methods [8], suggests that integrals of this form should be discretised by replacing $f(s)$ by an interpolating polynomial and treating the oscillatory term $\exp(i\omega s)$ exactly. The resonance-based idea (8) together with Filon-type approach opens up a plethora of possibilities to construct low-regularity integrators with many more degrees of freedom; which is a stepping stone to construct symmetric [5, 1, 9] and even symplectic resonance-based schemes [15].

3. RESULTS AND APPLICATIONS

Resonance-based schemes can be constructed for a large range of differential equations; here we consider two of them in slightly more detail.

3.1. The isotropic Landau–Lifshitz equation. Applicable to the simulation of vortex filaments in fluids and spin states in ferromagnetism, the isotropic Landau–Lifshitz (LL) equation describes the dynamics of a vector field $\mathbf{T}(t) : \mathbb{T} = [-\pi, \pi] \rightarrow \mathbb{S}^2$ under the flow

$$(10) \quad \mathbf{T}_t = \mathbf{T} \wedge \mathbf{T}_{xx}.$$

Through a nonlinear gauge transformation (the so-called

Hasimoto transform) the LL equation can be related to a unique cubic nonlinear Schrödinger equation. This mapping allows for an efficient low-regularity approximation, via the FLOWRH (Fast-Low-Regularity-Hasimoto) transform combined with resonance-based schemes for the NLSE. An important example lies in the accurate and fast simulation of the vortex filament shown in Fig. 1 (which corresponds to a solution in $\mathcal{C}([0, T]; H^{3/2-})$ in (10)) [5].

3.2. Navier Stokes equations.

Resonance-based schemes have also been successfully developed for the incompressible Navier–Stokes (NS) equations

$$\begin{aligned} \partial_t u + u \cdot \nabla u - \mu \Delta u + \nabla p &= 0 \\ \nabla \cdot u &= 0 \end{aligned}$$

posed on a bounded domain $\Omega \subset \mathbb{R}^d$ with set initial condition ([13]). A similar construction to that described in section 2 can be applied in this case, leading to the semi-implicit integrator

$$\begin{aligned} (11) \quad u_n + \tau_n P_X [e^{\tau_n \mu A} u_{n-1} \cdot \nabla u_n] \\ = e^{\tau_n \mu A} u_{n-1}. \end{aligned}$$

where $P_X : L^2(\Omega)^d \rightarrow \dot{L}^2$

is the L^2 -orthogonal projection onto the divergence-free subspace and $A = P_X \Delta$. Coupled with finite-elements as a spatial discretisation the low regularity integrator (11) allows for improved computational performance for Navier–Stokes equations under lower regularity assumptions than classical schemes require.

4. CONCLUSIONS AND OPEN QUESTIONS

Albeit resonance-based schemes are a fairly recent development in the numerical approximation of evolution equations they are seeing an increasing amount of success in

the accurate simulation of a wide range of PDEs. Nevertheless, many important questions remain, and amongst them in particular relevant to the ECCOMAS readership is the scalability of these methods to real-life computational applications.

Furthermore resonance-based schemes may offer a novel approach to the reliable computation of blow-up phenomena and PDEs in presence of randomness [3]. In context of structure preservation, many exciting questions remain open including proofs of long-time behaviour and symplecticity boiling down to a fundamental but yet open question in computational mathematics for nonlinear PDEs: *How – and to what extent – can we reproduce the qualitative behaviour of nonlinear PDEs in a finite dimensional (discrete) world?*

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