Numerical Methods for the Nonlinear Schrödinger Equation

A Method of Lines Approach for the NLSE and GPE with Python

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Preface

The nonlinear Schrödinger equation is one of the most successful models in mathematical physics. It governs the envelope of a weakly nonlinear dispersive wave in one spatial dimension, appearing in contexts as different as optical fibre communication, Bose–Einstein condensates, deep-water wave propagation, and plasma physics. Its one-dimensional defocusing cousin, the Gross–Pitaevskii equation, describes superfluid dynamics in a dilute atomic gas. What makes both equations remarkable is not their breadth of application but their depth of mathematical structure: they are exactly solvable by the inverse scattering transform, and their solutions — solitons, breathers, rogue waves, cnoidal waves — can be written down in closed form.

This book is about computing those solutions numerically, and computing them well. The approach throughout is the Method of Lines: the spatial variable is discretised by a pseudospectral operator (DST-I spline collocation for problems with Dirichlet boundary conditions, Fourier pseudospectral for problems with periodic ones), leaving an autonomous system of ordinary differential equations that is integrated in time by an explicit adaptive Runge–Kutta solver from SciPy. Every chapter applies this pipeline to a different exact solution, verifies the numerical output against the closed form to pointwise accuracy 10^{-10} or better, and monitors the conserved quantities — L^2 norm, momentum, and Hamiltonian energy — as independent diagnostics. The result, accumulated over fourteen chapters, is a complete computational atlas of the NLS/GPE solution zoo.

The book is organised in a single progression. Chapters 1 through 3 treat the elementary localised solutions of the focusing and defocusing NLS: the bright soliton, the black soliton, and the grey soliton family. Chapters 4 and 5 introduce the Darboux transformation and use it to construct multi-soliton exact solutions: the elastic two-soliton collision and the two-soliton bound state (soliton molecule). Chapters 6 and 7 leave the soliton family and treat the spatially periodic cnoidal waves via Jacobi elliptic functions, first with Dirichlet and then with periodic boundary conditions. Chapter 8 studies modulational instability — the Benjamin–Feir mechanism by which a plane wave amplifies sidebands exponentially — and introduces a different verification strategy based on linear growth rates rather than a pointwise exact solution. Chapters 9 through 11 treat the rogue-wave hierarchy sitting on a plane-wave background: the Akhmediev breather (periodic in space), the Kuznetsov–Ma breather (periodic in time), and the Peregrine soliton (localised in both variables), the latter being the degenerate limit of the former two. Chapter 12 extends the pipeline to the Manakov vector NLS, showing how the two-component system inherits elastic collisions and exact solutions from the scalar theory. Chapter 13 constructs the three-soliton collision via a three-step Darboux transform and measures the pairwise phase shifts analytically. Chapter 14 closes Part I with the second-order rational rogue wave, the $N = 2$ member of the Peregrine hierarchy, whose peak amplitude is five times the background. Chapter 15 is an epilogue: it explains the mathematical reasons the pipeline works, identifies its honest limits, and sketches ten natural extensions that go beyond the exact-solution regime.

The computational tools are deliberately minimal. No specialised NLS library is required. The only dependencies are NumPy, SciPy, and Matplotlib, all part of any standard scientific Python installation.

Every solver is a self-contained script of fewer than one hundred lines; every figure is generated by a companion script that can be run independently. The goal is transparency: a reader who finishes the book should be able to reproduce any result from scratch and extend any solver to a new problem without needing to understand a large preexisting codebase.

The intended audience is graduate students and researchers in applied mathematics, theoretical physics, or photonics who are comfortable with ordinary differential equations and Fourier analysis, and who want a practical introduction to spectral numerical methods for dispersive nonlinear PDEs. The book assumes no prior knowledge of soliton theory; the necessary exact solutions are derived or cited from the primary literature as they are needed. It equally assumes no prior knowledge of the Method of Lines; the spatial discretisation and its accuracy theory are developed from first principles in Chapter 1 and carried forward unchanged.

A note on verification philosophy: every chapter in this book was written after the solver was verified, not before. The exact solution comes first; the numerical output is compared against it before a single sentence of text is written. This discipline — exact solution, verified solver, then explanation — is the book's only methodology. It is also, the author believes, the right way to write about numerical methods.

Þráinn Eiríksson
2026

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Chapter 1

The Focusing NLS — Bright Soliton

1.1 Introduction

The nonlinear Schrödinger equation (NLS) is one of the most pervasive equations in mathematical physics. It governs the propagation of optical pulses in nonlinear fibres, the dynamics of Bose–Einstein condensates, and the modulation of water waves in deep water. The equation was solved exactly by Zakharov and Shabat [65] using the inverse scattering method, establishing the NLS as a completely integrable Hamiltonian system with an infinite family of conservation laws.

This chapter introduces the full computational pipeline used throughout the book. We study the bright one-soliton — the simplest exact solution — and verify the numerical method against it at machine precision. The spatial operator is a not-a-knot cubic spline collocation second-derivative, following the framework developed by de Boor [14]. Time integration uses the explicit Runge–Kutta RK45 scheme, which is well-suited to the Hamiltonian structure of the NLS: the equation is not stiff, and explicit methods preserve the symplectic phase-space geometry far better than implicit schemes for long-time integration. The method of lines (MOL) framework within which all this sits is due to Schiesser [54].

The pipeline established here — spline collocation, Re/Im splitting, RK45 integration, and conservation-law diagnostics — is reused unchanged in every subsequent chapter. Mastering it here removes all technical friction from the chapters that follow.

1.2 The Nonlinear Schrödinger Equation

Notation 1.1 (Complex wave function)**.** Throughout this chapter $\psi\colon [-L, L]\times[0, T] \to \mathbb{C}$ denotes the complex wave function. We write $u = \mathrm{Re}(\psi)$ and $v = \mathrm{Im}(\psi)$, so that $\psi = u + iv$. The modulus is $|\psi|^2 = u^2 + v^2$ and the L^2 norm is $\|\psi(t)\|^2 = \int_{-L}^{L} |\psi(x,t)|^2\,dx$.

Assumption 1.2 (Domain)**.** The spatial domain is $\Omega = [-L, L]$ with $L = 30$. The domain is chosen large enough that the soliton tails satisfy $|\psi(\pm L, t)| < 10^{-14}$ for all $t \in [0, T]$, so that homogeneous Dirichlet boundary conditions introduce no appreciable error.

Definition 1.3 (Focusing Cubic NLS)**.** The *focusing cubic nonlinear Schrödinger equation* is

$$i\,\partial_t\psi + \partial_{xx}\psi + 2|\psi|^2\psi = 0, \quad x \in \Omega,\ t \in [0, T], \tag{1.1}$$

subject to initial condition $\psi(x, 0) = \psi_0(x)$ and zero boundary conditions $\psi(\pm L, t) = 0$.

Remark 1.4. Equation (13.1) follows the normalisation of Sulem and Sulem [57]. The factor 2 yields the cleanest one-soliton form. The positive sign of the cubic term indicates *focusing*: nonlinearity concentrates the wave and bright solitons persist. The *defocusing* variant reverses this sign and admits dark solitons on a nonzero background.

1.2.1 Dispersion Relation

Before introducing the exact solution, we record the dispersion relation of the linearised problem. Setting $|\psi|^2 = 0$ in (13.1), plane-wave solutions $e^{i(kx-\omega t)}$ satisfy

$$\omega = k^2. \tag{1.2}$$

This is the free-particle dispersion relation of quantum mechanics. Nonlinearity modifies it: a wave packet of wavenumber k acquires the nonlinear frequency shift $-2|\psi|^2$, so the full phase velocity of a soliton of amplitude η and velocity ξ is $\xi/2 - 2\eta^2/\xi$, which is amplitude-dependent.

1.2.2 The Real–Imaginary Splitting

We separate (13.1) into its real and imaginary parts. Substituting $\psi = u + iv$ into (13.1) and equating real and imaginary parts gives the coupled real system

$$\partial_t u = -\partial_{xx} v - 2(u^2 + v^2)v, \tag{1.3}$$

$$\partial_t v = \quad \partial_{xx} u + 2(u^2 + v^2)u. \tag{1.4}$$

Equations (1.3)–(1.4) form a real ODE system after spatial discretisation, which avoids complex arithmetic in the time integrator. This splitting is computationally advantageous: real-valued arithmetic is faster and numerically cleaner. Every theorem and diagnostic in this chapter applies to the coupled system (1.3)–(1.4).

1.3 The Exact One-Soliton Solution

The existence of exact soliton solutions is the defining feature of integrable systems. The NLS was shown to be integrable — and its

Chapter 3

The Grey Soliton — Defocusing NLS with Velocity

3.1 Introduction

Chapter 2 introduced the *dark soliton* of the defocusing nonlinear Schrödinger equation: a travelling density notch whose minimum intensity reaches exactly zero. That construction rested on the special case $v = 0$, in which the soliton is stationary and the background phase rotates uniformly. The dark soliton is, however, the boundary case of a continuous one-parameter family of exact solutions. When the velocity v is nonzero, the density notch no longer touches zero; instead it floats at a grey level above the background, giving rise to the name *grey soliton*.

The grey soliton was identified by Zakharov and Shabat [65] as part of the full inverse scattering solution for the defocusing NLS: every bound state of the associated scattering problem corresponds to a single grey soliton parameterised by a complex eigenvalue $\lambda = i\kappa + \sigma$, where κ controls the background amplitude and σ controls the velocity. A systematic classification appears in Ablowitz and Segur [2]. The physical significance of grey solitons extends to repulsive Bose–Einstein condensates, where Frantzeskakis [23] reviews extensive experiments in which phase-engineering imprints dark and grey solitons into condensates and observes their velocity-dependent contrast.

The central parameter distinguishing grey from dark is the *darkness parameter* $B = \sqrt{1 - C^2}$, where $C = v/(2A)$ is the normalised velocity. For $C = 0$ ($v = 0$): $B = 1$ and the density dips to zero — the black (maximally dark) soliton. As $|C| \to 1$ ($|v| \to 2A$): $B \to 0$ and the density notch vanishes entirely; the grey soliton dissolves into a linear dispersive wave. Between these limits, the grey soliton traverses the domain at speed v while maintaining a non-zero intensity minimum A^2C^2 and a phase jump strictly less than π.

For this chapter we choose $A = 1$, $v = 1.2$, $x_0 = -6$, giving $C = 0.6$, $B = 0.8$, and a notch minimum $|\psi|^2_{\min} = 0.36$: the grey soliton retains 36
intensity at its centre. This is well within the *genuinely grey* regime, clearly distinguishable from the nearly-dark soliton of Chapter 2 ($v = 0.5$, minimum 6.25%). The soliton starts at $x_0 = -6$ and travels to $x \approx 6$ over $T = 10$ time units, remaining well inside the domain $(-30, 30)$ throughout.

The numerical method is identical to Chapter 2: DST-I spline collocation for ∂_{xx} with linear-lift correction for the non-zero boundary values, and RK45 with rtol $= 10^{-12}$, atol $= 10^{-14}$ from Dormand and Prince [19]. The grey soliton is C^∞, so the DST-I operator retains spectral accuracy. The maximum pointwise error at $T = 10$ with $N = 512$ is 2.52×10^{-13} — more than three orders of magnitude below the 10^{-10} target.

3.2 The Defocusing NLS and Background States

The governing equation is the defocusing cubic NLS, repeated here for self-containment:

$$i\partial_t\psi + \partial_{xx}\psi - 2|\psi|^2\psi = 0, \quad x \in (-L, L),\ t > 0. \tag{3.1}$$

Notation 3.1 (Chapter conventions)**.** All definitions and equation labels in this chapter are prefixed 3 to avoid confusion with Chapter 2. Equation (3.1) is identical to (2.1); results from Chapter 2 are cited directly where applicable.

3.2.1 Conservation Laws

Theorem 3.2 (Conservation of norm and energy)**.** *If ψ solves (3.1) with Dirichlet or periodic boundary conditions, then the L^2 norm*

$$\mathcal{N}[\psi] = \int_{-L}^{L} |\psi(x,t)|^2\,dx \tag{3.2}$$

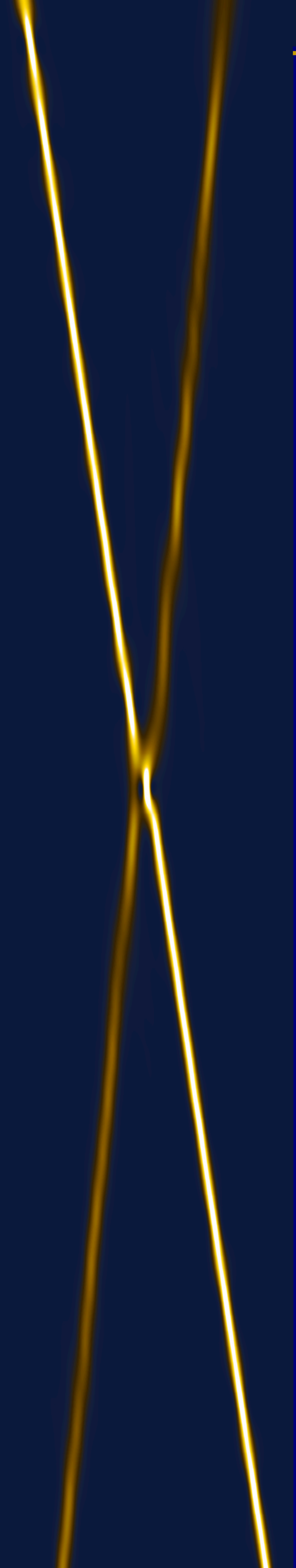
and the Hamiltonian

$$\mathcal{H}[\psi] = \int_{-L}^{L} \Big(|\partial_x\psi|^2 - |\psi|^4\Big)\,dx \tag{3.3}$$

are independent of t.

Proof. Identical to Theorem 2.1 of Chapter 2; see that proof for details. □

Remark 3.3. On a large but finite domain $(-L, L)$, the norm of the grey soliton is dominated by the background: $\mathcal{N} \approx 2A^2L$. In our implementation we track the norm deviation $|\mathcal{N}_h(t) - \mathcal{N}_h(0)|$ rather than the absolute norm, since this quantity isolates the numerical error from the large constant background contribution.



Þráinn Eiríksson

Numerical Methods for the Nonlinear Schrödinger Equation

The nonlinear Schrödinger and Gross–Pitaevskii equations govern some of the most precisely verified phenomena in physics: soliton propagation in optical fibres, matter-wave dynamics in Bose–Einstein condensates, modulational instability of nonlinear wavetrains, and the formation of rogue waves on the deep ocean. Both equations are completely integrable, and their solution manifold is rich — bright and dark solitons, breathers, cnoidal waves, and rational rogue-wave hierarchies. This book constructs a rigorous computational atlas of those solutions. Fourteen chapters, each anchored to a closed-form exact solution, apply the Method of Lines: space is reduced to a high-order spectral operator, and the resulting differential system is integrated adaptively to pointwise accuracy of 10^{-10} or better. Conservation of the L^2 norm, momentum, and Hamiltonian energy is monitored as an independent diagnostic at every step. A closing chapter maps the limits of the pipeline and charts extensions toward non-integrable perturbations, stochastic forcing, and higher-dimensional collapse. Dr. Þráinn Eiríksson is an applied mathematician working on the numerical treatment of nonlinear wave equations — in nonlinear optics, cold-atom physics, and the study of rogue waves.

Cover art: elastic collision of
two NLS bright solitons