Time Integration of Wave Turbulence Problems

Exponential Integrators and IMEX

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MOTIVATIONS

- Wave turbulence models are stiff systems.
- Long-time simulations are required to study statistically-stationary state.
- **We cannot be limited by small time step-sizes!**

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The basic ODE system for wave turbulence is separated into linear and (weakly) nonlinear components,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z} = \mathbf{L}\mathbf{z} + \mathbf{N}(\mathbf{z}), \tag{1}$$

and $\epsilon \ll 1$ is the ratio of time scales between the two.

Exponential Integrators

The change of variable via $\mathbf{v} = \exp(-t\mathbf{L})\mathbf{z}$ yields a new ODE,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v} = \exp(-t\mathbf{L})\mathbf{N}(\exp(t\mathbf{L})\mathbf{v}) =: \mathbf{f}(\mathbf{v}, t). \tag{2}$$

Integrating Factor [1] applies quadrature to the whole integrand:

$$\mathbf{z}(t) = \exp(t\mathbf{L})\left[\mathbf{z}(0) + \int_0^t \mathbf{f}(\mathbf{v}(\tau), \tau)\mathrm{d}\tau\right] \tag{3}$$

Exponential Time Differencing [2] exactly solves :

$$\mathbf{z}(t) = \exp(t\mathbf{L})\left[\mathbf{z}(0) + \int_0^t \exp(-\tau\mathbf{L})\mathbf{p}_s(\tau)\mathrm{d}\tau\right] \tag{4}$$

where $\mathbf{N}(\mathbf{z}(\tau)) \approx p_0 + p_1\tau + \cdots + p_s\tau^s$.

[1] B. Minchev and W. Wright, "A review of exponential integrators for first order semi-linear problems," Preprint Numerics, vol. 2, pp. 1–45, 2005.
[2] S. M. Cox and P. C. Matthews, "Exponential time differencing for stiff systems," Journal of Computational Physics, vol. 176, no. 2, pp. 430–455, 2002.

IMEX (IMPLICIT-EXPLICIT)

Let $\mathrm{IM}(\mathbf{L}, \mathbf{z}_n, \mathbf{z}_{n-1}, \cdots)$ represent a linear implicit scheme, and $\mathrm{EX}(\mathbf{N}, \mathbf{z}_{n-1}, \mathbf{z}_{n-2}, \cdots)$ an explicit scheme. An IMEX scheme using these two schemes is

$$\frac{\mathbf{z}_n - \mathbf{z}_{n-1}}{h} = \mathrm{IM}(\mathbf{L}, \mathbf{z}_n, \mathbf{z}_{n-1}, \cdots) + \mathrm{EX}(\mathbf{N}, \mathbf{z}_{n-1}, \mathbf{z}_{n-2}, \cdots). \quad (5)$$

Rearrange to get

$$\mathcal{D}\mathbf{z}_n = \mathrm{RHS}(\mathbf{L}, \mathbf{N}, \mathbf{z}_{n-1}, \mathbf{z}_{n-2}, \cdots), \quad (6)$$

where $\mathcal{D}$ is a linear operator we need to invert and the RHS evaluated explicitly.

Rational Approximation of Matrix Exponential

Our novel approach: we consider near-minimax approximations instead of the standard Padé approximation ($h \to 0$).

- This can be easily implemented for IF methods.
- AAA-Lawson Algorithm in `chebfun` package in MATLAB (see [3])
- Let $\tilde{R}_n(z)$ be the rational approximation found by AAA-Lawson.

Then, our modified AAA-Lawson rational approximant is forced to be convergent,

$$R_n(z) := \tilde{R}_n(z) - \tilde{R}_n(0) + 1. \tag{7}$$

[3]Y. Nakatsukasa and L. N. Trefethen, "An algorithm for real and complex rational minimax approximation," 2019.

Resonant Triad

Let's consider a single triad,

$$\dot{z}_1 = \mathrm{i}\omega_1 z_1 + \epsilon C_1 z_2^* z_3^*,$$
$$\dot{z}_2 = \mathrm{i}\omega_2 z_2 + \epsilon C_2 z_1^* z_3^*,$$
$$\dot{z}_3 = \mathrm{i}\omega_3 z_3 + \epsilon C_3 z_1^* z_2^*.$$

The condition $C_1 + C_2 + C_3 = 0$ ensures energy conservation while the condition $\omega_1 + \omega_2 + \omega_3 = 0$ makes this system a *resonant* triad.

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{z} = \mathbf{L}_{RT}\mathbf{z} + \mathbf{N}_{RT}(\mathbf{z}) \tag{8}$$

$$\mathbf{L}_{RT} = \begin{bmatrix} \mathrm{i}\omega_1 & 0 & 0 \\ 0 & \mathrm{i}\omega_2 & 0 \\ 0 & 0 & \mathrm{i}\omega_3 \end{bmatrix}, \qquad \mathbf{N}_{RT}(\mathbf{z}) = \epsilon \begin{bmatrix} C_1 z_2^* z_3^* \\ C_2 z_1^* z_3^* \\ C_3 z_1^* z_2^* \end{bmatrix}, \qquad \text{and } \mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}.$$

QUICK MULTI-SCALE ASYMPTOTIC ANALYSIS

Step 1: Find the leading order solution. Expand with an asymptotic ordering by ϵ and add slow-time variable, $\tau = \epsilon t \Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} = \partial_t + \epsilon\partial_\tau$.

$$z_i(t,\tau) = z_{i,0}(t,\tau) + \epsilon z_{i,1}(t,\tau) + \mathcal{O}(\epsilon^2), \tag{9}$$

Substituting into RT system:

$$\mathcal{O}(1): \quad \partial_t z_{i,0} = \mathrm{i}\omega_i z_{i,0}, \tag{10}$$

$$\mathcal{O}(\epsilon): \quad \partial_t z_{i,1} = \mathrm{i}\omega_i z_{i,1} - \partial_\tau z_{i,0} + C_i z_{j,0}^* z_{k,0}^*, \tag{11}$$

and the leading order solution is

$$z_{i,0}(t) = z_{i,0}(0)e^{\mathrm{i}\omega_i t}.$$

Step 2: Force the leading order solution to have slowly-varying amplitudes.

$$z_{i,0} = A_i(\tau)e^{\mathrm{i}\omega_i t} \tag{12}$$

Using this in the $\mathcal{O}(\epsilon)$ equation gives us

$$\partial_t z_{i,1} = \exp(\mathrm{i}\omega_i t)\left(-\frac{\mathrm{d}}{\mathrm{d}\tau}A_i + C_i A_j^* A_k^*\right) + \mathrm{i}\omega_i z_{i,1}.$$

Step 3: Find the solvability condition at $\mathcal{O}(\epsilon)$. To avoid secular growth, we **need**

$$\frac{\mathrm{d}}{\mathrm{d}\tau}A_i = C_i A_j^* A_k^*. \tag{13}$$

Multi-scale Analysis Summary and goals

- $\frac{\mathrm{d}}{\mathrm{d}\tau}A_i = C_i A_j^* A_k^*$ describes the slow amplitude evolution that directly connects to the slow energy transfer.
- We want our discretizations to **preserve** the above **asymptotic** behavior.
- Our time-steps should scale to slow-time $\mathcal{O}(\epsilon^{-1})$. That is, $h\omega_{\max}$ need not be $\ll 1$.
- Standard stability analysis for numerical ODEs: $h \to 0$ with fixed final time T.
- Our analysis: fix h, let $\epsilon \to 0$ and $T = \mathcal{O}(\epsilon^{-1}) \to \infty$.

IF-EULER

Recall, we are numerically solving the integral in

$$\mathbf{z}(t) = \exp(t\mathbf{L}) \left[\mathbf{z}(0) + \int_0^t \mathbf{f}(\mathbf{v}(\tau), \tau)\mathrm{d}\tau\right].$$

Discretized: $\mathbf{z}_n = \exp(h\mathbf{L})\left[\mathbf{z}_{n-1} + h\mathbf{N}(\mathbf{z}_{n-1})\right]$

Step 1: The IF-Euler difference equations are

$$z_i^n = e^{\mathrm{i}\omega_i h} z_i^{n-1} + \epsilon C_i h e^{\mathrm{i}\omega_i h} (z_j^{n-1})^* (z_k^{n-1})^*,$$

which has leading order solution

$$z_{i,0}^n \approx e^{\mathrm{i}\omega_i n h} z_{i,0}^0.$$

Step 2: Now introduce an order ϵ correction and a slow modulation

$$z_i^{n-1} = A_i(\epsilon(n-1)h)e^{\mathrm{i}\omega_i(n-1)h} + \epsilon z_{i,1}^{n-1}.$$

Then the $\mathcal{O}(\epsilon)$ term, $z_{i,1}$, has difference equation,

$$z_{i,1}^{n} = e^{\mathrm{i}\omega_i h} z_{i,1}^{n-1} + \text{other terms}.$$

Step 3: Using the above recurrence relation gives us

$$\begin{aligned} z_{i,1}^{n} = \quad & e^{\mathrm{i}\omega_i nh} z_{i,1}^{0} \\ & + e^{\mathrm{i}\omega_i nh}\left[\frac{1}{\epsilon}(A_i(0) - A_i(\epsilon nh) + C_i h \sum_{m=0}^{n-1} A_j^*(\epsilon mh) A_k^*(\epsilon mh)\right] \end{aligned}$$

Need solvability condition to avoid breakdown of asymptotic ordering!

Rearranging the solvability condition gives us

$$A_i(\epsilon nh) - A_i(0) = C_i \epsilon h \sum_{m=0}^{n-1} A_j^*(\epsilon mh) A_k^*(\epsilon mh),$$

which is the Riemann sum for

$$\int_0^{n\times\epsilon h} \frac{\mathrm{d}}{\mathrm{d}\tau} A_i(\tau)\mathrm{d}\tau = C_i \int_0^{n\times\epsilon h} A_j^*(\tau) A_k^*(\tau)\mathrm{d}\tau.$$

Finally, we result in

$$\frac{\mathrm{d}}{\mathrm{d}\tau} A_i = C_i A_j^* A_k^*.$$

Good!

General IFRK Analysis

IFRK schemes with butcher tableau $\mathbf{A}, \mathbf{b}, \mathbf{c}$ computes

$$\mathbf{k}_i = \exp(c_i h\mathbf{L})\mathbf{y}_{n-1} + h\sum_{j=1}^{i-1} a_{ij}\exp((c_i - c_j)h\mathbf{L})\mathbf{N}(\mathbf{k}_j) \tag{14}$$

$$\mathbf{y}_n = \exp(h\mathbf{L})\mathbf{y}_{n-1} + h\sum_{j=1}^{s} b_j\exp((1 - c_j)h\mathbf{L})\mathbf{N}(\mathbf{k}_j). \tag{15}$$

Discrete-asymptotic analysis leads to

$$\frac{\mathrm{d}}{\mathrm{d}\tau}A_i = C_i\left(\sum_{l=1}^{s} b_l\right)A_j^* A_k^* = C_i A_j^* A_k^*. \tag{16}$$

Still good!

ETD METHODS

Recall that ETD methods solve this integral form

$$\mathbf{z}(t) = \exp(t\mathbf{L})\left[\mathbf{z}(0) + \int_0^t \exp(-\tau\mathbf{L})\mathbf{N}(\mathbf{z}(\tau))\mathrm{d}\tau\right].$$

If we approximate $\mathbf{N}(\cdot)$ over $[t_{n-1}, t_n]$ with an s-degree polynomial,

$$\mathbf{N}(t) \approx \mathbf{p}_s(\tau) := p_0 + p_i\tau + \cdots + p_s\tau^s,$$

the full ETD scheme is then,

$$\mathbf{y}_n = \exp(h\mathbf{L})\left[\mathbf{y}_{n-1} + \sum_{i=0}^{s} p_i \int_0^h \exp(-\tau\mathbf{L})\tau^i\mathrm{d}\tau\right]. \tag{17}$$

Here we introduce a family of functions that deal with these sorts of integrals. We have $\varphi_0(h\mathbf{L}) := \exp(h\mathbf{L})$, and for $l \geq 1$,

$$\varphi_l(h\mathbf{L}) = \frac{\exp(h\mathbf{L})}{h^l(l-1)!}\int_0^h \exp(-\tau\mathbf{L})\tau^{l-1}\mathrm{d}\tau = \frac{\varphi_{l-1}(h\mathbf{L}) - \frac{1}{(l-1)!}}{h\mathbf{L}},$$

where the recurrence relation is derived from integration by parts.

ETD1 [2]

ETD1 approximates the integrand with a constant,

$$\mathbf{z}_n = \exp(h\mathbf{L})\mathbf{z}_{n-1} + \varphi_1(h\mathbf{L})\mathbf{N}(\mathbf{z}_{n-1}),$$

and the RT model discretization is

$$z_i^n = e^{\mathrm{i}\omega_i h} z_i^{n-1} + \epsilon C_i h \varphi_1(\mathrm{i}\omega_i h)(z_j^{n-1})^*(z_k^{n-1})^*.$$

Details are omitted but discrete-asymptotic analysis yields

$$\frac{\mathrm{d}}{\mathrm{d}\tau} A_i = C_i \varphi_1(-\mathrm{i}\omega_i h) A_j^* A_k^*,$$

which converges to correct RHS as $h \to 0$, but we are not interested in that limit.

General ETDRK

An explicit ETDRK scheme computes

$$\mathbf{k}_i = \exp(c_i h\mathbf{L})\mathbf{y}_{n-1} + h\sum_{j=1}^{i-1} a_{ij}(h\mathbf{L})\mathbf{N}(\mathbf{k}_j), \tag{18}$$

$$\mathbf{y}_n = \exp(h\mathbf{L})\mathbf{y}_{n-1} + h\sum_{j=1}^{s} b_j(h\mathbf{L})\mathbf{N}(\mathbf{k}_j), \tag{19}$$

where $a_{ij}(\cdot)$ and $b_j(\cdot)$ are often written in terms of the φ_l functions.
The discrete-asymptotic analysis yields

$$\frac{\mathrm{d}}{\mathrm{d}\tau}A_i = C_i\left(\sum_{l=1}^{s} b_l(\mathrm{i}h\omega_i)\exp(\mathrm{i}(c_l-1)h\omega_i)\right)A_j^*A_k^*$$

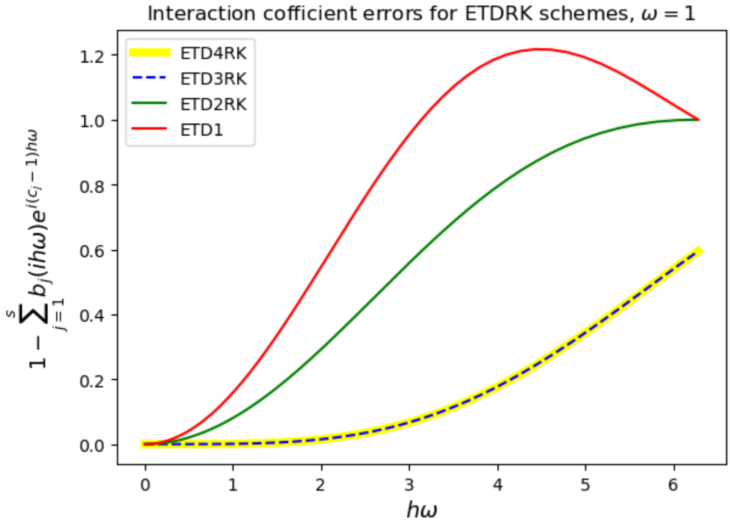

Figure: Interaction coefficient errors in ETDRK methods.

IMEX-Euler

IMEX-Euler uses backward Euler for the implicit linear solve and forward Euler for the explicit nonlinear solve,

$$(\mathbf{I} - h\mathbf{L})\mathbf{z}_n = \mathbf{z}_{n-1} + h\mathbf{N}(\mathbf{z}_{n-1}).$$

The leading order solution decays to zero,

$$z_{i,0}^{n} = \left(\frac{1}{1 - \mathrm{i}h\omega_i}\right)^{n} z_{i,0}^{0}.$$

Here, *dissipative errors* dominate.

CN-Euler

Crank-Nicholson is free of dissipative errors,

$$\left(\mathbf{I} - \frac{h}{2}\mathbf{L}\right)\mathbf{z}_n = \left(\mathbf{I} + \frac{h}{2}\mathbf{L}\right)\mathbf{z}_{n-1} + h\mathbf{N}(\mathbf{z}_{n-1}),$$

and its RT difference equations are

$$z_i^n = \frac{1 + \mathrm{i}h\omega_i/2}{1 - \mathrm{i}h\omega_i/2} z_i^{n-1} + \frac{h}{1 - \mathrm{i}h\omega_i/2}\epsilon C_i (z_j^{n-1})^* (z_k^{n-1})^*.$$

The leading order solution does not decay to zero,

$$z_{i,0}^n = r_i^n z_{i,0}^0, \qquad r_i = \frac{1 + \mathrm{i}h\omega_i}{1 - \mathrm{i}h\omega_i},$$

but now exhibits dispersive errors. Further analysis shows that this incorrectly models the resonant transfer of energy.

RT Numerical Results

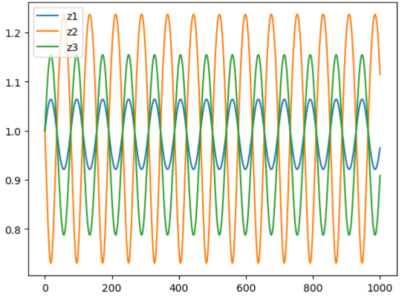

Figure: The ground truth amplitude evolution of the RT model with $\omega_1 = -1, \omega_2 = 3, \omega_3 = -2$ and $\epsilon =$1e-2, computed by RK4 with $h =$1e-5.

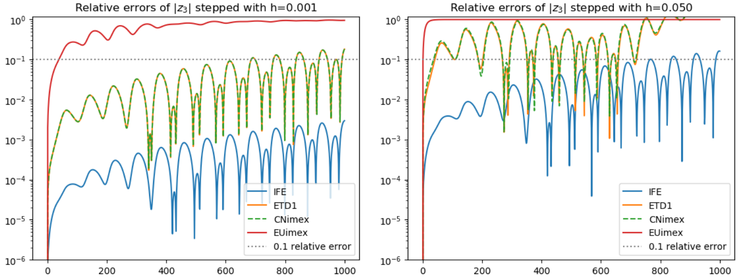

Figure: Relative errors of a single wave in a resonant triad system. Both plots display the errors for IFE, ETD1, IMEX-Euler, and CN-Euler, where the left plot is for $h = 0.001$ and the right plot, $h = 0.050$.

MMT Background

The MMT model is a 1D model of dispersive wave interactions that exhibits a medium-complexity weak wave turbulence (see [4]).

$$\mathrm{i}\partial_t \psi = |\partial_x|^{1/2}\psi + \left(|\psi|^2\,\psi\right). \tag{20}$$

The linear operator in Fourier space is $\mathbf{L}_{MMT} := -\mathrm{i} \times \operatorname{diag}\left(\{|k|^{1/2}\}_{k=-N/2+1}^{N/2}\right) + \mathbf{F} + \mathbf{D}$, where $\mathbf{F}$ and $\mathbf{D}$ refer to forcing and damping defined via

$$\mathbf{F}(k) = \begin{cases} 0.2, & 6 \leq |k| \leq 9 \\ 0, & \text{otherwise} \end{cases} \quad \text{and } \mathbf{D}(k) = -196.61|k|^{-8} - 2.51\times 10^{-57}|k|^{16},$$

and the nonlinear function in physical space is $\mathbf{N}(\psi) := -\mathrm{i}|\psi|^2\psi$.

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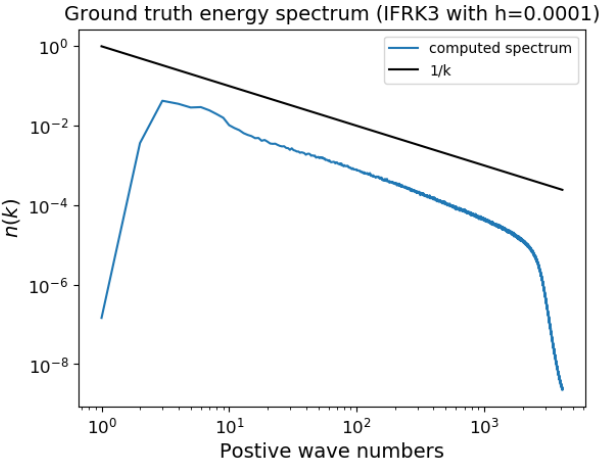
[4]V. Zakharov, F. Dias, and A. Pushkarev, “One-dimensional wave turbulence,” Physics Reports, vol. 398, no. 1, pp. 1–65, 2004.

ENERGY SPECTRUM



Convergence of IFRK

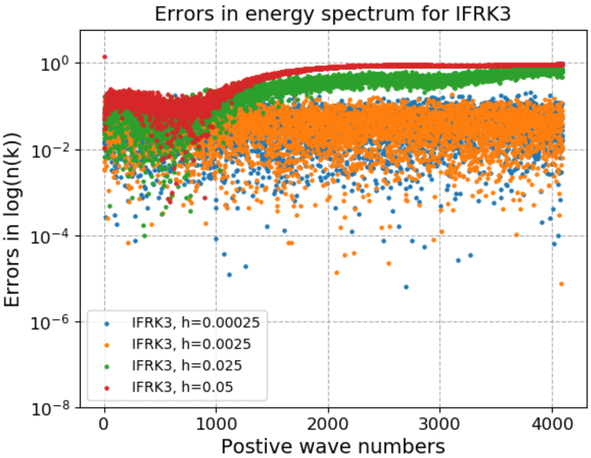


Figure: The log errors of the energy spectrum compared against the ground truth for IFRK3 with various step-sizes are shown.

COMPARISON BETWEEN IFRK3, EDRK3, ARK3 AND ARK4

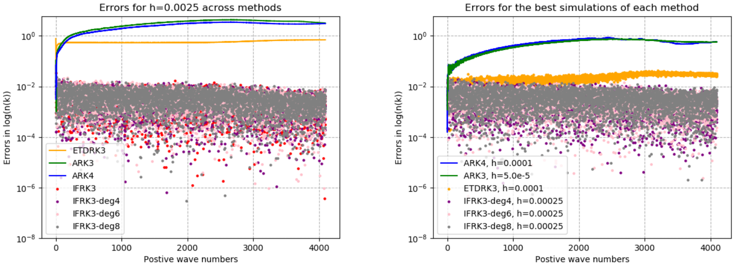


Figure: Left: The log errors of various methods for fixed $h = 0.0025$. Right: The log errors of the best variants of each method.

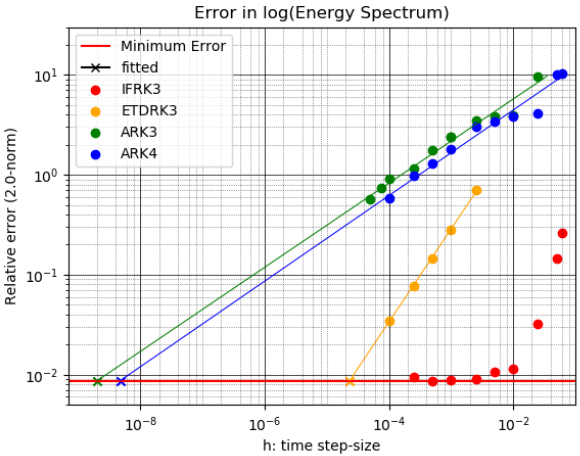


Figure: 2-norm relative errors for various methods and time step-sizes.

Takeaways and Future Work

- IF is the better exponential integrator than ETD for wave turbulence.
- ETD methods insert error into interaction coefficient.
- IMEX methods treats resonances incorrectly (and therefore the energy transfer).
- Near-minimax rational approximations yield great results in IFRK schemes.
- Try for larger 2D and 3D models!

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[1] B. Minchev and W. Wright, “A review of exponential integrators for first order semi-linear problems,” *Preprint Numerics*, vol. 2, pp. 1–45, 2005.

[2] S. M. Cox and P. C. Matthews, “Exponential time differencing for stiff systems,” *Journal of Computational Physics*, vol. 176, no. 2, pp. 430–455, 2002.

[3] Y. Nakatsukasa and L. N. Trefethen, “An algorithm for real and complex rational minimax approximation,” 2019.

[4] V. Zakharov, F. Dias, and A. Pushkarev, “One-dimensional wave turbulence,” *Physics Reports*, vol. 398, no. 1, pp. 1–65, 2004.

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