Numerical Schemes for 3-Wave Kinetic Equations

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Helsinki, November 23, 2023

OUTLINE OF THE TALK

1. **Brief introduction to wave kinetic**
   - Wave Kinetic: The Physical History
2. **Numerics of wave kinetic equations**
   - A finite volume scheme (Joint work with Walton)
   - A deep learning scheme (Joint work with Walton and Bensoussan)

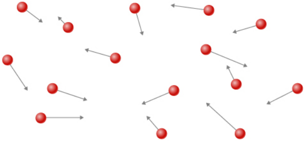
BRIEF INTRODUCTION TO WAVE KINETIC THEORY

Wave Turbulence: The Physical History

What is Wave Kinetic?

- Waves $\longrightarrow$ Wave Equations

- Particles $\longrightarrow$ Kinetic Equations



- Wave Turbulence (Wave Kinetic Theory) $\longrightarrow$ Using Kinetic Equations to describe (Weak) Nonlinear Waves

Physical History: Formal Derivations + Applications

- Origin in the works of Peierls (1929), Hasselmann (1961), Benney-Saffman-Newell (1966), Zakharov (1966)
- Vast range of applications:
  - Oceanography and climate science [1]
  - Quantum physics (work of Pomeau)
  - Inertial waves due to rotation
  - Alfvén wave turbulence in the solar wind
  - Waves in plasmas of fusion devices

  and many others

[1] Irene Gamba, Leslie Smith, MBT. On the wave turbulence theory for stratified flows in the ocean, M3AS, 2020

3-WKE

- Nonnegative wave density, $f(t,k)$, at wavenumber $k \in \mathbb{R}^n$, with $n \geq 2$ and initial condition $f_0(k) \geq 0$, the evolution is determined by

$$\begin{aligned} \partial_t f(t,k) &= Q[f](t,k), \\ f(0,k) &= f_0(k), \end{aligned} \tag{1}$$

where

$$Q = \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\Big[R_{k,k_1,k_2} - R_{k_1,k,k_2} - R_{k_2,k,k_1}\Big]\mathrm{d}k_1\mathrm{d}k_2, \tag{2}$$

and

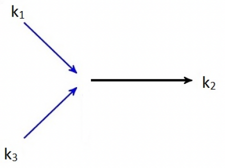
$$R_{k,k_1,k_2} := |V_{k,k_1,k_2}|^2\delta(k-k_1-k_2)\delta(\omega-\omega_1-\omega_2)(f_1f_2 - ff_1 - ff_2), \tag{3}$$

$\omega = \omega(k), \omega_1 = \omega(k_1), \omega_2 = \omega(k_2)$

- In this talk we take

$$|V_{k,k_1,k_2}|^2 = (|k||k_1||k_2|)^\gamma,\ n = 3,\ \text{and } \omega(k) = |k|^s, \tag{4}$$

$f = f(k), f_1 = f(k_1), f_2 = f(k_2)$



NUMERICS OF WAVE KINETIC EQUATIONS

Previous Works

1. C. Connaughton, Numerical solutions of the isotropic 3-wave kinetic equation, Physica D: Nonlinear Phenomena, 238 (2009), pp. 2282-2297.
2. C. Connaughton and P. Krapivsky, Aggregation-fragmentation processes and decaying three-wave turbulence, Physical Review E, 81 (2010), p. 035-303.
3. C. Connaughton and A. C. Newell, Dynamical scaling and the finite-capacity anomaly in three-wave turbulence, Physical Review E, 81 (2010), p. 036-303

Assumptions on isotropic solutions $f(t,k) = f(t,\omega)$

- The solutions follow a self-similar hypothesis, called dynamic scaling

$$f(t,\omega) \approx s(t)^a F\left(\frac{\omega}{s(t)}\right) \tag{5}$$

- The energy is not conserved and assumed to grow

$$\int_0^\infty \omega f(t,\omega)d\omega = \int_0^\infty s(t)^a F\left(\frac{\omega}{s(t)}\right)\omega d\omega \backsim \mathcal{O}\Big(s(t)^{a+2}\Big). \tag{6}$$

We then obtain the system

$$\dot{s}(t) = s^\zeta, \text{ with } \zeta = \gamma + a + 2 \text{ and } aF(x) + x\dot{F}(x) = Q[F](x). \tag{7}$$

Further assumptions: $F(x) \backsim x^{-n}$, when $x \backsim 0$ and $n = \gamma + 1$.

Previous Works

- Work [2] Considers infinite capacity case, the degree of homogeneity γ is considered in the interval $[0, 1)$

$$\int_0^\infty xF(x)dx \tag{8}$$

is well-defined. However, there is a problem in the finite capacity case: when $\gamma > 1$, this integral becomes singular.

- Work [3] considers both infinite capacity ($0 \leq \gamma \leq 1$) and finite capacity cases ($\gamma > 1$). In the finite capacity case, the solution is considered before the first blow-up time $t < t_1^*$. However, to solve (7), a hypothesis is needed: the total energy of the solution is assumed to grow linearly in time

$$\int_0^\infty \omega f(t,\omega)d\omega = Jt. \tag{9}$$

- Another challenging technical issue is that the integration (8) with $F(x) \backsim x^{-\frac{\gamma+3}{2}}$ for small x . As thus, other assumptions need to be imposed on the solution itself.

$\longrightarrow$ **We need rigorous numerical schemes with no assumption**

A FINITE VOLUME SCHEME

TREATING THE FORWARD CASCADE PART

Treating the forward cascade part of the collision operator

Isotopic 3-wave kinetic equation with only the forward cascade collision operator (Connaughton's terminology)

$$\partial_t f(t,\omega) \;=\; Q[f(t,\omega)]$$

$$Q[f](t,\omega) \;=\; \int_0^\omega [a(\omega_1,\omega-\omega_1)f(\omega_1)f(\omega-\omega_1) - a(\omega,\omega_1)f(\omega)f(\omega_1)$$
$$- a(\omega,\omega-\omega_1)f(\omega)f(\omega-\omega_1)]\mathrm{d}\omega_1 \;-2\int_0^\infty [a(\omega,\omega_1)f(\omega)f(\omega_1)$$
$$- a(\omega+\omega_1,\omega_1)f(\omega+\omega_1)f(\omega_1) - a(\omega_1+\omega,\omega)f(\omega)f(\omega_1+\omega)]\mathrm{d}\omega_1$$

where $a(\omega_1,\omega_2) \;=\; (\omega_1\omega_2)^{\gamma/2}$.

Energy cascade: $\int_0^R f(t,\omega)d\omega \;\le\; \mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$ **as** $t\to\infty$,

Smoluchowski coagulation equation

$$\partial_t f(t,\omega) \;=\; \mathbb{Q}[f(t,\omega)]$$

$$\mathbb{Q}[f](t,\omega) \;=\; \int_0^\omega a(\omega_1,\omega-\omega_1)f(\omega_1)f(\omega-\omega_1)\mathrm{d}\omega_1 \;-2\int_0^\infty a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1$$

Key idea of Filbet-Laurencot's scheme (SIAM Sci. Comp. 2003)

$$\partial_t f(t,\omega) = \mathbb{Q}[f(t,\omega)]$$

$$\mathbb{Q}[f](t,\omega) = \int_0^\omega a(\omega_1,\omega-\omega_1)f(\omega_1)f(\omega-\omega_1)\mathrm{d}\omega_1 - 2\int_0^\infty a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1$$

where a satisfies $a(\omega_1,\omega_2) = (\omega_1\omega_2)^\gamma$.
Test function $\phi(\omega) = \omega$:

$$\int_0^c \partial_t f(t,\omega)\omega \mathrm{d}\omega = \int_0^c\int_0^\omega \omega a(\omega_1,\omega-\omega_1)f(\omega_1)f(\omega-\omega_1)\mathrm{d}\omega_1\mathrm{d}\omega$$

$$-2\int_0^c\int_0^\infty \omega a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1\mathrm{d}\omega$$

$$= 2\int_0^c\int_0^{c-\omega} \omega a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1\mathrm{d}\omega - 2\int_0^c\int_0^\infty \omega a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1\mathrm{d}\omega$$

Rearranging the RHS, we find

$$\int_0^c \partial_t f(t,\omega)\omega \mathrm{d}\omega = -2\int_0^c\int_{c-\omega}^\infty \omega a(\omega,\omega_1)f(\omega_1)f(\omega)\mathrm{d}\omega_1\mathrm{d}\omega$$

Key idea of Filbet-Laurencot's scheme (SIAM Sci. Comp. 2003 2003)

$$\int_0^c \partial_t f(t,\omega)\omega \mathrm{d}\omega \;=\; -2\int_0^c\int_{c-\omega}^{\infty} \omega a(\omega,\omega_1)f(\omega_1)f(\omega)\mathrm{d}\omega_1\mathrm{d}\omega$$

Taking the derivative

$$\partial_t f(t,c)c \;=\; -2\partial_c\int_0^c\int_{c-\omega}^{\infty} \omega a(\omega,\omega_1)f(\omega_1)f(\omega)\mathrm{d}\omega_1\mathrm{d}\omega$$

Truncating

$$\partial_t f(t,c)c \;=\; -2\partial_c\int_0^c\int_{c-\omega}^{R} \omega a(\omega,\omega_1)f(\omega_1)f(\omega)\mathrm{d}\omega_1\mathrm{d}\omega$$

After that, apply any FVM scheme to solve the truncated problem.

A similar identity for the gain part of the collision operator - Walton-MBT SIAM Scientific Computing 2023

$$\partial_t f(t,\omega) \;=\; \mathbb{Q}[f(t,\omega)]$$

$$\begin{aligned}\mathbb{Q}[f](t,\omega) \;=\; & \int_0^\omega [a(\omega_1,\omega-\omega_1)f(\omega_1)f(\omega-\omega_1) - a(\omega,\omega_1)f(\omega)f(\omega_1) \\ & - a(\omega,\omega-\omega_1)f(\omega)f(\omega-\omega_1)]\mathrm{d}\omega_1 \\ & - 2\int_0^\infty [a(\omega,\omega_1)f(\omega)f(\omega_1) - a(\omega+\omega_1,\omega_1)f(\omega+\omega_1)f(\omega_1) \\ & - a(\omega_1,\omega)f(\omega)f(\omega_1)]\mathrm{d}\omega_1\end{aligned}$$

Key: Test function. Let $\phi(\omega)$ be a test function, we have a nice identity

$$\int_0^\infty \partial_t f(t,\omega)\phi(\omega)\mathrm{d}\omega \;=\; \int_0^\infty\int_0^\infty a(\omega,\omega_1)f(\omega)f(\omega_1)[\phi(\omega+\omega_1)-\phi(\omega)-\phi(\omega+\omega_1)]\mathrm{d}\omega\mathrm{d}\omega_1$$

Main Idea

Let $\phi(\omega)$ be a test function, we have

$$\int_0^\infty \partial_t f(t,\omega)\phi(\omega)\mathrm{d}\omega \;=\; \int_0^\infty \int_0^\infty a(\omega,\omega_1)f(\omega)f(\omega_1)[\phi(\omega+\omega_1)-\phi(\omega)-\phi(\omega_1)]\mathrm{d}\omega\mathrm{d}\omega_1$$

If we choose $\phi(\omega)=\chi_{[0,c]}(\omega)$ (Filbet-Laurencot's choice $\phi(\omega)=\omega\chi_{[0,c]}(\omega)$)

$$\int_0^\infty \partial_t f(t,\omega)\chi_{[0,c]}(\omega)\mathrm{d}\omega \;=\; \int_0^\infty \int_0^\infty a(\omega,\omega_1)f(\omega)f(\omega_1)[\chi_{[0,c]}(\omega+\omega_1)-\chi_{[0,c]}(\omega)-\chi_{[0,c]}(\omega_1)]$$

Taking the derivative

$$\begin{aligned}\partial_t f(t,c) \;&=\; -2\partial_c \int_0^\infty \int_0^c a(\omega,\omega_1)f(\omega)f(\omega_1)\mathrm{d}\omega_1\mathrm{d}\omega \\ &+\partial_c \int_0^c \int_0^c a(\omega,\omega_1)f(\omega)f(\omega_1)\chi_{[0,c]}(\omega+\omega_1)\mathrm{d}\omega\mathrm{d}\omega_1\end{aligned}$$

Finite Volume Method

- Let $i \in \{1, 2, \dots, M\} = I_h^M$, with the maximum stepsize $h \in (0, 1)$.
- The cells, pivots and step-size are

$$K_i = [x_{i-1/2}, x_{i+1/2})_{i \in I_h^M}, \quad \{x_i\}_{i \in I_h^M} = \frac{x_{i+1/2} + x_{i-1/2}}{2}, \quad \{h_i\}_{i \in I_h^M} = x_{i+1/2} - x_{i-1/2},$$

  with the boundary nodes $x_{1/2} = 0$ and $x_{M+1/2} = R$, the truncation parameter.
- Set $T_N = \{0, \dots, T\}$ with $N + 1$ nodes with fixed time step $\Delta t = \frac{T}{N}$, and denote by $t_n = \Delta t \cdot n$ for $n \in \{0, \dots, N\}$.

- We approximate the forward cascade equation with

$$g^{n+1}(x_i) = g^n(x_i) + \lambda_i\Big(Q^n_{i+1/2}\Big[\frac{g}{x}\Big] - Q^n_{i-1/2}\Big[\frac{g}{x}\Big]\Big), \tag{10}$$

where $\lambda_i = \frac{p_i \Delta t}{h_i}$, and

$$Q^n_{i+1/2}\Big[\frac{g}{x}\Big] - Q^n_{i-1/2}\Big[\frac{g}{x}\Big] = -2\Big(Q^n_{1,i+1/2}\Big[\frac{g}{x}\Big] - Q^n_{1,i-1/2}\Big[\frac{g}{x}\Big]\Big)$$
$$+\Big(Q^n_{2,i+1/2}\Big[\frac{g}{x}\Big] - Q^n_{2,i-1/2}\Big[\frac{g}{x}\Big]\Big),$$

with

$$Q^n_{1,i+1/2}\Big[\frac{g}{x}\Big] = \sum_{m=1}^{i} h_m \frac{g^n(p_m)}{p_m}\left(\sum_{j=1}^{i} h_j \frac{g^n(p_j)}{p_j} a(p_m,p_j)\chi\Big\{x_{i+1/2} < p_m + p_j\Big\}\right), \tag{11}$$

$$Q^n_{2,i+1/2}\Big[\frac{g}{x}\Big] = \sum_{m=1}^{M} h_m \frac{g^n(p_m)}{p_m}\left(\sum_{j=1}^{M} h_j \frac{g^n(p_j)}{p_j} a(p_m,p_j)\chi\Big\{x_{i+1/2} < p_m + p_j\Big\}\right), \tag{12}$$

where we have used the midpoint rule to approximate the integrals.

- The ℓ-th moment, $\mathcal{M}^\ell(t_n)$, is approximated by

$$\mathcal{M}^\ell(t_n) = \sum_{i=1}^{M} h_i g^n(x_i) x_i^\ell, \tag{13}$$

  with $\ell \in \mathbb{N}$.
- The initial condition $g_0(x) \geq 0$ is approximated by

$$g^0(x_i) = \frac{1}{h_i} \int_{K_i} g_0(x) \mathrm{d}x \approx g_0(x_i).$$

CFL type condition

- If the time step, Δt satisfies

$$\Delta t R^{\gamma+1}\|g^0\|_{L^\infty(0,R)} \leq \frac{\gamma}{16}\min_{i\in I_h^M} h_i, \tag{14}$$

then, for all $n \geq 0$ and $i \in I_h^M$ we have $g_i^n \geq 0$, and further,

$$\|g^{n+1}\|_{L^\infty(0,R)} \leq C(\gamma)\|g^n\|_{L^\infty(0,R)},$$

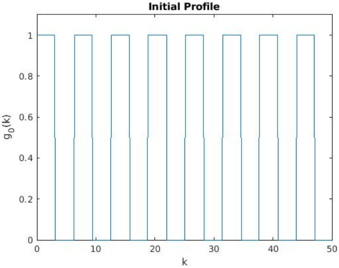
with $C(\gamma) \in [\frac{15}{16}, 1]$ so that finally,

$$\|g^n\|_{L^\infty(0,R)} \leq \|g^0\|_{L^\infty(0,R)}, \tag{15}$$

for all $n \geq 0$.

Numerical Tests - Finite Volume Scheme (Walton -MBT SIAM Sci. Comp. 2023)

- Key technique: New transformation that turns the integro-differential equation into a hyperbolic PDEs $\longrightarrow$ capture the long time dynamics



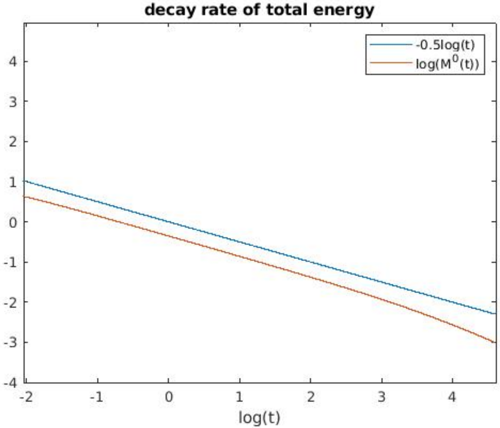


Figure: Log of the decay rate: The blue line is the log of $\frac{1}{\sqrt{t}}$, the orange one is the log of the numerical cascade rate. The 2 lines seem to be parallel, which means the orange one is approximately $\frac{C}{\sqrt{t}}$ $\longrightarrow$ **The bound is optimal**.

TREATMENT OF THE COMPLETE COLLISION OPERATOR

Main Idea

- Forward cascade part:

$$\partial_t f(t,c) = -2\partial_c \int_0^\infty \int_0^c a(\omega,\omega_1) f(\omega) f(\omega_1) \mathrm{d}\omega_1 \mathrm{d}\omega$$

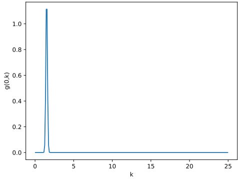
$$+\partial_c \int_0^c \int_0^c a(\omega,\omega_1) f(\omega) f(\omega_1) \chi_{[0,c]}(\omega+\omega_1) \mathrm{d}\omega \mathrm{d}\omega_1$$

- Full equation:

$$\begin{aligned}\partial_t f(t,c) =& 2\partial_c \Big[\int_0^\infty \int_c^{c+\omega_1} f(\omega_1) f(\omega_2) (\omega_1-\omega_2)^2 \mathrm{d}\omega_2 d\omega_1 \\ & - \int_0^c \int_{c-\omega_1}^{\omega_1} f(\omega_1) f(\omega_2)(\omega_1-\omega_2)^2 \mathrm{d}\omega_2 \mathrm{d}\omega_1 \\ & - 4 \int_0^c \int_c^\infty f(\omega_1) f(\omega_2) \omega_1 \omega_2 \mathrm{d}\omega_2 \mathrm{d}\omega_1 - 4 \int_0^c \int_0^{\omega_1} f(\omega_1) f(\omega_2) \omega_1 \omega_2 \mathrm{d}\omega_2 \mathrm{d}\omega_1 \\ & - 2 \int_0^c f^2(\omega_1) \omega_1^2 \mathrm{d}\omega_1 - 2 \int_{\frac{c}{2}}^c f(\omega_1)^2 \omega_1^2 \mathrm{d}\omega_1 \Big]\end{aligned}$$

Numerical Tests

$$g(0,k) = 1.26157\,\exp(-50(k-1.5)^2) \tag{16}$$



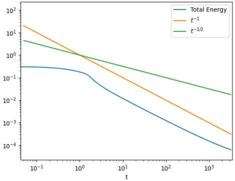
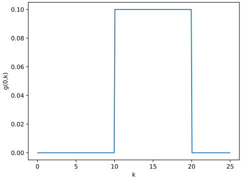


Figure: Decay rate of total energy.

Numerical Tests

$$g(0,k) = \begin{cases} \frac{1}{10} & \text{if } 10 \le k \le 20 \\ 0 & \text{otherwise} \end{cases} \tag{17}$$



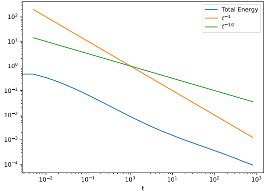


Figure: Decay rate of total energy.

A DEEP LEARNING SCHEME

$$
\partial_t f(t,c) \;=\; -2\partial_c \int_0^\infty \int_0^c a(\omega,\omega_1) f(\omega) f(\omega_1) \mathrm{d}\omega_1 \mathrm{d}\omega
$$

$$
+\partial_c \int_0^c \int_0^c a(\omega,\omega_1) f(\omega) f(\omega_1) \chi_{[0,c]}(\omega+\omega_1) \mathrm{d}\omega \mathrm{d}\omega_1 = \partial_c \mathcal{Q}[f](t,c)
$$

Define a neural network approximation, $f(t,c;\theta)$ to be a solution to the optimization problem

$$
f(t,c;\theta^*) = \min_{\theta\in\Theta} J[f](t,c;\theta),
$$

with $\theta^* \in \Theta$ a minimizing set of parameters of the functional

$$
J[f](t,c;\theta) = \|\mathcal{R}(t,c;\theta)\|^2_{L^2(\mathbb{R}^+\times\mathbb{R}^+)} + \|f(0,c;\theta) - f_0(p)\|^2_{L^2(\mathbb{R}^+)},
$$

where, $\mathcal{R}$ denotes the residual operator of the evolution equation defined by

$$
\mathcal{R}(f,c;\theta) = \partial_t f(t,c;\theta) - \partial_c \mathcal{Q}[f](t,c;\theta).
$$

Numerical Tests - Deep Learning (Walton -MBT-Bensoussan 2022)

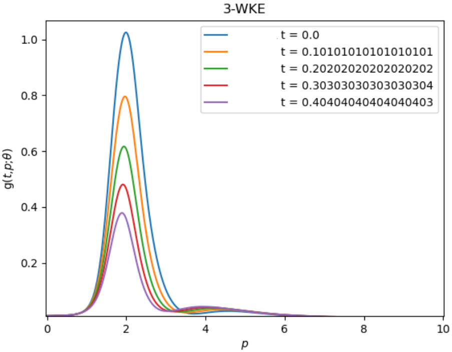


Figure: A few snapshots of the NN approximation. The positivity of the solution is preserved. The functional is approximated via a Quasi-Monte Carlo method with sample points drawn from the Sobol sequence in the unit square and then transformed to some truncated rectangle of the time, wavenumber domain. The architecture was chosen to have 2 hidden layers, each with 128 units and sigmoidal activation functions. The loss was minimized using tensorflows implementation of ADAM.

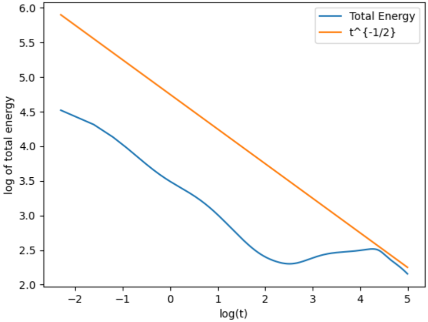


Figure: Log-Log plot of the total energy as predicted up to $t = 148$

THANK YOU SO MUCH FOR YOUR ATTENTION!

Supported by NSF DMS-2204795, DMS-2044626, DMS-1814149