A hyperbolic augmented model for the Nonlinear Schrödinger equation

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Joint work with
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Euler-Korteweg equations

The equations write :

$$\begin{cases} \rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \\ (\rho\mathbf{u})_t + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p(\rho) = \rho\nabla\left(K(\rho)\Delta\rho + \frac{1}{2}K'(\rho)|\nabla\rho|^2\right) \end{cases}$$

where $\rho = \rho(\mathbf{x}, t)$, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ and $(\mathbf{x}, t) \in \mathbb{R}^d \times [0, T]$

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- $K(\rho) = \sigma$: **Compressible flow with surface tension**

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- $K(\rho) = \frac{1}{4\rho}$: **Quantum hydrodynamics**

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Main objective

Given the Quantum hydrodynamics system :

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Ultimate Motivation

To obtain a hyperbolic approximation model of Euler-Korteweg equations in the general case , $i.e$ for generic $K(\rho)$.

Outline

The Non-Linear Schrödinger equation

Expressed in terms of the complex scalar field $\psi(\mathbf{x}, t)$:

$$i\psi_t + \frac{1}{2}\Delta\psi - f(|\psi|^2)\psi = 0$$

- It has a wide range of applications:
  - Nonlinear optics
  - Quantum fluids
  - Surface gravity waves
- It is integrable in the 1-d case [Zakharov, Shabat 1972]

  $\Rightarrow$ Obtaining analytical solutions is possible.

Defocusing NLS equation

Particular case of a cubic non-linearity $f(|\psi|^2) = |\psi|^2$:

$$i\psi_t + \frac{1}{2}\Delta\psi - |\psi|^2\,\psi = 0$$

The Madelung transform (1927)

$$\psi(\mathbf{x},t) = \sqrt{\rho(\mathbf{x},t)}e^{i\theta(\mathbf{x},t)} \qquad\qquad \mathbf{u} = \nabla\theta$$

$$\begin{cases} \rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \\ (\rho\mathbf{u})_t + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + \left(\frac{\rho^2}{2} - \frac{1}{4}\Delta\rho\right)\mathbf{I_d} + \frac{1}{4\rho}\nabla\rho\otimes\nabla\rho\right) = 0 \end{cases}$$

$\Rightarrow$ Corresponds to the Euler-Korteweg quantum hydrodynamic system in the case of a potential flow (irrotational velocity field).

Lagrangian for Quantum hydrodynamics system

The hydrodynamic form of NLS equation admits the following Lagrangian:

$$\mathcal{L} = \int_{\Omega_t} \left(\frac{\rho \left|\mathbf{u}\right|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{\left|\nabla \rho\right|^2}{2} \right) \, d\Omega$$

Hamilton's principle : $a = \displaystyle\int_{t_0}^{t_1} \mathcal{L} \, dt$

$+$

Differential constraint : $\rho_t + \mathrm{div}(\rho \mathbf{u}) = 0$

$\downarrow$

$$(\rho \mathbf{u})_t + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \frac{1}{4\rho} \nabla \rho \otimes \nabla \rho \right) + \nabla \left(\frac{\rho^2}{2} - \frac{1}{4} \Delta \rho \right) = 0$$

Augmented Lagrangian - Attempt 1

Original Lagrangian

$$\mathcal{L}(\mathbf{u}, \rho, \nabla\rho) = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla\rho|^2}{2} \right) d\Omega$$

$$\rho_t + \mathrm{div}(\rho\mathbf{u}) = 0$$

'Augmented' Lagrangian approach

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta) \qquad (\eta \longrightarrow \rho)$$

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla\eta|^2}{2} - \frac{\rho}{2\alpha} \left(\frac{\eta}{\rho} - 1 \right)^2 \right) d\Omega$$

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$\Longrightarrow$ Time to derive the Euler-Lagrange equations !

Hints on calculus of variations

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla \eta|^2}{2} - \frac{\rho}{2\alpha} \left(\frac{\eta}{\rho} - 1 \right)^2 \right) d\Omega$$

$\tilde{\mathcal{L}}(\overbrace{\mathbf{u}, \rho}^{\delta \mathbf{x}}, \underbrace{\eta, \nabla \eta}_{\delta \eta}) \Rightarrow$ Two Euler-Lagrange equations

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$$\tilde{\mathcal{L}}(\overbrace{\mathbf{u}, \rho}^{\delta \mathbf{x}}, \underbrace{\eta, \nabla \eta}_{\delta \eta}) \Rightarrow \text{Two Euler-Lagrange equations}$$

- Virtual displacement of the continuum ($\delta \mathbf{x}$):

$$(\rho \mathbf{u})_t + \operatorname{div} \left(\rho \mathbf{u} \otimes \mathbf{u} + \frac{1}{4\rho} \nabla \eta \otimes \nabla \eta \right) + \nabla \left(\frac{\rho^2}{2} - \frac{|\nabla \eta|^2}{4\rho} + \frac{\eta}{\alpha} \left(1 - \frac{\eta}{\rho} \right) \right) = 0$$

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- η variation ($\delta\eta$) :

$$\frac{1}{4\rho^2} \nabla\rho \cdot \nabla\eta - \frac{1}{4\rho} \Delta\eta = \frac{1}{\alpha} \left(1 - \frac{\eta}{\rho} \right)$$

Preliminary system

Thus the system of governing equations now writes :

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Idea : Include $\dot{\eta}$ into the Lagrangian !

Augmented Lagrangian - Attempt 2

Augmented Lagrangian approach

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta, \dot{\eta}) \qquad \alpha, \beta \ll 1$$

$$\tilde{\mathcal{L}} = \int_{\Omega_t} \left(\rho\frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho}\frac{|\nabla\eta|^2}{2} - \frac{\rho}{2\alpha}\left(\frac{\eta}{\rho} - 1\right)^2 + \frac{\beta\rho}{2}\dot{\eta}^2 \right) d\Omega$$

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Order reduction

1. We denote $w = \dot{\eta}$. Thus :

$$w = \eta_t + \mathbf{u} \cdot \nabla \eta \quad \Longrightarrow \quad \boxed{(\rho\eta)_t + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w}$$

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Important : $\mathbf{p}(\mathbf{x}, t = 0) = \nabla \eta(\mathbf{x}, t = 0)$

Augmented NLS system

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\begin{cases}
\rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \\
(\rho\mathbf{u})_t + \operatorname{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + \left(\frac{\rho^2}{2} - \frac{|\mathbf{p}|^2}{4\rho} + \frac{\eta}{\alpha}(1-\frac{\eta}{\rho})\right)\mathbf{Id} + \frac{1}{4\rho}\mathbf{p}\otimes\mathbf{p}\right) = 0 \\
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(\rho\eta)_t + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w \\
\mathbf{p}_t + \operatorname{div}\left((\mathbf{p}\cdot\mathbf{u} - w)\,\mathbf{I_d}\right) = 0, \qquad (\mathbf{curl}(\mathbf{p}) = 0)
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- Main question : Is this system hyperbolic ?

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$\Rightarrow$ Strongly hyperbolic in one dimension of space.

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$\Rightarrow$ Strongly hyperbolic in one dimension of space.

$\Rightarrow$ Weakly hyperbolic in multi-dimensions.

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(\rho w)_t + \operatorname{div}\left(\rho w \mathbf{u} - \frac{1}{4\beta\rho}\mathbf{p}\right) = \frac{1}{\alpha\beta}\left(1 - \frac{\eta}{\rho}\right) \\
(\rho\eta)_t + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w \\
\mathbf{p}_t + \operatorname{div}\left((\mathbf{p}\cdot\mathbf{u} - w)\,\mathbf{I_d}\right) = 0, \qquad (\mathbf{curl}(\mathbf{p}) = 0)
\end{cases}
$$

- Main question : Is this system hyperbolic ?

$\Rightarrow$ Strongly hyperbolic in one dimension of space.

$\Rightarrow$ Weakly hyperbolic in multi-dimensions. **+ curl constraint**

Augmented NLS system

$$\begin{cases} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \operatorname{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \left(\frac{\rho^2}{2} - \frac{|\mathbf{p}|^2}{4\rho} + \frac{\eta}{\alpha}(1 - \frac{\eta}{\rho})\right) \mathbf{Id} + \frac{1}{4\rho} \mathbf{p} \otimes \mathbf{p}\right) = 0 \\ (\rho w)_t + \operatorname{div}\left(\rho w \mathbf{u} - \frac{1}{4\beta\rho}\mathbf{p}\right) = \frac{1}{\alpha\beta}\left(1 - \frac{\eta}{\rho}\right) \\ (\rho\eta)_t + \operatorname{div}(\rho\eta\mathbf{u}) = \rho w \\ \mathbf{p}_t + \operatorname{div}\left((\mathbf{p}\cdot\mathbf{u} - w)\,\mathbf{I_d}\right) = 0, \qquad (\mathbf{curl}(\mathbf{p}) = 0) \end{cases}$$

- Main question : Is this system hyperbolic ?

⇒ Strongly hyperbolic in one dimension of space.

⇒ Weakly hyperbolic in multi-dimensions. **+ curl constraint**

⇒ Strongly hyperbolic upgrade proposed in *Busto & al. 2021*.

Hyperbolicity of augmented NLS

1-d case: $\mathbf{u} = (u, 0, 0)^T$ and $\mathbf{p} = (p, 0, 0)^T$:

$$\mathbf{U}_t + A(\mathbf{U})\mathbf{U}_x = \mathbf{S}(\mathbf{U}) :$$

Eigensystem of A :

$$\xi_1 = u \quad , \quad \mathbf{v_1} = \left(\frac{\rho}{\alpha\rho^3+\eta^2}, 0, 0, \frac{p}{\alpha\rho^3+\eta^2}, \frac{1}{2\eta-\rho}\right)^T$$

$$\xi_2 = u + \frac{1}{2\rho\sqrt{\beta}} \quad , \quad \mathbf{v_2} = (0, 0, \sqrt{\beta}, 2, 0)^T$$

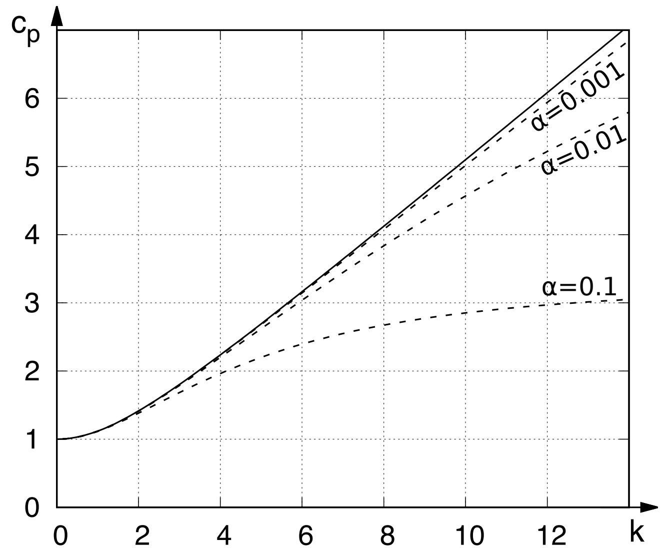
$$\xi_3 = u - \frac{1}{2\rho\sqrt{\beta}} \quad , \quad \mathbf{v_3} = (0, 0, -\sqrt{\beta}, 2, 0)^T$$

$$\xi_4 = u + \sqrt{\rho + \frac{\eta^2}{\alpha\rho^2}} \quad , \quad \mathbf{v_4} = \left(\rho, \sqrt{\rho + \frac{\eta^2}{\alpha\rho^2}}, 0, p, 0\right)^T$$

$$\xi_5 = u - \sqrt{\rho + \frac{\eta^2}{\alpha\rho^2}} \quad , \quad \mathbf{v_5} = \left(\rho, -\sqrt{\rho + \frac{\eta^2}{\alpha\rho^2}}, 0, p, 0\right)^T$$

$\Rightarrow$ **The system is always hyperbolic.**

Dispersion relation comparison



The dispersion relation $c_p = f(k)$ for the original model (continuous line) and the dispersion relation for the Augmented model (dashed lines) for different values of λ and for $\beta = 10^{-4}$

Numerical scheme: IMEX-Type

1-d system of equations to solve :

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}(\mathbf{U})$$

The idea is to solve the hyperbolic part explicitly and the source term implicitly in time according to the scheme ($\gamma = 1 - \frac{\sqrt{2}}{2}$):

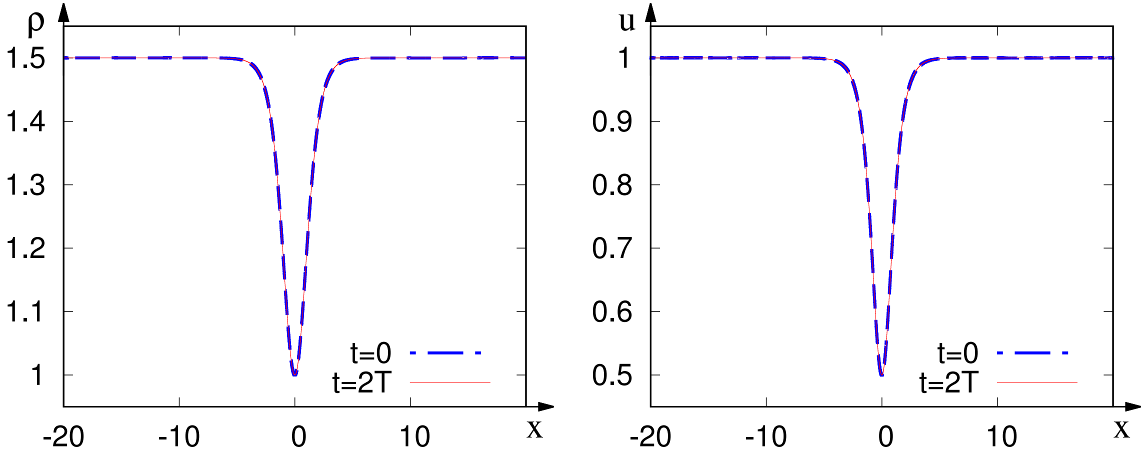
$$\mathbf{U}^{\star} = \mathbf{U}^{n} - \gamma \frac{\Delta t}{\Delta x}\left(F^{n}_{i+\frac{1}{2}} - F^{n}_{i-\frac{1}{2}}\right) + \gamma \Delta t \mathbf{S}(\mathbf{U}^{\star})$$

$$\mathbf{U}^{n+1} = \mathbf{U}^{n} - (\gamma - 1)\frac{\Delta t}{\Delta x}\left(F^{n}_{i+\frac{1}{2}} - F^{n}_{i-\frac{1}{2}}\right) - (2-\gamma)\frac{\Delta t}{\Delta x}\left(F^{\star}_{i+\frac{1}{2}} - F^{\star}_{i-\frac{1}{2}}\right) + (1-\gamma)\Delta t S(\mathbf{U}^{\star}) + \gamma \Delta t S(\mathbf{U}^{n+1})$$

- MUSCL reconstruction in space.
- Rusanov solver for the fluxes.

Grey Soliton solution

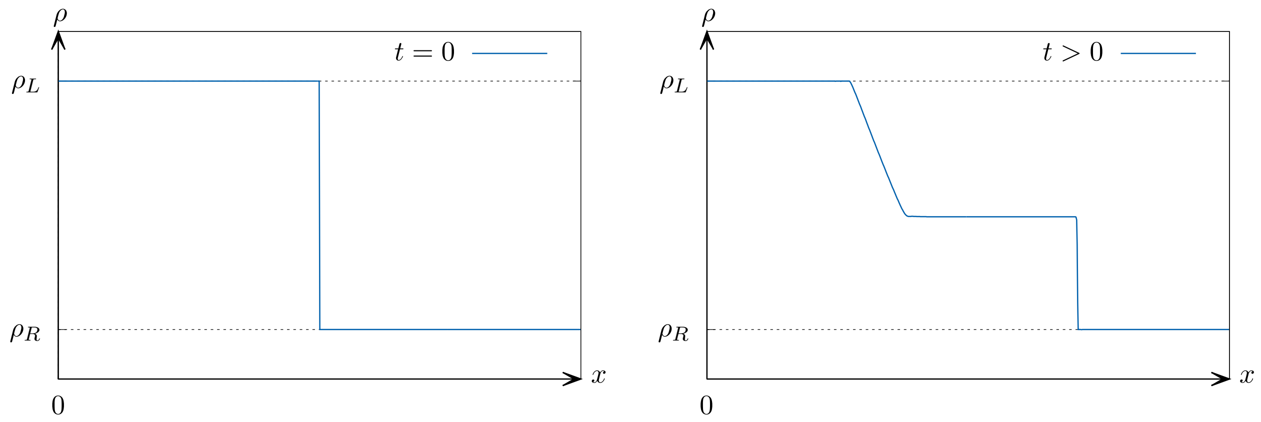
$$\rho(x,t) = b_1 - \frac{b_1 - b_3}{\cosh^2\left(\sqrt{b_1 - b_3}\,(x - Ut)\right)} \qquad u(x,t) = U - \frac{b_1\sqrt{b_3}}{\rho(x,t)}$$



Numerical profiles of ρ (left) and u (right) at $t = 0$ and $t = 2T$. The used domain is $L = [-20, 20]$ with $N = 100000$. Parameters used for the simulation are $U = 2, \beta = 10^{-4}, \alpha = 0.002$.

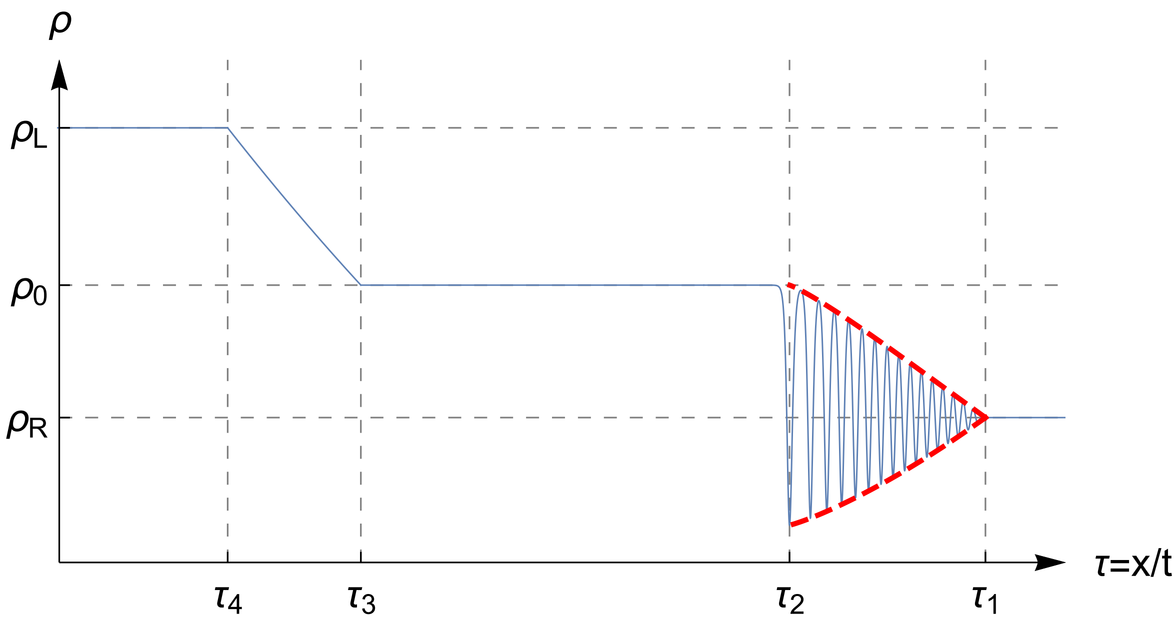
Shock waves for Euler equations

Riemann problem in dispersionless hydrodynamics governed by Euler Equations :



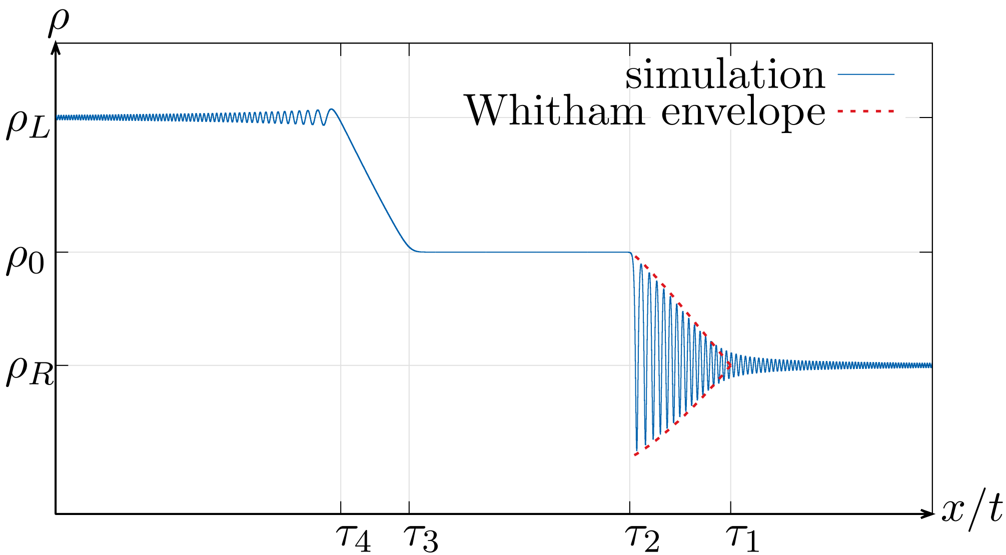
Shockwave solution to a Riemann problem for Euler Equations.

Dispersive Shock waves



Asymptotic profile of the solution to NLS equation (continuous line) for the Riemann problem $\rho_L = 2$, $\rho_R = 1$, $u_L = u_R = 0$. Oscillations shown at t=70

DSW Numerical results : ρ



Comparison of the numerical result (ρ) with the Whitham modulational profile of the DSW at $t = 70$. $\beta = 2.10^{-5}$, $\alpha = 10^{-3}$, $N = 100000$. The computational domain is $[-500, 500]$

Conclusion & Perspectives

Summary :

- A first order hyperbolic approximation of NLS equation was developed.
- Numerical results have shown good agreement in both stationary and non-stationary cases.

Current concerns :

- Extension to Navier-Stokes-Korteweg equations.
- Extension to cases with non-convex free energy. (Modeling diffuse interface multi-phase flows).

Future concerns (Non exhaustive list)

- Boundary conditions.
- Splitting approach to separate fast dispersive waves.
- Further analysis of numerics.

Thank you

Thank you for your attention !

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