An augmented Lagrangian Approach for the defocusing non-linear Schrödinger Equation

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20 August 2019

Introduction : Euler's equation for compressible fluids

A Lagrangian :

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

A Constraint :

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

$\Longrightarrow$ The corresponding Euler-Lagrange equation :

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

Dispersive models in mechanics

1. Surface waves with surface tension [Nikolayev, Gavrilyuk, Gouin 2006] :

$$\mathcal{L}(\mathbf{u}, h, \nabla h) = \int_{\Omega_t} \left(\frac{\rho_0 h \left|\mathbf{u}\right|^2}{2} - \frac{\rho_0 g h^2}{2} - \sigma \frac{\left|\nabla h\right|^2}{2} \right) d\Omega_t$$

2. Shallow water equations described by Serre-Green-Naghdi equations [Salmon (1998)]:

$$\mathcal{L}(u, h, \dot{h}) = \int_{\Omega_t} \left(\frac{hu^2}{2} - \frac{gh^2}{2} + \frac{h\dot{h}^2}{6} \right) d\Omega_t$$

Euler-Korteweg type systems

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

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

$K(\rho) = \sigma$: constant capillarity

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p(\rho) = \sigma\rho\nabla\left(\Delta\rho\right)$$

$K(\rho) = \frac{1}{4\rho}$: Quantum capillarity / DNLS equation

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

The Non-Linear Schrödinger equation

$$i\epsilon\psi_t + \frac{\epsilon^2}{2}\Delta\psi - f\left(|\psi|^2\right)\psi = 0 \qquad ; \qquad \epsilon = \frac{\hbar}{m}$$

- A wide range of applications: Nonlinear optics, quantum fluids, surface gravity waves
- Advantage : the equation is integrable. [Zakharov,Manakov 1974]
- Construction of analytical solutions is possible.

Problematic

Can we solve a dispersive problem by the means of hyperbolic equations ?

Outline

The defocusing NLS equation

In what follows we take : $f\left(|\psi|^2\right) = |\psi|^2$ and $\epsilon = 1$; $t' = \frac{t}{\epsilon}$ $x' = \frac{x}{\epsilon}$:

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

The Madelung transform

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

$$\begin{cases} \rho_t + \mathrm{div}(\rho\mathbf{u}) = 0 \\ (\rho\mathbf{u})_t + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + \Pi\right) = 0 \end{cases}$$

with : $\Pi = \left(\frac{\rho^2}{2} - \frac{1}{4}\Delta\rho\right)\mathbf{Id} + \frac{1}{4\rho}\nabla\rho\otimes\nabla\rho$

A Lagrangian for DNLS equation

For the previous set of equations, we can construct the Lagrangian:

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

Energy conservation law:

$$\frac{\partial E}{\partial t} + \mathrm{div}\left(E\mathbf{u} + \Pi\mathbf{u} - \frac{1}{4}\dot{\rho}\nabla\rho\right) = 0 \quad ; \qquad \dot{\rho} = \rho_t + \mathbf{u}\cdot\nabla\rho$$

where

$$E = \rho\frac{|\mathbf{u}|^2}{2} + \frac{\rho^2}{2} + \frac{1}{4\rho}\frac{|\nabla\rho|^2}{2}$$

Augmented Lagrangian approach

The objective

Obtain a new Lagrangian whose Euler-Lagrange equations :

- are hyperbolic
- approximate Schrödinger's equation in a certain limit

The idea

- Decouple $\nabla\rho$ from $\mathbf{u}$ and ρ, have it as an independent variable.

Augmented Lagrangian approach : Application to DNLS

DNLS Lagrangian :

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

'Augmented' Lagrangian approach [Favrie, Gavrilyuk, 2017]

$$\tilde{\mathcal{L}}(\mathbf{u}, \rho, \eta, \nabla\eta, \dot{\eta}) \qquad \mathbf{p} = \nabla\eta \qquad w = \dot{\eta}$$

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

$\frac{\lambda}{2}\rho \left(\frac{\eta}{\rho} - 1 \right)^2$: Penalty

$\frac{\beta\rho}{2}\dot{\eta}^2$: Regularizer

Augmented system Euler-Lagrange equations

The Augmented Lagrangian :

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

The constraint :

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

$\Longrightarrow$ We apply Hamilton's principle :

$$\boxed{a = \int_{t_0}^{t_1} \tilde{\mathcal{L}}\, dt \quad \Longrightarrow \quad \delta a = 0}$$

Types of variations

Two types of variations will be considered :

$$\tilde{\mathcal{L}}(\overbrace{\mathbf{u}, \rho, \dot{\eta}}^{I}, \underbrace{\dot{\eta}, \eta, \nabla\eta}_{II}) \qquad \dot{\eta} = \eta_t + \mathbf{u}\cdot\nabla\eta$$

- Type I : Virtual displacement of the continuum:

$$\hat{\delta}\rho = -\mathrm{div}(\rho\delta\mathbf{x}) \qquad \hat{\delta}\mathbf{u} = \dot{\delta\mathbf{x}} - \nabla\mathbf{u}\cdot\delta\mathbf{x} \qquad \delta\dot{\eta} = \hat{\delta}\mathbf{u}\cdot\nabla\eta$$

- Type II : Variations with respect to η

$$\delta\nabla\eta = \nabla\delta\eta \qquad \delta\dot{\eta} = (\delta\eta)_t + \mathbf{u}\cdot\nabla\delta\eta$$

Augmented system Euler-Lagrange Equations

- Type I : Virtual displacement of the continuum:

$$\boxed{(\rho\mathbf{u})_t + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u} + \mathbf{P}\right) = 0}$$

with :
$$\mathbf{P} = \left(\frac{\rho^2}{2} - \frac{1}{4\rho}\left|\mathbf{p}\right|^2 + \eta\lambda\left(1 - \frac{\eta}{\rho}\right)\right)\mathbf{Id} + \frac{1}{4\rho}\mathbf{p}\otimes\mathbf{p}$$

- Type II : Variations with respect to η:

$$\boxed{(\rho w)_t + \mathrm{div}\left(\rho w\mathbf{u} - \frac{1}{4\rho\beta}\mathbf{p}\right) = \frac{\lambda}{\beta}\left(1 - \frac{\eta}{\rho}\right)}$$

Closure of the system

1. Definition of $w = \dot{\eta}$

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

2. Evolution of $\mathbf{p} = \nabla\eta$

$$\begin{aligned} \nabla w &= \nabla(\eta_t + \mathbf{u}\cdot\nabla\eta) \\ &= (\nabla\eta)_t + \nabla(\mathbf{u}\cdot\nabla\eta) \\ \Longrightarrow \quad & (\nabla\eta)_t + \nabla(\mathbf{u}\cdot\nabla\eta - w) = 0 \\ \Longrightarrow \quad & \boxed{\mathbf{p}_t + \mathrm{div}((\mathbf{p}\cdot\mathbf{u} - w)\mathbf{Id}) = 0} \end{aligned}$$

2'. Initial condition for $\mathbf{p}$: $\mathbf{p}_{t=0} = (\nabla\eta)_{t=0}$

The full Augmented system

$$\begin{cases} \rho_t + \mathrm{div}(\rho \mathbf{u}) = 0 \\ (\rho \mathbf{u})_t + \mathrm{div}\left(\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{P}\right) = 0 \\ (\rho\eta)_t + \mathrm{div}(\rho\eta\mathbf{u}) = \rho w \\ (\rho w)_t + \mathrm{div}\left(\rho w \mathbf{u} - \frac{1}{4\rho\beta}\mathbf{p}\right) = \frac{\lambda}{\beta}\left(1 - \frac{\eta}{\rho}\right) \\ \mathbf{p}_t + \mathrm{div}\left((\mathbf{p}\cdot\mathbf{u} - w)\,\mathbf{Id}\right) = 0; \qquad \mathrm{curl}(\mathbf{p}) = 0 \end{cases}$$

$$\mathbf{P} = \left(\frac{\rho^2}{2} - \frac{1}{4\rho}\left|\mathbf{p}\right|^2 + \eta\lambda(1 - \frac{\eta}{\rho})\right)\mathbf{Id} + \frac{1}{4\rho}\mathbf{p}\otimes\mathbf{p}$$

- Closed system.
- What about hyperbolicity ?
- Values of λ and β ?

One-Dimensional case : Hyperbolicity

In order to study the hyperbolicity of this system, we write it in quasi-linear form :

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}(\mathbf{U})\frac{\partial \mathbf{U}}{\partial x} = \mathbf{q}$$

where:

$$\mathbf{U} = \begin{pmatrix} \rho, u, w, p, \eta \end{pmatrix}^T \qquad \mathbf{q} = \left(0, 0, \frac{1\lambda}{\beta\rho}\left(1 - \frac{\eta}{\rho}\right), 0, w \right)^T$$

$$\mathbf{A}(\mathbf{U}) = \begin{pmatrix} u & \rho & 0 & 0 & 0 \\ 1 + \frac{\lambda\eta^2}{\rho^3} & u & 0 & 0 & \frac{\lambda}{\rho}\left(1 - \frac{2\eta}{\rho}\right) \\ \frac{p}{4\beta\rho^3} & 0 & u & -\frac{1}{4\beta\rho^2} & 0 \\ 0 & p & -1 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{pmatrix}$$

One-Dimensional case : Hyperbolicity

The eigenvalues c of the matrix $\mathbf{A}$ are :

$$c = u,\ (c-u)^2_{\pm} = \frac{\left(\frac{1}{4\beta\rho^2} + \rho + \frac{\lambda\eta^2}{\rho^2}\right) \pm \sqrt{\left(-\frac{1}{4\beta\rho^2} + \rho + \frac{\lambda\eta^2}{\rho^2}\right)^2}}{2}.$$

The right-hand side is always positive. However, the roots can be multiple if

$$\frac{1}{4\beta\rho^2} = \rho + \frac{\lambda\eta^2}{\rho^2}.$$

In the case of multiple roots : We still get five linear independent eigenvectors. $\Longrightarrow$ $\boxed{\text{the system is always hyperbolic}}$

Values of λ and β

- Values have to be assigned : a criterion is needed.
- We can base this choice, for example, on the dispersion relation.

Original DNLS dispersion relation

$$c_p^2 = \rho_0 + \frac{k^2}{4}$$

Augmented DNLS dispersion relation

$$(c_p)^2 = \frac{\frac{1}{4\beta\rho_0^2} + \rho_0 + \lambda + \frac{\lambda}{\beta\rho_0^2 k^2} - \sqrt{\left(\frac{1}{4\beta\rho_0^2} + \rho_0 + \lambda + \frac{\lambda}{\beta\rho_0^2 k^2}\right)^2 - 4\left(\frac{\lambda}{\beta\rho_0 k^2} + \frac{\rho_0 + \lambda}{4\beta\rho_0^2}\right)}}{2}$$

Example estimation

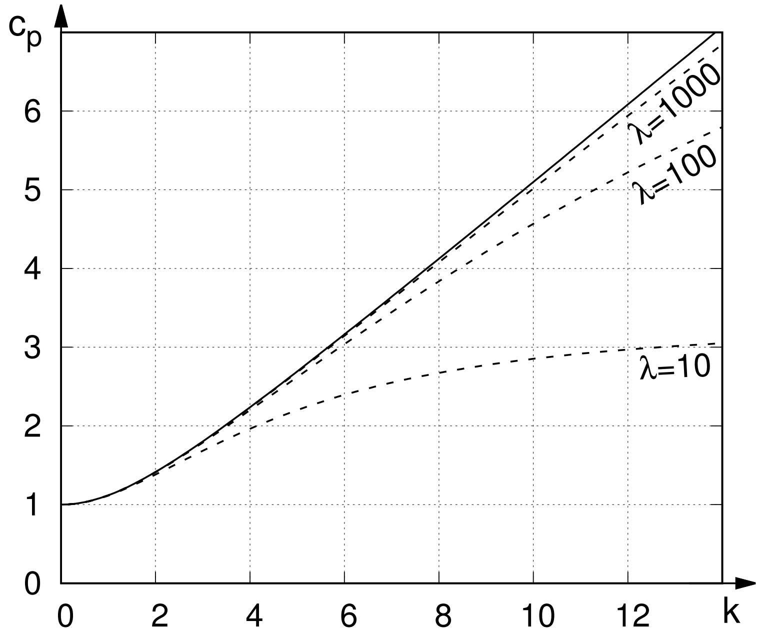

Figure 1: The dispersion relation $c_p = f(k)$ for the original model (continuous line) and the dispersion relation for the Augmented model (dashed lines) for different values of λ and for $\beta = 10^{-4}$

Numerical scheme : Hyperbolic step

1-d system of equations to solve :

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

Hyperbolic part:

1. Godunov scheme: $\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x}\left(\mathbf{F}^*_{i+\frac{1}{2}} - \mathbf{F}^*_{i-\frac{1}{2}}\right)$
2. Riemann Solver: Rusanov.

$$\mathbf{F}_{i+\frac{1}{2}} = \frac{1}{2}\left(\mathbf{F}(\mathbf{U}_{i+1}^n) - \mathbf{F}(\mathbf{U}_i^n)\right) - \frac{1}{2}\kappa^n_{i+\frac{1}{2}}\left(\mathbf{U}_{i+1}^n - \mathbf{U}_i^n\right)$$

where $\kappa^n_{i+\frac{1}{2}}$ is obtained by using the Davis approximation :

$$\kappa^n_{i+1/2} = \max_j(|c_j(\mathbf{U}_i^n)|, |c_j(\mathbf{U}_{i+1}^n)|),$$

where c_j are the eigenvalues of the Augmented system.

Numerical scheme : ODE step

Reduced to a second order ODE with constant coefficients which can be solved exactly in our case.

$$\left\{ \frac{d\rho}{dt} = 0; \quad \frac{d\rho u}{dt} = 0; \quad \frac{dp}{dt} = 0 \quad \frac{d\rho\eta}{dt} = \rho w \quad \frac{d\rho w}{dt} = \frac{\lambda}{\beta}\left(1 - \frac{\eta}{\rho}\right) \right.$$

Therefore, the exact solution is given by :

$$\begin{cases} \rho^{n+1} = \bar{\rho}^n \qquad u^{n+1} = \bar{u}^n \qquad p^{n+1} = \bar{p}^n \\ \eta^{n+1} = \bar{\rho}^n + (\bar{\eta}^n - \bar{\rho}^n)\cos(\Omega\Delta t) + \dfrac{\bar{w}^n}{\Omega}\sin(\Omega\Delta t) \\ w^{n+1} = \Omega(\bar{\rho}^n - \bar{\eta}^n)\sin(\Omega\Delta t) + \bar{w}^n\cos(\Omega\Delta t) \end{cases}$$

where $\Omega = \dfrac{\lambda}{\beta\rho^2}$.

A brief introduction to DSWs

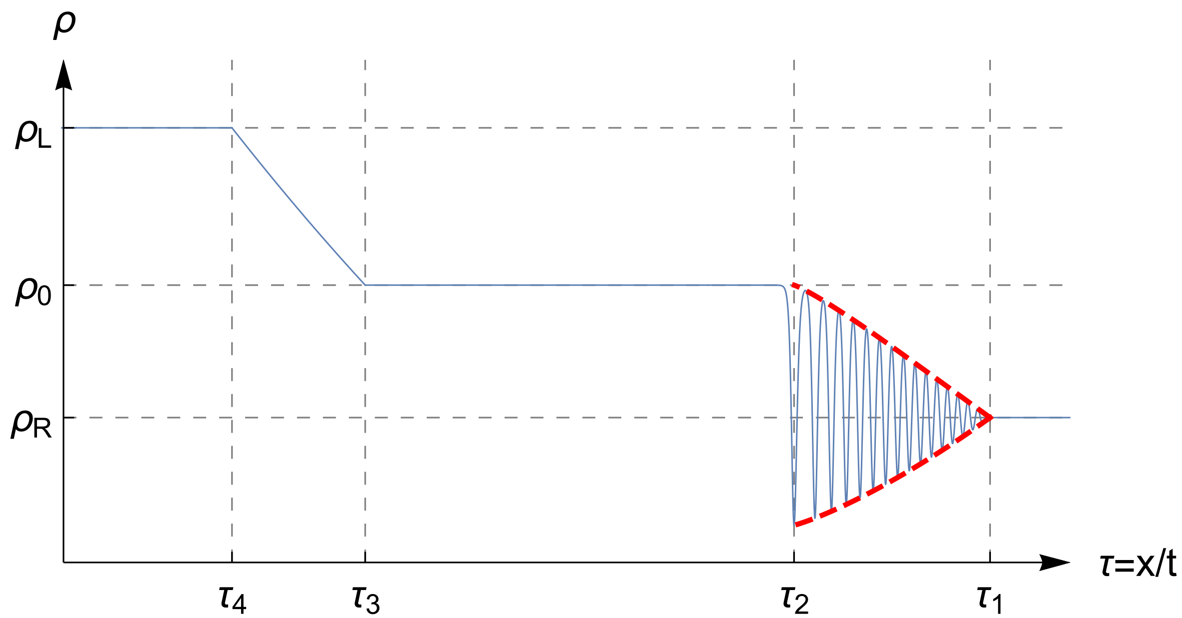

Figure 2: Asymptotic profile of the solution to NLS equation (continuous line) for the Riemann problem $\rho_L = 2$, $\rho_R = 1$, $u_L = u_R = 0$.
Oscillations shown at t=70

DSW Numerical results : ρ

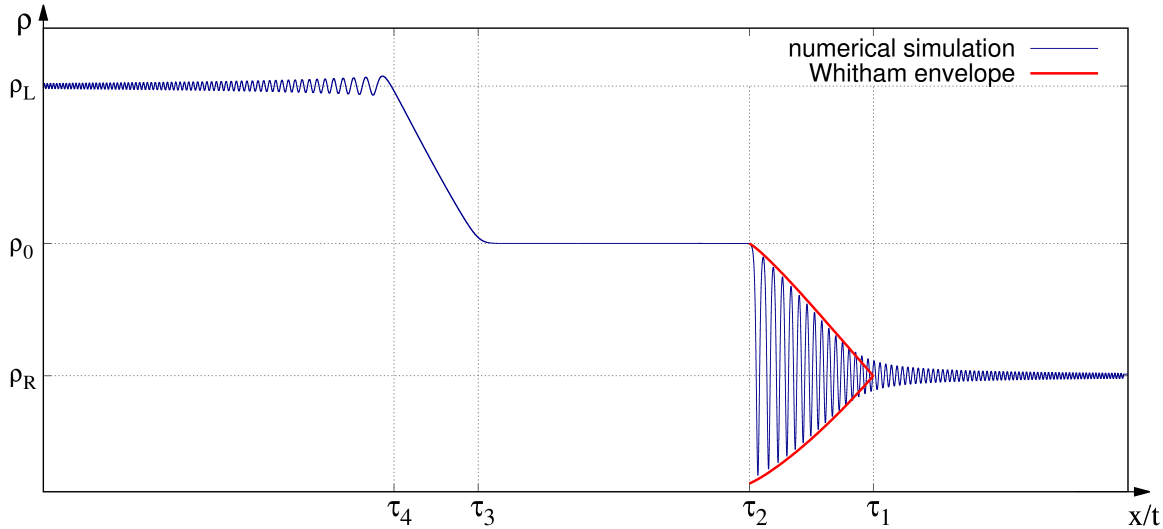

Figure 3: Comparison of the numerical result $\rho(x, t) = f(x/t)$ (blue line) with the asymptotic profile of the oscillations from Whitham's theory of modulations. t=70

DSW Numerical results : u

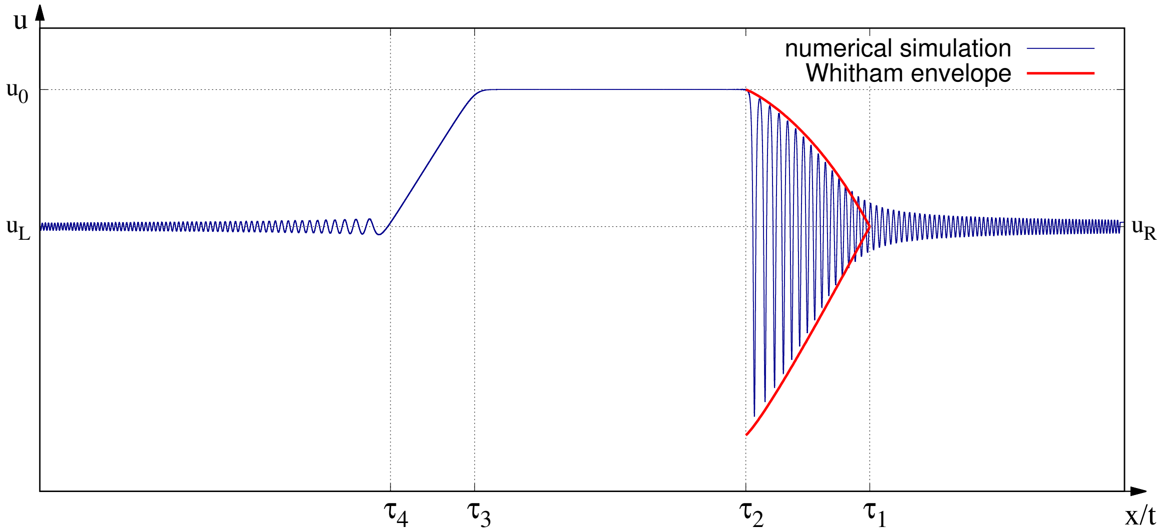

Figure 4: Comparison of the numerical result $u(x,t) = f(x/t)$ (blue line) with the asymptotic profile of the oscillations from Whitham's theory of modulations. t=70

vanishing oscillations at the left constant state

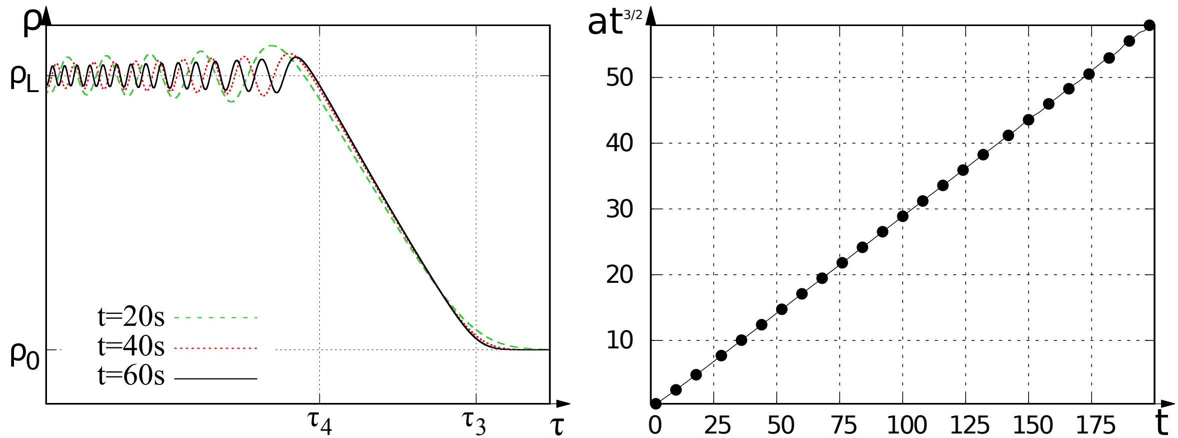

Figure 5: Vanishing oscillations at the vicinity of $\tau = \tau_4$. amplitude decreases as $\propto t^{-1/2}$.

Conclusions - perspectives

Conclusions :

- An approximate first order hyperbolic model for the defocusing nonlinear Schrödinger equation based on an augmented Lagrangian method.
- Tests were made for a non stationary solution (DSWs).

Perspectives (already done) :

- Obtained results for thin film flows with surface tension (another system of the Euler-Korteweg type)
- A more suitable numerical scheme (2nd order IMEX)

Perspectives (yet to be done) :

- Extension to the multidimensional case.
- Proper development of the boundary conditions.
- Further optimization of the numerical resolution.

Thank you for your attention :) !

F.A.Q :

- Obtaining the red envelope for the oscillatory wave train.
- What happens if you take a real discontinuity as initial condition ?
- How does the penalty method work.
- How we obtain both Euler Lagrange equations
- what boundary conditions do we use ?
- Do we have hyperbolicity in the multidimensional case ?
- Are the schemes we use Asymptotic Preserving ?
- Ensuring the curl-free constraint on $\mathbf{p}$ in multi-D.