

# Hyperbolic formulations of dispersive equations in continuum mechanics

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#### Feb 4th, 2022

# Surface tension / capillarity

- Euler-Korteweg equations : Fluid flow + <u>Surface tension</u>.
- Surface tension = Tendency of a fluid to shrink and minimize its surface.
- Examples in nature : Droplet shape, ripples on the water surface, water striders, etc...



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# Industrial applications

- Hydrophobic sprays (clothes, shoes, car glass, buildings, etc)
- Anti-icing liquids for plane wings, heating systems,...
- Nuclear evaporators, pharmaceutical applications...



Photo credits : Ave Calvar Martinez pexels.com



Colin cutler boldmethod.com

#### More theoretical examples



Photo credits (a) : Wan, W. et. al. Dispersive superfluid-like shock waves in nonlinear optics. Nature Phys 3, 46–51 (2007).

(b) : Hoefer, M. A et. al (2006). Dispersive and classical shock waves in Bose-Einstein condensates and gas dynamics. Physical Review A, 74(2).

(c) : Wikipedia, picture taken by Roger McLassus (Creative commons)

#### **Euler-Korteweg equations**

The equations write :

$$\begin{cases} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0\\ (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \rho \nabla \left( K(\rho) \Delta \rho + \frac{1}{2} K'(\rho) |\nabla \rho|^2 \right)\\ \text{where } \rho = \rho(\mathbf{x}, t), \ \mathbf{u} = \mathbf{u}(\mathbf{x}, t) \text{ and } (\mathbf{x}, t) \in \mathbb{R}^d \times [0, T] \end{cases}$$

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•  $K(\rho) = \sigma$ : Compressible flow with surface tension  $\begin{cases}
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• 
$$K(\rho) = \frac{1}{4\rho}$$
: Quantum hydrodynamics  

$$\begin{cases}
\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\
(\rho \mathbf{u})_t + \operatorname{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
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# Main objective

Given the Euler-Korteweg system of equations :

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#### **Ultimate Motivation**

Can we obtain a first-order hyperbolic reformulation of this model ?

# More than just hyperbolic

We want a new model that:

- approximates Euler-Korteweg in some limit.
- is derived from a variational principle.
- is in line with the laws of thermodynamics.
- can be solved numerically with accurate numerical methods.

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#### Hyperbolic equations

- Finite speed propagation (in line with relativity).
- Mathematically well-posed equations.
- A very rich literature on numerical methods.

# Outline

- From Euler-Korteweg to NLS equations
- 2 Hyperbolic NLS System
  - Augmented Lagrangian approach step 1
  - Augmented Lagrangian approach step 2
  - Numerical results
- 3 Thin film flows
  - Governing equations
  - Numerical results
- 4 Hyperbolic Navier-Stokes-Korteweg equations
  - The equations
  - Numerical results

# 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)

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

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

 $\Rightarrow$  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:

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

 $\begin{vmatrix} \mathsf{Hamilton's principle} : a = \int_{t_0}^{t_1} \mathcal{L} \, dt \\ + \\ \mathsf{Differential constraint} : \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \end{aligned}$ 

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

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

# Augmented Lagrangian - Attempt 1

Original Lagrangian

$$\mathcal{L}(\mathbf{u}, \rho, \nabla \rho) = \int_{\Omega_t} \left( \rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla \rho|^2}{2} \right) d\Omega$$
$$\rho_t + \operatorname{div}(\rho \mathbf{u}) = 0$$

#### '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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# Augmented Lagrangian - Attempt 1

**Original Lagrangian** 

$$\mathcal{L}(\mathbf{u}, \rho, \nabla \rho) = \int_{\Omega_t} \left( \rho \frac{|\mathbf{u}|^2}{2} - \frac{\rho^2}{2} - \frac{1}{4\rho} \frac{|\nabla \rho|^2}{2} \right) d\Omega$$
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 $\implies$  Time to derive the Euler-Lagrange equations !

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# Hints on calculus of variations

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

$$\delta \mathbf{x}$$

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

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• 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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•  $\eta$  variation  $(\delta \eta)$  :

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

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Winter School 2022, Trento

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#### Preliminary system

Thus the system of governing equations now writes :

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

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The obtained system :

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- × has an elliptic constraint.

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

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

# 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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 $\rho \sim 1$ 

## Augmented Lagrangian - Attempt 2

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

 $\tilde{c}$  (---  $\nabla$  c  $\dot{\nabla}$ 

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

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Order reduction

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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

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

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② We denote 
$$\mathbf{p}=
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 Again take :

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 Again take :

$$\nabla w = \nabla (\eta_t + \mathbf{u} \cdot \nabla \eta)$$

$$\implies \qquad \left| \mathbf{p}_t + \operatorname{div}((\mathbf{p} \cdot \mathbf{u} - w)\mathbf{I}_d) = 0 \right|$$

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2) We denote 
$$\mathbf{p}=
abla\eta.$$
 Again take :

$$\nabla w = \nabla (\eta_t + \mathbf{u} \cdot \nabla \eta)$$

$$\implies \qquad \mathbf{p}_t + \operatorname{div}((\mathbf{p} \cdot \mathbf{u} - w)\mathbf{I}_d) = 0$$

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

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

### 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 ?

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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- Main question : Is this system hyperbolic ?
- $\Rightarrow$  Strongly hyperbolic in one dimension of space.
- $\Rightarrow$  Weakly hyperbolic in multi-dimensions.

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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

- Main question : Is this system hyperbolic ?
- $\Rightarrow$  Strongly hyperbolic in one dimension of space.
- ⇒ Weakly hyperbolic in multi-dimensions. + curl constraint

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

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- Main question : Is this system hyperbolic ?
- $\Rightarrow$  Strongly hyperbolic in one dimension of space.
- $\Rightarrow$  Weakly hyperbolic in multi-dimensions. + curl constraint
  - $\Rightarrow$  Strongly hyperbolic upgrade proposed in *Busto & al. 2021*.

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

# 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:

$$\begin{aligned} \xi_{1} &= u &, \quad \mathbf{v_{1}} = \left(\frac{\rho}{\alpha\rho^{3} + \eta^{2}}, 0, 0, \frac{p}{\alpha\rho^{3} + \eta^{2}}, \frac{1}{2\eta - \rho}\right)^{T} \\ \xi_{2} &= u + \frac{1}{2\rho\sqrt{\beta}} &, \quad \mathbf{v_{2}} = (0, 0, \sqrt{\beta}, 2, 0)^{T} \\ \xi_{3} &= u - \frac{1}{2\rho\sqrt{\beta}} &, \quad \mathbf{v_{3}} = (0, 0, -\sqrt{\beta}, 2, 0)^{T} \\ \xi_{4} &= u + \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}} &, \quad \mathbf{v_{4}} = (\rho, \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}}, 0, p, 0)^{T} \\ \xi_{5} &= u - \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}} &, \quad \mathbf{v_{5}} = (\rho, -\sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}}, 0, p, 0)^{T} \end{aligned}$$

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

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

### 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  $\lambda$  and for  $\beta = 10^{-4}$ 

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

# 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  $(\gamma = 1 - \frac{\sqrt{2}}{2})$ :

$$\begin{aligned} \mathbf{U}^{\star} &= \mathbf{U}^{n} - \gamma \frac{\Delta t}{\Delta x} \left( F_{i+\frac{1}{2}}^{n} - F_{i-\frac{1}{2}}^{n} \right) + \gamma \Delta t \mathbf{S}(\mathbf{U}^{\star}) \\ \mathbf{U}^{n+1} &= \mathbf{U}^{n} - (\gamma - 1) \frac{\Delta t}{\Delta x} \left( F_{i+\frac{1}{2}}^{n} - F_{i-\frac{1}{2}}^{n} \right) - (2 - \gamma) \frac{\Delta t}{\Delta x} \left( F_{i+\frac{1}{2}}^{\star} - F_{i-\frac{1}{2}}^{\star} \right) \\ &+ (1 - \gamma) \Delta t S(\mathbf{U}^{\star}) + \gamma \Delta t S(\mathbf{U}^{n+1}) \end{aligned}$$

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

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### Grey Soliton solution



Numerical profiles of  $\rho$  (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  $U = 2, \beta = 10^{-4}, \alpha = 0.002$ .

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# Shock waves for Euler equations

Riemann problem in dispersionless hydrodynamics governed by Euler Equations :



Shockwave solution to a Riemann problem for Euler Equations.

Augmented Lagrangian approach - step 1 Augmented Lagrangian approach - step 2 Numerical results

### **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

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# DSW Numerical results : $\rho$



Comparison of the numerical result  $(\rho)$  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]

Governing equations Numerical results

# Thin film equations

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  - Governing equations
  - Numerical results
- Hyperbolic Navier-Stokes-Korteweg equations
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# Equations for thin films flow

Consider a thin film of liquid on an inclined horizontal plane which is moving under the effects of gravity :



Sketch of the setting.

Thin film flows  $\rightarrow$  Long wave approximation :  $\varepsilon = \frac{h}{L} \ll 1$ 

Governing equations Numerical results

# Governing equations

The dimensionless governing equations are obtained from Navier-Stokes equations as a leading order expansion in the long wave parameter  $\varepsilon$  [Lavalle,2015]:

$$\begin{aligned} h_t + (hU)_x &= 0\\ (hU)_t + \left(hU^2 + \frac{\cos\theta}{2F^2}h^2 + \frac{2\lambda^2}{225}h^5\right)_x &= \frac{\varepsilon\kappa_1}{F^2}hh_{xxx} + \frac{1}{\varepsilon Re}\left(\lambda h - \frac{3U}{h}\right) + o(\varepsilon)\\ Re &= \frac{\tilde{h}_N \tilde{U}_N}{\nu}, \ F = \frac{\tilde{U}_N}{\sqrt{g\tilde{h}_N}}, \ We = \frac{\rho}{\gamma}\tilde{h}_N \tilde{U}_N^2, \ \lambda = \frac{Re\sin\theta}{F^2}, \ \kappa_1 = \frac{\varepsilon F^2}{We} \end{aligned}$$

Equivalent system in dimensional variables :

$$\begin{aligned} h'_{t'} + (h'U')_{x'} &= 0\\ (h'U')_{t'} + \left(h'U'^2 + \frac{gh'^2}{2}\cos\theta + \frac{g^2\sin(\theta)^2}{\nu^2}h'^5\right)_{x'} - \frac{\sigma}{\rho}h'h'_{x'x'x'} &= gh'\sin(\theta) - \nu\frac{U'}{h'} \end{aligned}$$

Governing equations Numerical results

#### Considered system

$$\begin{cases} h_t + (hU)_x = 0\\ (hU)_t + \left(hU^2 + \frac{2\lambda^2}{225}h^5 + \frac{\cos\theta}{2F^2}h^2\right)_x - \frac{\varepsilon\kappa_1}{F^2}hh_{xxx} = \frac{1}{\varepsilon Re}\left(\lambda h - \frac{3U}{h}\right) \end{cases}$$

Additional difficulties :

- Model admits inherent dissipation.
- **2** New system should preserve asymptotics in  $\varepsilon$ .

Governing equations Numerical results

# Deriving the augmented system



Governing equations Numerical results

# Deriving the augmented system



Governing equations Numerical results

# Deriving the augmented system



Governing equations Numerical results

#### Augmented system

After applying Hamilton's principle, the augmented system writes :

$$\begin{aligned} h_t + (\rho u)_x &= 0, \\ (hu)_t + \left(hu^2 + \frac{h^2 \cos\theta}{2F^2} + \frac{2\lambda^2 h^5}{225} + \frac{\varepsilon \kappa_1 p^2}{2F^2} + \frac{\eta}{\alpha} \left(1 - \frac{\eta}{h}\right)\right)_x &= \frac{1}{\varepsilon Re} \left(\lambda h - \frac{3U}{h}\right) \\ (h\eta)_t + (h\eta u)_x &= \rho w, \\ (hw)_t + \left(hwu - \frac{\varepsilon \kappa_1 p}{\beta F^2}\right)_x &= \frac{1}{\alpha\beta} \left(1 - \frac{\eta}{\rho}\right), \\ p_t + (pu - w)_x &= 0 \end{aligned}$$

 $\implies$  How to choose  $\alpha$  and  $\beta$  in this setting ?

Governing equations Numerical results

# Asymptotic study

- Too many small parameters :  $\alpha, \beta, \varepsilon$ .
- $\implies$  We pose  $\alpha = \varepsilon^m$  and  $\beta = \varepsilon^p$ .
- Expand phase velocities of both systems in  $\varepsilon$ :

$$c_p = c_{p_0} + \varepsilon c_{p_1} + \varepsilon^2 c_{p_2} + \dots$$

then choose m and p so that :



Phase speeds of both systems are consistent.

Neutral stability curves of both systems are consistent.

#### After tedious calculations

Phase speeds are consistent to 2nd order if  $\alpha = o(\varepsilon)$  and  $\beta = o(\varepsilon^3)$ 

What about stability analysis ?

Governing equations Numerical results

### Stability analysis



Neutral stability curves in the (k, Re) plane for the original model (blue continuous line) and the augmented model for various scalings of  $\alpha$  and  $\beta$  with respect to  $\varepsilon$ . Parameters are  $\theta = 6.4^{\circ}$ , We = 0.184, F = 0.847 and  $\varepsilon = 0.006$ .

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### One last step before results

In order to compare with experimental results, 2nd order viscosity must be added to the model :

$$(hu)_t + \left(hu^2 + \frac{h^2}{2F^2}\cos\theta + \frac{2\lambda^2 h^5}{225}\right)_x = \frac{1}{\varepsilon Re} \left(\lambda h - \frac{3u}{h}\right) + \frac{\varepsilon \kappa_1}{F^2} hh_{xxx} + \frac{9\varepsilon}{2Re} (hu_x)_x$$

On the discrete level, we use centered finite differences :

$$(hu_x)_x = \left( (hu_x)_{i+\frac{1}{2}} - (hu_x)_{i-\frac{1}{2}} \right) / \Delta x$$
$$(hu_x)_{i+\frac{1}{2}} = h_{i+\frac{1}{2}} \left( u_{i+1} - u_{i-1} \right) / \Delta x$$

From Euler-Korteweg to NLS equations Hyperbolic NLS System Thin film flows

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Hyperbolic Navier-Stokes-Korteweg equations

# Liu & Gollub's experiment (1994)



Dimensionless water height as a function of space (dimensioned), in the setting of the Liu & Gollub experiment, for an imposed frequency of 1.5Hz. (Obtained through numerical simulation). Parameters used here are : Re = 19.33,  $\kappa = 1.440.10^{-4}$ , Fr = 0.8476,  $\theta = 6.4^{\circ}$ 

Governing equations Numerical results

### Results for different frequencies



Governing equations Numerical results

# Thorough comparison for 1.5Hz



Superimposed numerical simulation with the experimental result for  $\tilde{f} = 1.5 Hz$ .

- $\implies$  Very good agreement in both shape and values.
- $\implies$  Involved waveslengths are correctly captured by the model.

Governing equations Numerical results

### Test for a nonlinear surface tension

the same approach was used in the case of a nonlinear surface tension term :

$$\mathcal{L} = \int_{\Omega_t} \left( \frac{1}{2} \tilde{h} \tilde{U}^2 - \frac{1}{2} g \tilde{h}^2 - \frac{\sigma}{\rho} \sqrt{1 + \tilde{h}_{\tilde{x}}^2} \right) d\Omega$$

Corresponding augmented Lagrangian is given by :

$$\mathcal{L} = \int_{\Omega_t} \left( \frac{1}{2} \tilde{h} \tilde{U}^2 + \frac{1}{2} \tilde{\beta} \tilde{h} \tilde{w}^2 - \frac{1}{2} g \tilde{h}^2 - \frac{\sigma}{\rho} \sqrt{1 + \tilde{p}^2} + \frac{\tilde{h}}{2\tilde{\alpha}} \left( 1 - \frac{\tilde{\eta}}{\tilde{h}} \right)^2 \right) d\Omega$$

 $\implies$  Corresponding system of equations is shown hyperbolic.

Governing equations Numerical results

# Results



Comparison of the obtained numerical results (solid lines) with the converged numerical solutions shown in *Bresch et.al* [2020] (dots), at t = 5ms. Parameters used here are  $g = 9.81m.s^{-2}$ ,  $\sigma = 0.0728Kg.s^{-2}$ ,  $\rho = 1000Kg.m^{-3}$ ,  $h_0 = 2.725mm$ .  $\tilde{\alpha} = 10^{-3}m^{-2}s^2$  and  $\tilde{\beta} = 10^{-5}$ . Results are shown with a mesh resolution of n = 5000.

Governing equations Numerical results

# Preliminary conclusion

- A generic approach to build a first order hyperbolic approximation of Euler-Korteweg equations was developed.
- Analytical, asymptotic and numerical comparisons between the original and augmented system were done.
- Numerical results have shown very good agreement for two specific systems : Defocusing NLS and thin films flows in stationary and non stationary cases.
- Extension to nonlinear forms of capillary term was shown successful.

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Governing equations Numerical results

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- Extension to nonlinear forms of capillary term was shown successful.
- × Still used finite differences ( $\times$ ) for Laplace operator ( $\times \times \times$ ).
- X Model is not perfectly hyperbolic for viscous flows.

The equations Numerical results

# Hyperbolic Navier-Stokes-Korteweg equations

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  - The equations
  - Numerical results

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# Navier-Stokes-Korteweg systems

Viscous tensor is added to Euler-Korteweg equations:

$$\begin{cases} \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0\\ (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \underline{\underline{K}} + \underline{\underline{S}} \end{cases}$$

where the (dispersive) Korteweg stress tensor is given by:

$$\underline{\underline{K}} = \rho \nabla \left( K(\rho) \Delta \rho + \frac{1}{2} K'(\rho) |\nabla \rho|^2 \right)$$

and the (viscous) Navier-Stokes stresses are given by

$$\underline{\underline{S}} = \mu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} \operatorname{div}(\mathbf{u}) \mathbf{I} \right)$$
The equations Numerical results

## General difficulties with NSK system

Main difficulties are given by

- Nonlinear High-order terms.
- **2** Very constricting CFL time-stepping.
- Often coupled with non-convex equations of state (unphysical negative pressure), for example

$$p = \frac{\rho RT}{1 - b\rho} - a\rho^2, \qquad a > 0, \ b > 0$$

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The equations Numerical results

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- A Hyperbolic reformulation of Euler-Korteweg systems was just presented.
- A hyperbolic reformulation of Navier-Stokes Equations (Godunov-Peshkov-Romenski) was presented in the previous lecture.
- The idea : Combine both models.

The equations Numerical results

# Hyperbolic NSK = Hyperbolic EK + Hyperbolic NS

$$\begin{array}{ll} \mathsf{Ma.C} & \rho_t + \operatorname{div}(\rho \mathbf{u}) = 0 \\ \mathsf{Mo.B} & (\rho \mathbf{u})_t + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \mathbf{PId} + K(\rho)\mathbf{p} \otimes \mathbf{p} - \sigma) = 0 \\ \eta \text{ evolution} & (\rho \eta)_t + \operatorname{div}(\rho \eta \mathbf{u}) = \rho w \\ \eta - \mathsf{E-L} & (\rho w)_t + \operatorname{div}\left(\rho w \mathbf{u} - \frac{K(\rho)}{\beta}\mathbf{p}\right) = \frac{\lambda}{\beta}\left(1 - \frac{\eta}{\rho}\right) \\ \mathbf{p} \text{ evolution} & \mathbf{p}_t + \nabla\left(\mathbf{p} \cdot \mathbf{u} - w\right) = 0 \\ \mathsf{Distortion} & \mathbf{A}_t + \nabla(\mathbf{Au}) + \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)^T\right) \cdot \mathbf{u} = 0 \\ \mathsf{HM} & (\rho \mathbf{J})_t + \operatorname{div}(\rho \mathbf{J} \otimes \mathbf{u} + T\mathbf{I}) = -\rho \mathbf{H} \end{array}$$

with  $\sigma = -\rho \mathbf{A}^T E_{\mathbf{A}}$  and  $\mathbf{P}$  is the hyperbolic Korteweg stress.

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## GLM-curl cleaning approach

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# GLM-curl cleaning approach

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- By definition  $\mathbf{curl}(\mathbf{p}) = 0$ .
- Theoretically satisfied, but not numerically guaranteed.

The equations Numerical results

# GLM-curl cleaning approach

- By definition  $\mathbf{p} = \nabla \eta$ .
- By definition  $\mathbf{curl}(\mathbf{p}) = 0$ .
- Theoretically satisfied, but not numerically guaranteed.

In order to avoid spurious errors on  ${\bf curl}({\bf p})$  we use GLM-curl cleaning [3]:

$$\mathbf{p}_t - \nabla w + \left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)^T \mathbf{p} + \left(\frac{\partial \mathbf{p}}{\partial \mathbf{x}}\right) \mathbf{u} + 2a_c \rho \, \operatorname{\mathbf{curl}}(\psi) = 0$$
$$\psi_t + \left(\frac{\partial \psi}{\partial \mathbf{x}}\right)^T \mathbf{u} - \frac{a_c}{2\rho} \operatorname{\mathbf{curl}}(\mathbf{p}) = 0$$

with fast cleaning speed  $a_c$  that propagates  $\mathbf{curl}(\mathbf{p})$  errors.

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## About non-convex energy

Take barotropic Euler equations for example. Energy is given by :

$$E = W(\rho) + \frac{1}{2}\rho|\mathbf{u}|^2$$

Eigenvalues of the PDE are given by :

$$\lambda_1 = u - c, \quad \lambda_2 = u, \quad \lambda_3 = u + c$$

where c is given by :  $c = \sqrt{\rho W''(\rho)}$ .  $\implies$  Complex values for non-convex energy!.

The equations Numerical results

## Recall Hyperbolic NLS equation eigenvalues

$$\begin{split} \xi_{1} &= u &, \quad \mathbf{v_{1}} = (\frac{\rho}{\alpha\rho^{3} + \eta^{2}}, 0, 0, \frac{p}{\alpha\rho^{3} + \eta^{2}}, \frac{1}{2\eta - \rho})^{T} \\ \xi_{2} &= u + \frac{1}{2\rho\sqrt{\beta}} &, \quad \mathbf{v_{2}} = (0, 0, \sqrt{\beta}, 2, 0)^{T} \\ \xi_{3} &= u - \frac{1}{2\rho\sqrt{\beta}} &, \quad \mathbf{v_{3}} = (0, 0, -\sqrt{\beta}, 2, 0)^{T} \\ \xi_{4} &= u + \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}} &, \quad \mathbf{v_{4}} = (\rho, \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}}, 0, p, 0)^{T} \\ \xi_{5} &= u - \sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}} &, \quad \mathbf{v_{5}} = (\rho, -\sqrt{\rho + \frac{\eta^{2}}{\alpha\rho^{2}}}, 0, p, 0)^{T} \end{split}$$

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- Fast dispersive characteristics cover-up for non-convex regions!
- Restores hyperbolicity even for non-convex internal energy.

In summary

The equations Numerical results

The hyperbolic Navier-Stokes-Korteweg we propose

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The equations Numerical results

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The equations Numerical results

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The equations Numerical results

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- **(5)** generally requires usual linear in  $\Delta x$  time-stepping.

The equations Numerical results

## Ostwald Ripening with 3 bubbles



Ostwald ripening with three bubbles (Obtained with a  $P_3P_3$  ADER-DG scheme + Periodic boundary conditions + WENO3 subcell limiting on a  $96 \times 96$  grid)

The equations Numerical results

## Ostwald Ripening with 14 bubbles



Ostwald ripening test case with 14 bubbles (Obtained with a  $P_3P_3$ ADER-DG scheme + Periodic boundary conditions + WENO3 subcell limiting on a  $192 \times 192$  grid)

Firas DHAOUADI

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The equations Numerical results

## **Conclusion & Perspectives**

#### Summary :

- A first order hyperbolic reformulation of general dispersive and diffusive continuum mechanics equations is presented
- Particular attention was given to Navier-Stokes-Korteweg equations.

#### **Current concerns :**

- Flux splitting approaches to separate fast characteristics from the rest.
- Extension to more general and nonlinear energies depending on other forms of the gradient of macroscopic variables.
- Better schemes for exactly conserving the curl-free and/or divergence-free constraints.

The equations Numerical results

# Thank you

# Thank you for your attention !



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Studies in Applied Mathematics, 142(3):336–358, 2019.



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