

Metamaterials: time-domain numerical methods for dispersive and nonlinear media

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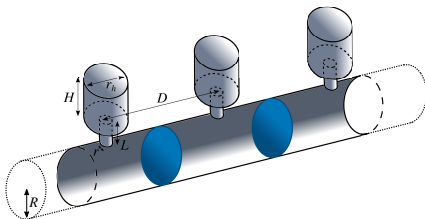
Laboratoire de Mécanique et d'Acoustique, Marseille, France

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Part I

Introduction

Example 1/3: resonant waveguide



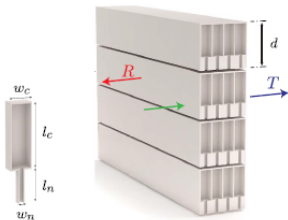
- guide connected with membranes and Helmholtz resonators (Fang et al, 2006)
 - 1D plane mode, $\lambda \gg D$: homogenization

$$\partial_x \left(\frac{1}{\hat{\rho}(\omega)} \partial_x \hat{p} \right) + \omega^2 \hat{\kappa}^{-1}(\omega) \hat{p} = 0$$

$$\left| \begin{array}{l} \hat{\rho}(\omega) = \rho_0 \left(1 - \frac{\Omega_\rho^2}{\omega^2 - \omega_\rho^2} \right), \quad \hat{\kappa}^{-1}(\omega) = \kappa_0^{-1} \left(1 - \frac{\Omega_\kappa^2}{\omega^2 - \omega_\kappa^2 - i\gamma\omega} \right) \\ \omega_\kappa = c_0 \sqrt{\frac{A}{LV}}, \quad \Omega_\kappa = \omega_\kappa \sqrt{\frac{V}{SD}}, \quad \Omega_\rho = \sqrt{\frac{K}{\rho_m}} \end{array} \right.$$

- ✓ frequency-dependence of the effective density and compressibility
- ✓ large amplitude: nonlinear Burgers' equation (Sugimoto, 1995)

Example 2/3: resonant metasurface



📖 Romero-Garcia et al, CR Physique (2020)

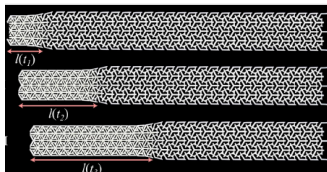
- reduction of size: thin row of **resonant scatterers**
 - subwavelength resonators ($d \ll \lambda$)
 - matched-asymptotic expansions + homogenisation = **interface** (simpler)

$$\begin{cases} \llbracket \hat{p} \rrbracket_a = \mathbf{B} \cdot \langle \nabla \hat{p} \rangle_a \\ \llbracket \hat{v} \cdot \mathbf{n} \rrbracket_a = \mathbf{C} : \langle \nabla \hat{v} \rangle_a + \mathcal{D}_\infty(\omega) \langle \operatorname{div} \hat{v} \rangle_a \end{cases}$$

$$\mathcal{D}_\infty(\omega) = \alpha_0 - \sum_{r \geq 1} \alpha_r^2 \frac{\omega^2}{\omega^2 - \omega_r^2}$$

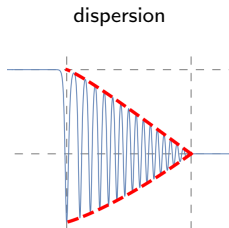
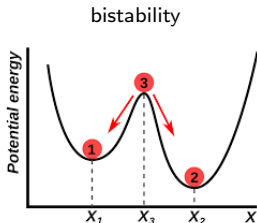
✓ **frequency-dependent** jump conditions

Example 3/3: deployable structures



Khajehtourian-Kochmann EML (2020)

- continuum approximation
 - ✓ **nonlinearities**: finite deformations + bistability
 - ✓ **dispersion**: travelling wave



Position of the problem

- **dispersion**, frequency-dependant parameters:
 - natural formulation in the frequency domain
 - in time domain: convolution products

$$\hat{\rho}(\omega) \times \hat{v}(\mathbf{x}, \omega) \mapsto \rho(t) \star v(\mathbf{x}, t)$$

✗ non-local in time, huge storage

- **nonlinearities**:

✗ generation of harmonics = difficulties in the frequency domain

✗ non-smooth solutions

✗ not uniqueness of solution

- **interface** conditions:

✗ available numerical tools?

✗ accuracy + efficiency?

Sketch of this Lecture

Objective: toolbox for time-domain simulations in metamaterials

- time-domain formulations:
 - dispersion, nonlinearity
- numerical methods:
 - schemes, splitting, interfaces
- illustration through many examples

remarks:

- ✓ no justification of models (topic of other Lectures!)
- ✓ very incomplete panel of numerical methods
- ✓ algorithms in 1D

Part II

Mathematical modeling

How to formulate resonant parameters in time?

- frequency-domain acoustics

$$\begin{cases} i\omega \hat{\rho}(\omega) \hat{\mathbf{v}} + \nabla \hat{p} = \mathbf{0} \\ i\omega \hat{\kappa}^{-1}(\omega) \hat{p} + \operatorname{div} \hat{\mathbf{v}} = 0 \end{cases}$$

frequency-dependent parameters

$$\hat{\rho}(\omega) = \rho_0 \left(1 - \frac{\Omega_\rho^2}{\omega^2 - \omega_\rho^2} \right), \quad \hat{\kappa}^{-1}(\omega) = \kappa_a^{-1} \left(1 - \frac{\Omega_\kappa^2}{\omega^2 - \omega_\kappa^2 - i\gamma\omega} \right)$$

- strategy:

formalism of **auxiliary fields** = additional fields \leadsto local-in-time PDE

✓ Maxwell equations (📖 Gralak-Tip 10, Vinales 16, Cassier-Joly 17)

✓ fractional derivatives (📖 Matignon 10)

Auxiliary fields

- conservation of momentum + effective density

$$\begin{cases} i\omega \hat{\rho} \hat{\mathbf{v}} + \nabla \hat{p} = \mathbf{0} \\ \hat{\rho}(\omega) = \rho_a \left(1 - \frac{\Omega_\rho^2}{\omega^2 - \omega_\rho^2} \right) \end{cases}$$

auxiliary field $\hat{\mathbf{w}}$

$$\begin{cases} i\omega \rho_a \hat{\mathbf{v}} + i\omega \rho_a \Omega_\rho^2 \hat{\mathbf{w}} + \nabla \hat{p} = \mathbf{0} \\ (-\omega^2 + \omega_\rho^2) \hat{\mathbf{w}} = \hat{\mathbf{v}} \end{cases}$$

inverse Fourier transform in time

$$\begin{cases} \rho_a \frac{\partial \mathbf{v}}{\partial t} + \rho_a \Omega_\rho^2 \frac{\partial \mathbf{w}}{\partial t} + \nabla p = \mathbf{0} \\ \frac{\partial^2 \mathbf{w}}{\partial t^2} + \omega_\rho^2 \mathbf{w} = \mathbf{v} \end{cases}$$

- conservation of mass + effective compressibility: auxiliary field \mathbf{r}

$$\begin{cases} i\omega \hat{\kappa}^{-1}(\omega) \hat{p} + \text{div } \hat{\mathbf{v}} = 0 \\ \hat{\kappa}^{-1}(\omega) = \kappa_a^{-1} \left(1 - \frac{\Omega_\kappa^2}{\omega^2 - \omega_\kappa^2 - i\gamma\omega} \right) \end{cases} \Rightarrow \begin{cases} \frac{\partial p}{\partial t} + \Omega_\kappa^2 \frac{\partial \mathbf{r}}{\partial t} + \kappa_a \text{div } \mathbf{v} = 0 \\ \frac{\partial^2 \mathbf{r}}{\partial t^2} + \gamma \frac{\partial \mathbf{r}}{\partial t} + \omega_\kappa^2 \mathbf{r} = p \end{cases}$$

First-order augmented system

- additional auxiliary fields $\mathbf{u} = \frac{\partial \mathbf{w}}{\partial t}$ and $q = \frac{\partial r}{\partial t}$

$$\left\{ \begin{array}{l} \rho(t) \star \frac{\partial \mathbf{v}}{\partial t} + \nabla p = \mathbf{0} \\ \hat{\kappa}^{-1}(t) \star \frac{\partial p}{\partial t} + \operatorname{div} \mathbf{v} = 0 \end{array} \right. \rightarrow \left\{ \begin{array}{l} \frac{\partial \mathbf{v}}{\partial t} + \frac{1}{\rho_a} \nabla p + \Omega_\rho^2 \mathbf{u} = \mathbf{0} \\ \frac{\partial p}{\partial t} + \kappa_a \operatorname{div} \mathbf{v} + \Omega_\kappa^2 q = 0 \\ \frac{\partial \mathbf{u}}{\partial t} - \mathbf{v} + \omega_\rho^2 \mathbf{w} = \mathbf{0} \\ \frac{\partial \mathbf{w}}{\partial t} - \mathbf{u} = \mathbf{0} \\ \frac{\partial q}{\partial t} - p + \gamma q + \omega_\kappa^2 r = 0 \\ \frac{\partial r}{\partial t} - q = 0 \end{array} \right.$$

- compact writing $\mathbf{U} = (\mathbf{v}, p, \mathbf{u}, \mathbf{w}, q, r)^\top$

$$\frac{\partial}{\partial t} \mathbf{U} + \sum_{j=1}^d \mathbf{A}_j \frac{\partial}{\partial x_j} \mathbf{U} = \mathbf{S} \mathbf{U} \quad (\mathbf{x} \in \mathbb{R}^d, t > 0)$$

Formulation of conservation laws

- **first-order system** with source term

$$\frac{\partial}{\partial t} \mathbf{U} + \sum_{j=1}^d \frac{\partial}{\partial x_j} \mathbf{f}_j(\mathbf{U}) = \mathbf{g}(\mathbf{U}), \quad (\mathbf{x} \in \mathbb{R}^d, t > 0)$$

\mathbf{f}_j **flux** function, \mathbf{g} **relaxation** + **diffusion** term

divergence theorem: variation of \mathbf{U} = flux on boundary + variation in volume

- 1D examples:

- linear advection: $\partial_t u + a \partial_x u = 0$

- linear advection-reaction: $\partial_t u + a \partial_x u = -\alpha u$

- inviscid Burgers: $\partial_t u + \partial_x \left(\frac{u^2}{2} \right) = 0$

- nonlinear elasticity: $\partial_t \mathbf{U} + \partial_x \mathbf{f}(\mathbf{U}) = \mathbf{0}$

$$\mathbf{U} = (\varepsilon, v)^\top, \quad \mathbf{f}(\mathbf{U}) = \left(-v, -\frac{1}{\rho} \sigma(\varepsilon) \right)^\top, \quad \text{with } \sigma(\varepsilon) \text{ **constitutive law**}$$

Hyperbolic PDEs

$$\frac{\partial}{\partial t} U + \sum_{j=1}^d \frac{\partial}{\partial x_j} f_j(U) = g(U)$$

- jacobians $A_j = \frac{\partial}{\partial U} f_j(U)$

- space dimension $d > 1$: $\mathbf{k} = (k_1, \dots, k_d)^\top \in \mathbb{R}^d$, $A(\mathbf{k}) = \sum_{j=1}^d k_j A_j$

Property (hyperbolicity)

The system is hyperbolic if the matrix $A(\mathbf{k})$ is diagonalizable for all $\mathbf{k} \in \mathbb{R}^d \setminus \{0\}$ with real eigenvalues.

✓ **well-posed** problem + finite velocity of energy

✓ example: 1D acoustics

$$\left| \begin{array}{l} \frac{\partial}{\partial t} U + A \frac{\partial}{\partial x} U = 0 \\ U = \begin{pmatrix} v \\ p \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ \kappa & 0 \end{pmatrix} \end{array} \right.$$

$$\text{Sp}(A) = \left\{ \pm \sqrt{\frac{\kappa}{\rho}} \right\} \Rightarrow \text{hyperbolic}$$

Property for nonlinear waves

1D homogeneous **nonlinear** system

$$\begin{cases} \frac{\partial}{\partial t} \mathbf{U} + \frac{\partial}{\partial x} \mathbf{f}(\mathbf{U}) = \mathbf{0} \\ \mathbf{U}(x, 0) = \mathbf{U}_0(x) \end{cases}$$

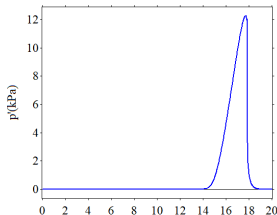
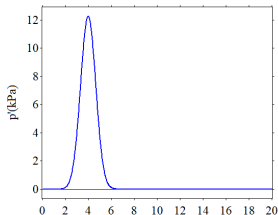
Property (shocks)

The following two properties hold:

- (i) discontinuities (ie shocks) develop in finite time t^*
- (ii) the shock speed s satisfies the Rankine-Hugonot conditions $[[\mathbf{f}(\mathbf{U})]] = s [[\mathbf{U}]]$

✓ example: Burgers 1D

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) = 0, \quad t^* = -\frac{1}{\min u'_0(x)}$$



Part III

Numerical modeling

Conservative schemes

1D **homogeneous** nonlinear system

$$\partial_t U + \partial_x f(U) = 0$$

- **finite-volume** schemes:

- uniform grid in space and time $x_i = i \Delta x$, $t_{n+1} = t_n + \Delta t$
- integration on $[x_{i-1/2}, x_{i+1/2}] \times [t_n, t_{n+1}]$
- approximations: mean value U_i^n , numerical flux $F_{i+1/2}^n$

$$U_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t_n) dx \approx U(x_i, t_n), \quad F_{i+1/2}^n \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(U(x_{i+1/2}, t)) dt$$

- **discrete conservative form**

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n)$$

- ✓ estimation of $F_{i+1/2}^n \mapsto$ families of **schemes**

Some examples (1D linear acoustics)

- notations:

- conservation law

$$\frac{\partial}{\partial t} \mathbf{U} + \mathbf{A} \frac{\partial}{\partial x} \mathbf{U} = \mathbf{0}$$

- numerical flux

$$\mathbf{F}_{i+1/2}^n \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \mathbf{A} \mathbf{U}(x_{i+1/2}, t) dt$$

- elementary schemes:

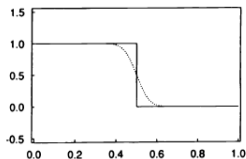
Godunov scheme ($|\mathbf{A}| = \mathbf{R} |\Lambda| \mathbf{R}^{-1}$)

$$\mathbf{F}_{i+1/2}^n = \frac{1}{2} (\mathbf{A} \mathbf{U}_i^n + \mathbf{A} \mathbf{U}_{i+1}^n) - \frac{1}{2} |\mathbf{A}| (\mathbf{U}_{i+1}^n - \mathbf{U}_i^n)$$

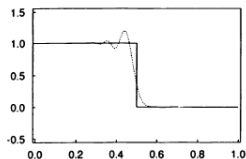
Lax-Wendroff scheme

$$\mathbf{F}_{i+1/2}^n = \frac{1}{2} (\mathbf{A} \mathbf{U}_i^n + \mathbf{A} \mathbf{U}_{i+1}^n) - \frac{\Delta t}{2 \Delta x} \mathbf{A}^2 (\mathbf{U}_{i+1}^n - \mathbf{U}_i^n)$$

Godunov



Lax-Wendroff



Numerical analysis

- **local truncation error**

- error due to one step of discretization
- example: discretization of the ODE $u' - \lambda u = 0$

Euler explicit	0	=	$\frac{u^{n+1} - u^n}{\Delta t} - \lambda u^n$
exact solution	$L(t_n)$	=	$\frac{u(t_{n+1}) - u(t_n)}{\Delta t} - \lambda u(t_n)$
Taylor expansion		=	$\frac{u(t_n) + \Delta t u'(t_n) + O(\Delta t^2) - u(t_n)}{\Delta t} - \lambda u(t_n)$
ODE		=	$\underbrace{u'(t_n) - \lambda u(t_n)}_{=0} + O(\Delta t)$

- **stability**

- linear amplification of the errors due to discretization
- Courant-Friedrichs-Lewy condition (CFL):

$$\max c \frac{\Delta t}{\Delta x} \leq 1$$

Theorem (Lax-Richtmyer)

Local error of order q + stability \Rightarrow global error of order q

Importance of the conservative form

- conservative form

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) = 0$$

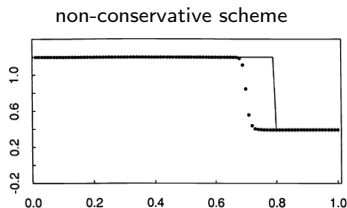
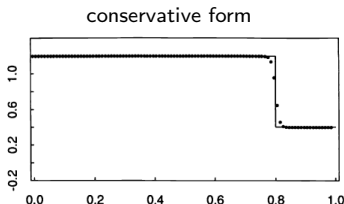
- conservative Godunov scheme

- non-conservative form (smooth solution):

$$\partial_t u + u \partial_x u = 0$$

- non-conservative scheme

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} u_i^n (u_i^n - u_{i-1}^n)$$



(LeVeque, 1993)

✓ conservative form → Rankine-Hugoniot → correct shock speed

To go further

- linear PDE: **high-order** ($k \geq 4$)

Arbitrary **DER**ivatives = **ADER** schemes

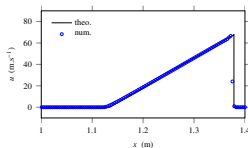
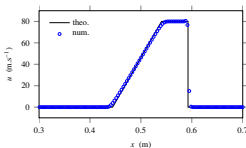
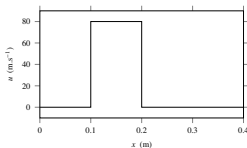
generalization of Lax-Wendroff


explicit, two-step, spatially centered

- **nonlinear PDE**

✗ non-smoothness + non-uniqueness

✓ high-order (in the smooth part) and low-order (near the shock)



 Benjamin et al, Acustica (2017)

Relaxation and dissipation

- nonlinear hyperbolic system with **linear source term**

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

✗ naive direct discretization: $\Delta t \leq \min\left(\frac{\Delta x}{c_{\max}}, \frac{2}{\varrho(S)}\right)$

Strang splitting (propagation and relaxation)

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t} U + \frac{\partial}{\partial x} f(U) = 0 \quad (H_p) \\ \frac{\partial}{\partial t} U = S U \quad (H_r) \end{array} \right.$$

$$U^{n+1} = H_r\left(\frac{\Delta t}{2}\right) \circ H_p(\Delta t) \circ H_r\left(\frac{\Delta t}{2}\right) U^n$$

- **propagation** step: finite-volume scheme with flux limiters

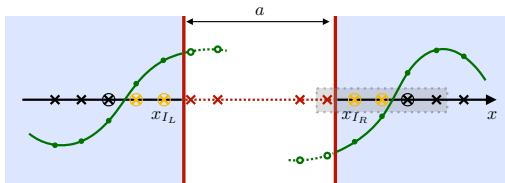
$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left(F_{i+1/2}^n - F_{i-1/2}^n \right), \quad \Delta t \leq \frac{\Delta x}{c_{\max}}$$

- **relaxation** step: exact solution

$$H_r(\tau) U_i = \exp(S\tau) U_i$$

Interfaces

- difficulties:
 - ✗ geometry: structured grid (poor geometry) vs unstructured grid (CFL $\Delta t \searrow$)
 - ✗ physics: nonlinear contacts, frequency-dependent metasurfaces, etc
 - ✗ maths: non-smoothness of the solution across interfaces
- strategy: **immersed interface method**
 - ✓ modification of the numerical values used by the scheme
 - ✓ modified values based on geometry and jump conditions
 - ✓ preprocessing step



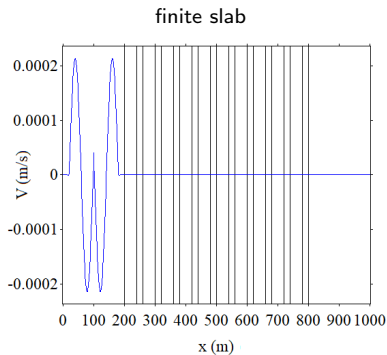
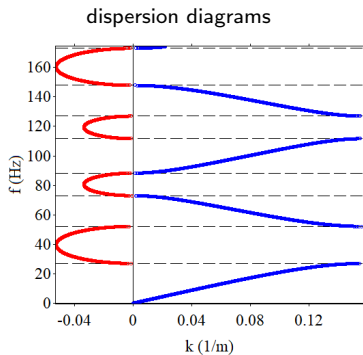
- stencil
- ✗ regular point
- ✗ irregular point
- point used in Taylor exp.
- ✗ phantom point
- numerical solution

Part IV

Numerical examples

Periodic medium 1D

- periodic medium, cell of length h
 - ✓ Bloch-Floquet theory: $U(x+h) = U(x) e^{ikh}$, k solved on a single cell
 - ✓ $k \in \mathbb{C}$: existence of **forbidden bands**
- example: $f = 30$ Hz ([video](#)), $f = 60$ Hz ([video](#))



Periodic medium 2D

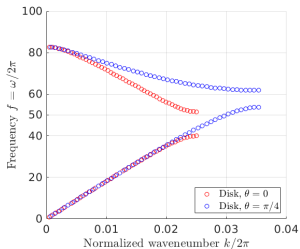
- fluid / fluid configuration

✓ $f = 30$ Hz: no gap (video)

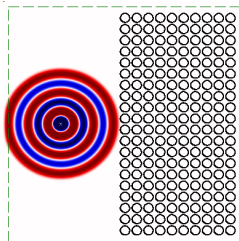
✓ $f = 45$ Hz: gap at $\theta = 0$ (video)

✓ $f = 58$ Hz: gap at $\theta = \pi/4$ (video)

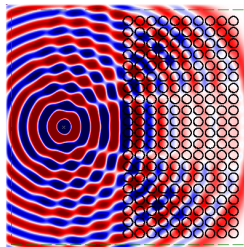
dispersion at $\theta = 0$ and $\theta = \pi/4$



$f = 45$ Hz



$f = 45$ Hz

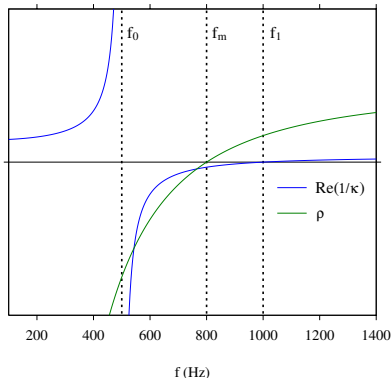


Dispersive medium 1D (1/3)

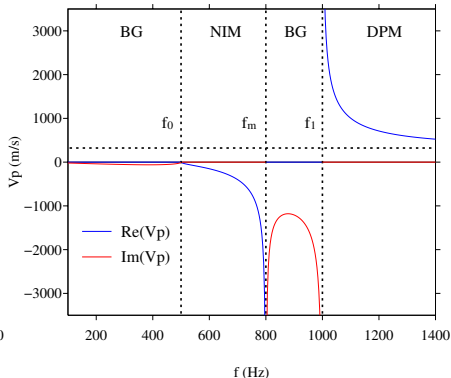
- Drude / Drude-Lorentz effective model

$$\hat{\rho}(\omega) = \rho_a \left(1 - \frac{\Omega_\rho^2}{\omega^2} \right) \quad \hat{\kappa}^{-1}(\omega) = \kappa_a^{-1} \left(1 - \frac{\Omega_\kappa^2}{\omega^2 - \omega_\kappa^2} \right)$$

effective parameters



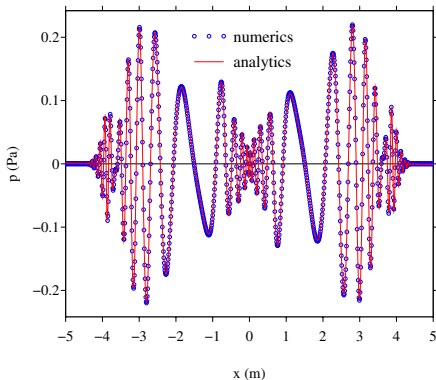
phase velocity



Dispersive medium 1D (2/3)

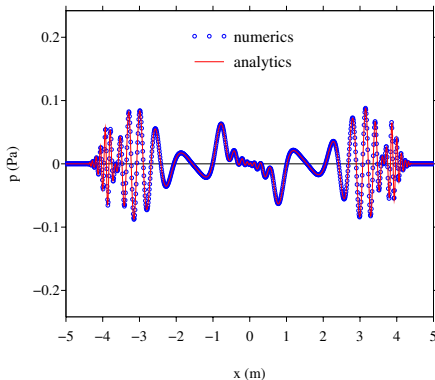
- inviscid case ($\gamma = 0$) or dissipative case ($\gamma = 400$)
- ✓ comparison with semi-analytical solution (Fourier)
- ✓ backward propagative waves at frequencies $\in [f_0, f_m]$ (NIM)
- ✓ pure sinus: [video](#)

inviscid case ($\gamma = 0 \text{ s}^{-1}$)



[video](#)

dissipative case ($\gamma = 400 \text{ s}^{-1}$)



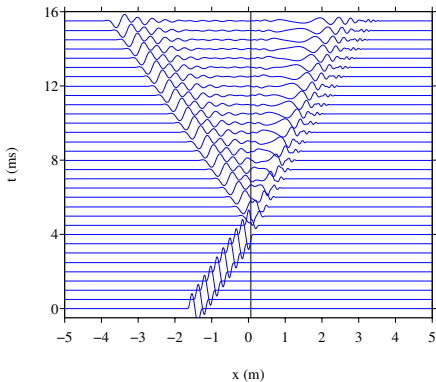
[video](#)

Dispersive medium 1D (3/3)

- interface fluid / metamaterial

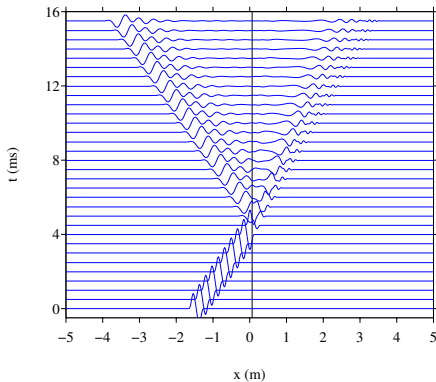
✓ **dispersive** transmitted wave

inviscid case ($\gamma = 0 \text{ s}^{-1}$)



video

dissipative case ($\gamma = 400 \text{ s}^{-1}$)

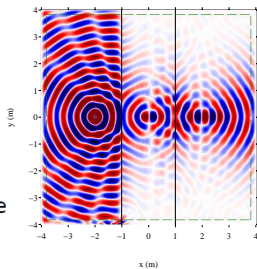
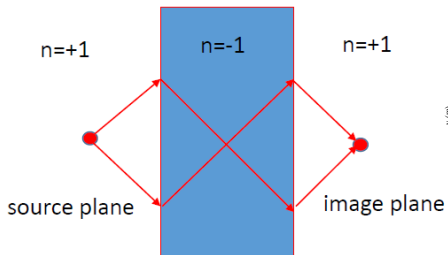


video


Dispersive medium 2D (1/2)

- Pendry Lens

- ✓ resonant medium in the slab



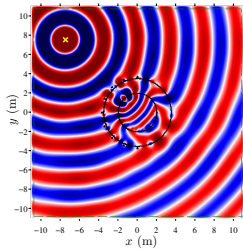
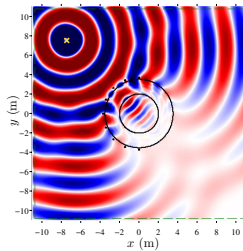
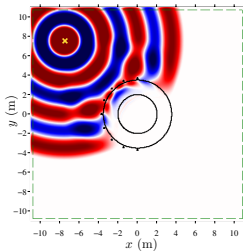
video

 Bellis-Lombard, Wave Motion 2019

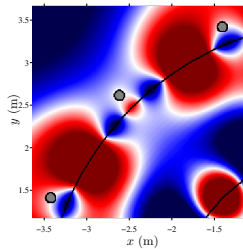
Dispersive medium 2D (2/2)

- external cloak

📖 Guenneau-Lombard-Bellis, APL (2021)




video



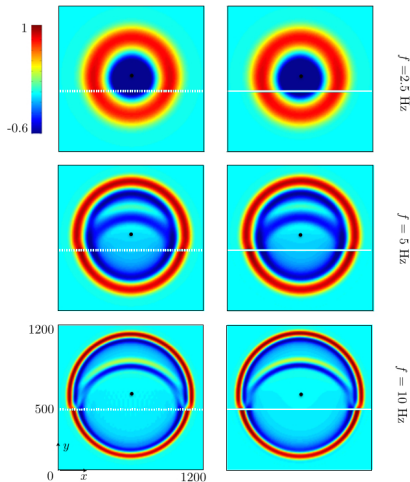
video

Interface homogenization: non-resonant case

- line of rigid scatterers

 Lombard-Maurel-Marigo, JCP (2017)

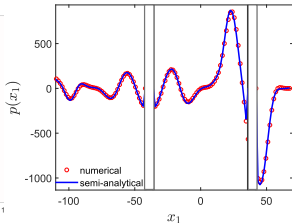
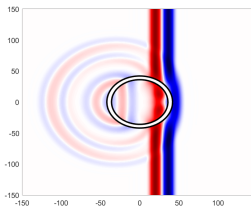
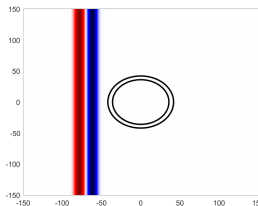
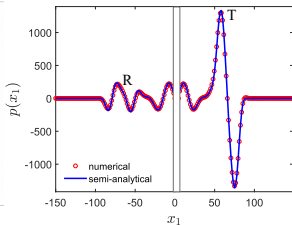
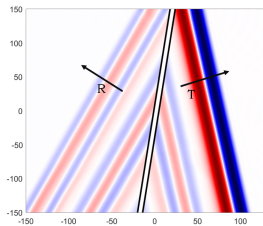
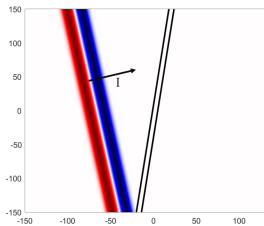
$$\begin{cases} \llbracket p \rrbracket = N \langle \partial_n p \rangle \\ \llbracket v_n \rrbracket = C_1 \langle \partial_n v_n \rangle + C_2 \langle \partial_\tau v_\tau \rangle \end{cases}$$



Interface homogenization: resonant case (1/2)


- **resonant metasurface** (Touboul-Lombard-Bellis, JCP 2020)

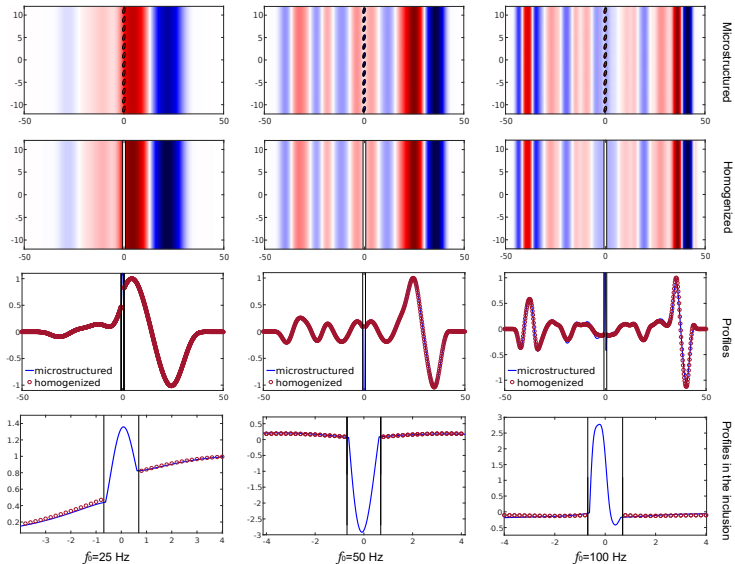
$$\begin{cases} \llbracket \hat{p} \rrbracket_a = \mathbf{B} \cdot \langle \nabla \hat{p} \rangle_a \\ \llbracket \hat{\mathbf{v}} \cdot \mathbf{n} \rrbracket_a = \mathbf{C} : \langle \nabla \hat{\mathbf{v}} \rangle_a + \mathcal{D}_\infty(\omega) \langle \text{div } \hat{\mathbf{v}} \rangle_a, \end{cases} \quad \mathcal{D}_\infty(\omega) = \alpha_0 - \sum_{r \geq 1} \alpha_r^2 \frac{\omega^2}{\omega^2 - \omega_r^2}$$



Interface homogenization: resonant case (2/2)

- full field vs homogenization

 Touboul-Pham-Maurel-Marigo-Lombard-Bellis, JElas 2020



Nonlinear media: acoustic solitons (1/2)

- guide connected with Helmholtz resonators (O. Richoux, LAUM)



📖 Sugimoto, JFM 1995

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(a u + b \frac{(u)^2}{2} \right) = c \frac{\partial^{-1/2}}{\partial t^{-1/2}} \frac{\partial u}{\partial x} + d \frac{\partial^2 u}{\partial x^2} - e \frac{\partial p}{\partial t} \\ \frac{\partial^2 p}{\partial t^2} + f \frac{\partial^{3/2} p}{\partial t^{3/2}} + g p - m \frac{\partial^2 (p)^2}{\partial t^2} + n \left| \frac{\partial p}{\partial t} \right| \frac{\partial p}{\partial t} = h u \end{cases}$$

✓ **nonlinear propagation:** a , b


✓ **oscillator:** g

✓ **coupling:** e , h

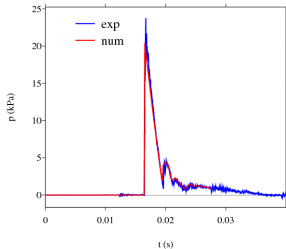
✓ **attenuation:** bulk d , fractional c and f , nonlinear m and n

Nonlinear media: acoustic solitons (2/2)

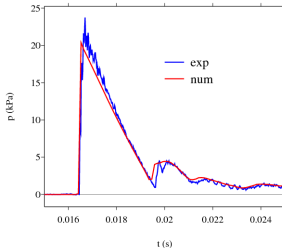
- comparisons experiences / simulations

 Richoux-Lombard-Mercier, Wave Motion 2015

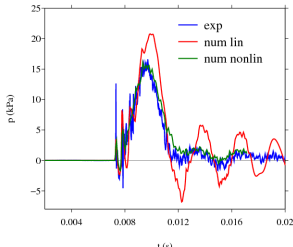
no resonators



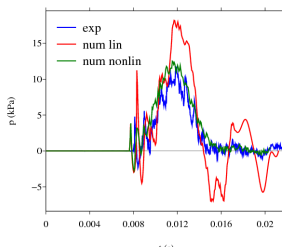
no resonators (zoom)



height $H = 7$ cm



height $H = 13$ cm



Part V

Conclusion

Take-home message

- **time-domain** studies:
 - ✓ possible even if frequency dependent parameters
 - ✓ advantages: nonlinearities, transients, etc
 - ✓ good **formalism**: hyperbolic models, conservative form, dedicated schemes
- bibliography:
 - 📖 R. LeVeque, Numerical Methods for Conservation Laws (1993)
 - 📖 M. Touboul, PhD Thesis (2021)
 - 📖 Author's webpage at LMA

Thanks for your attention!

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