COMSOL CONFERENCE
2015 BOSTON

Modeling Metamaterials with a Time-Domain Perfectly Matched Layer (PML) Formulation

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TALK OUTLINE

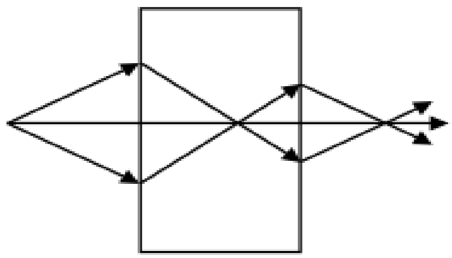
- Motivation: metamaterials
- PMLs formulation for elastic waves
- Why COMSOL?
- On stability and group velocity
- PML formulation for fluid-solid medium
- Molding metamaterial lens in time-domain
- Limitations: metamaterials within the PML
- Summary

METAMATERIALS

Veselago (1960s):

What if both **ε** and **μ** are negative?

Opposite group velocity
Negative refractive Index
Focusing using a slab



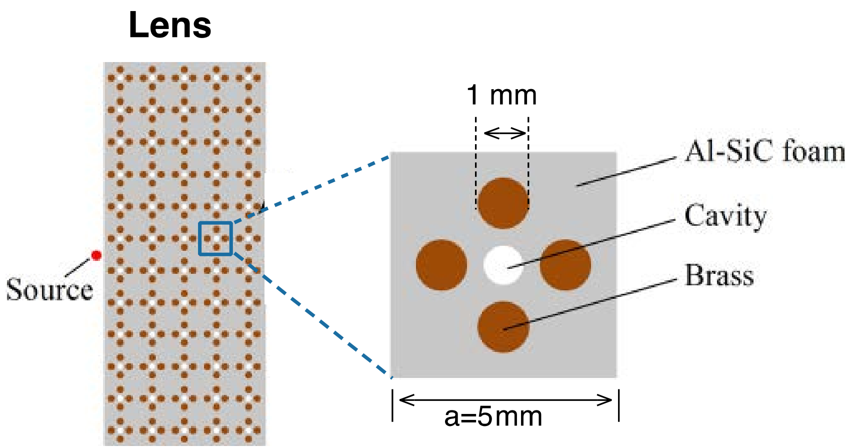
Pendry(~2000):

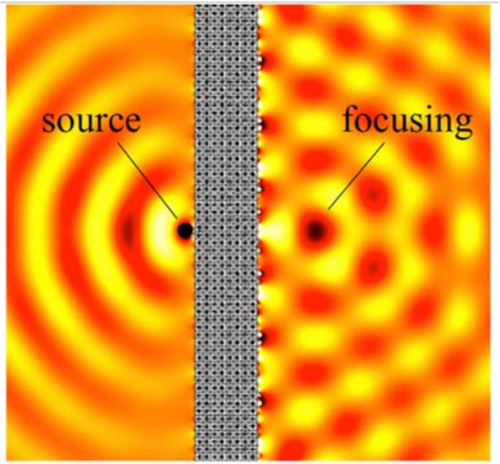
Perfect Lens: evanescent waves amplified
Transformation optics: cloaking

For **Acoustic :** It is the **density** and the **stiffness**

Acoustic metamaterials is an active area of research with potential application in acoustic insulation, filtering, cloaking, canceling out aberration, and super-lensing

MOTIVATION: ACOUSTIC SUPER-LENSING





Zhou *et al.,* Appl. Phys. Lett. 105, 233506 (2014)

a<<λ: Metamaterials with effective parameters

We want it in TIME DOMAIN using PML

CHALLENGES

PML for elastic wave equation

- Usually first order (not for COMSOL)
- Big number of equation

Komatitsch *et al* (2007)

	No PML	PML without total	PML with total	C-PML
2D	5	10	15	13
3D	9	24	33	27

- Stability for some materials

Fluid-solid coupling

- Two equation for different physics (acoustic, elastic)
- Coupling boundary conditions
- No reported PML formulation for the fluid-solid problem

Objectives

Our goal is develop time-domain models in order to simulate wave propagation in solids, fluids, and metamaterials, that are numerically efficient and easy to implement, especially for an unbounded domain.

ORIGINAL WAVE EQUATIONS IN 2D

Acoustic wave in fluids

$$\frac{1}{K}\frac{\partial^2 p}{\partial t^2} - \sum_{j=1}^{2}\frac{\partial}{\partial x_j}\left(\frac{1}{\rho_F}\frac{\partial p}{\partial x_j}\right) = 0$$

Elastic wave in solids

$$\rho_S\,\frac{\partial^2 u_i}{\partial t^2} - \sum_{j=1}^{2}\frac{\partial}{\partial x_j}\left(\sum_{k,l=1}^{2} C_{ijkl}\frac{\partial u_k}{\partial x_l}\right) = 0$$

Coupling at Fluid-solid interface

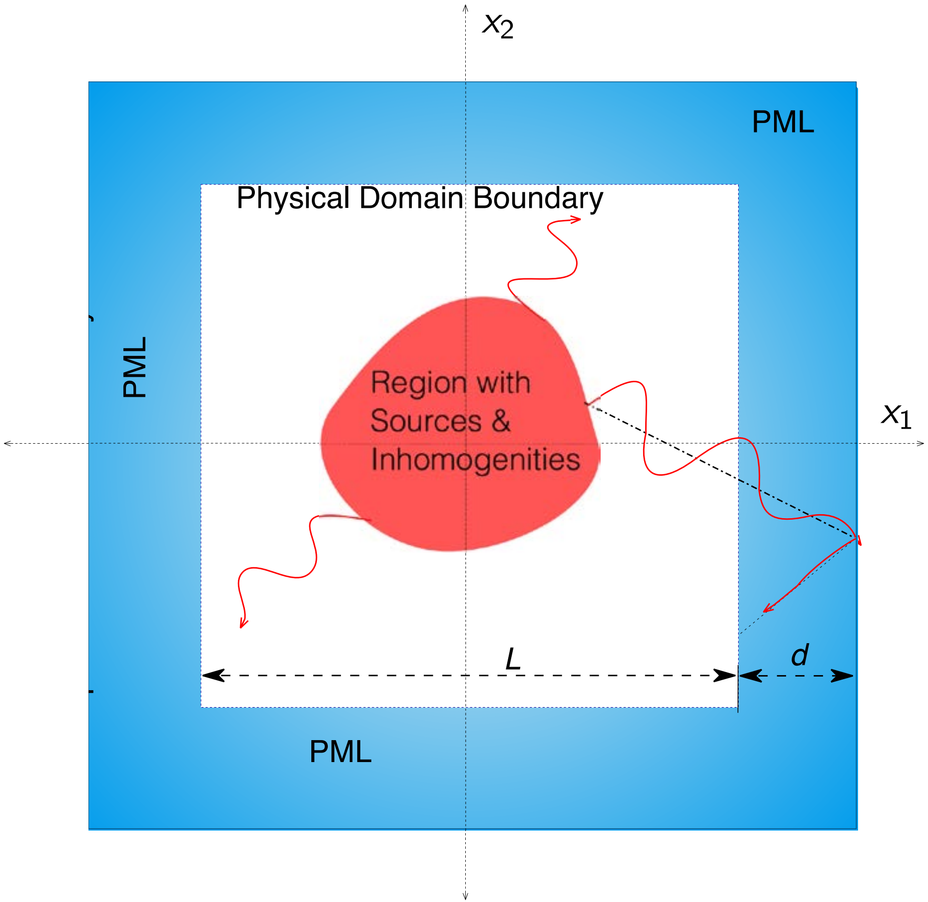
Form continuity of normal velocity:

$$\sum_{j=1}^{2} n_{F_j}\frac{1}{\rho_F}\frac{\partial p}{\partial x_j} = -\sum_{j=1}^{2} n_{F_j}\frac{\partial^2 u_j}{\partial t^2}$$

Form continuity traction:

$$\sum_{j,k,l=1}^{2} n_{S_j}\,C_{ijkl}\frac{\partial u_k}{\partial x_l} = -n_{S_i}\,p$$

Perfectly Matched Layer (PML)



PML FORMULATION FOR ELASTIC WAVES

Two second order equations (same as the original problem)+ four auxiliary equations

$$\tilde{\rho}_S \left(\frac{\partial^2 u_i}{\partial t^2} + b \frac{\partial u_i}{\partial t} + c\, u_i \right) = \sum_{j=1}^{2} \frac{\partial}{\partial x_j} \left(\sum_{k,l=1}^{2} \tilde{C}_{ijkl} \frac{\partial u_k}{\partial x_l} + a_j w_{ij} \right)$$

$$\frac{\partial w_{ij}}{\partial t} + \beta_j\, w_{ij} = \sum_{k=1}^{2} \frac{C_{ijkj}}{\alpha_j} \frac{\partial u_k}{\partial x_j},$$

$$\tilde{\rho}_S(\mathbf{x}) = \alpha_1 \alpha_2\, \rho_S$$

$$\tilde{C}_{ijkl}(\mathbf{x}) = \frac{\alpha_1 \alpha_2\, C_{ijkl}}{\alpha_j \alpha_l}$$

$$a_j(\mathbf{x}) = \frac{\alpha_1 \alpha_2}{\alpha_j} \left(\frac{\beta_1 \beta_2}{\beta_j} - \beta_j \right)$$

$$b(\mathbf{x}) = \beta_1 + \beta_2$$

$$c(\mathbf{x}) = \beta_1 \beta_2$$

And, the weak form for use in FEM (COMSOL)

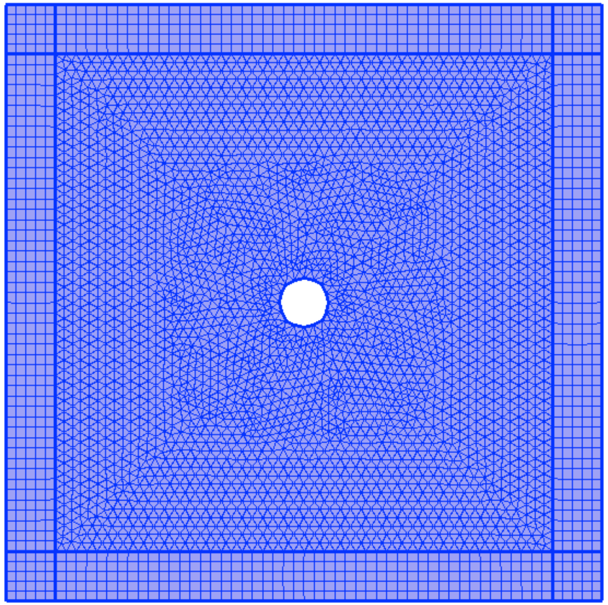
$$\int_{\Omega_S} \left[\sum_{j=1}^{2} \left(\sum_{k,l=1}^{2} \tilde{C}_{ijkl} \frac{\partial u_k}{\partial x_l} + a_j w_{ij} \right) \frac{\partial \phi_i}{\partial x_j} + \tilde{\rho}_S \left(\frac{\partial^2 u_i}{\partial t^2} + b \frac{\partial u_i}{\partial t} + c\, u_i \right) \phi_i \right] \mathrm{d}\Omega_S = 0,$$

$$\int_{\Omega_S} \left(\frac{\partial w_{ij}}{\partial t} + \beta_j\, w_{ij} - \sum_{k=1}^{2} \frac{C_{ijkj}}{\alpha_j} \frac{\partial u_k}{\partial x_j} \right) \psi_{ij}\, \mathrm{d}\Omega_S = 0$$

Assi and Cobbold, *Math. Mech. Solids*, (2015). doi: 10.1177/1081286515569266

Why Comsol ?

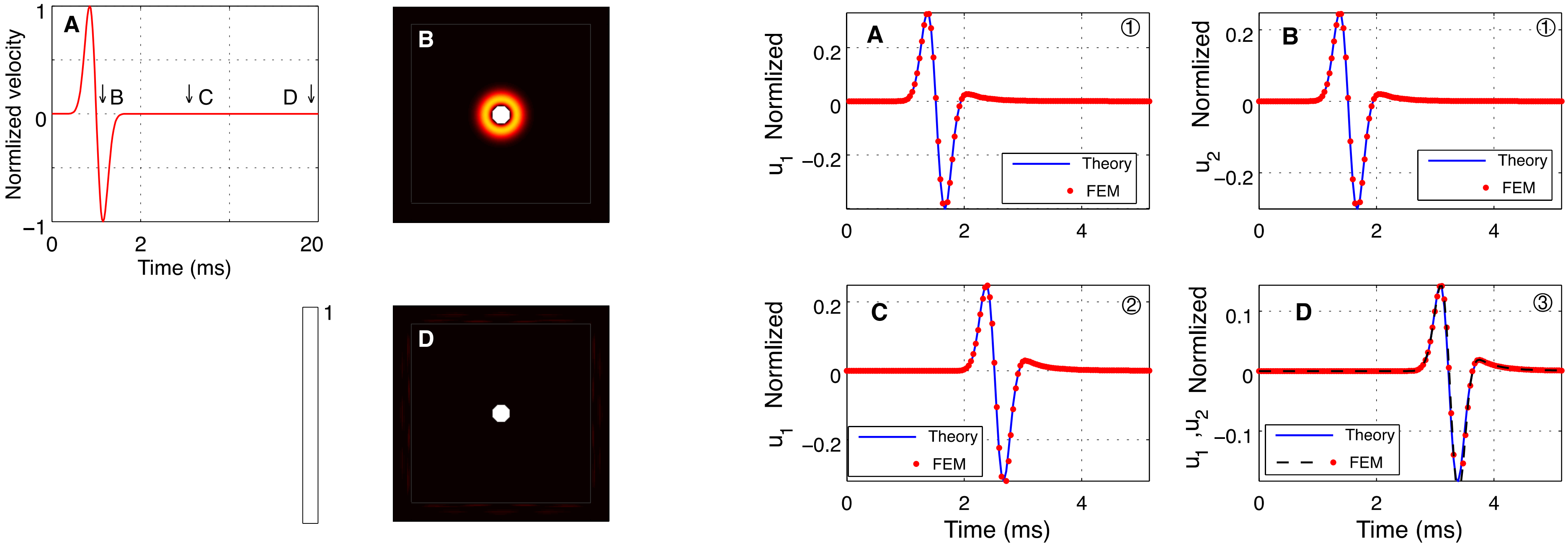
- **We need more than a black box, but we don't want to reinvent the wheel.**
- The Mathematics Interface
- Can access the mass and stiffness matrices
- FEM mesh captures the details of periodic structure better than FD grid.



$$h_0 = \frac{1}{N}\frac{c_{\min}}{f_c}$$

$$\Delta t \simeq \frac{h_0}{c_{\max}}$$

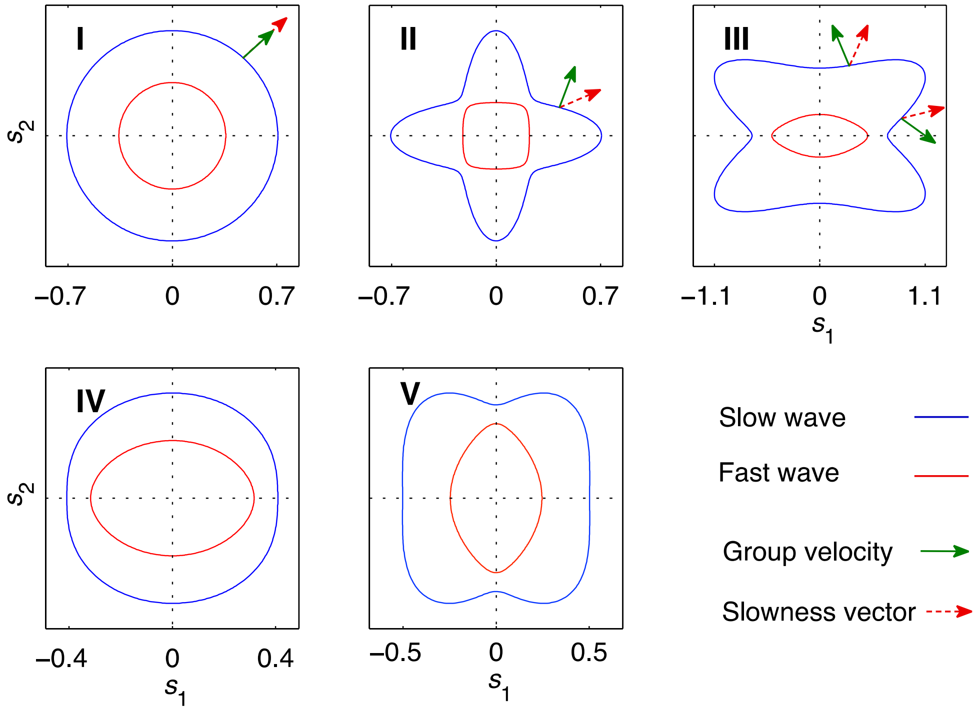
MODEL VALIDATION: ISOTROPIC SOLID



On group velocity & stability

From the dispersion relation, $F_0(\omega, k_1, k_2)$,

The **Slowness Curves**



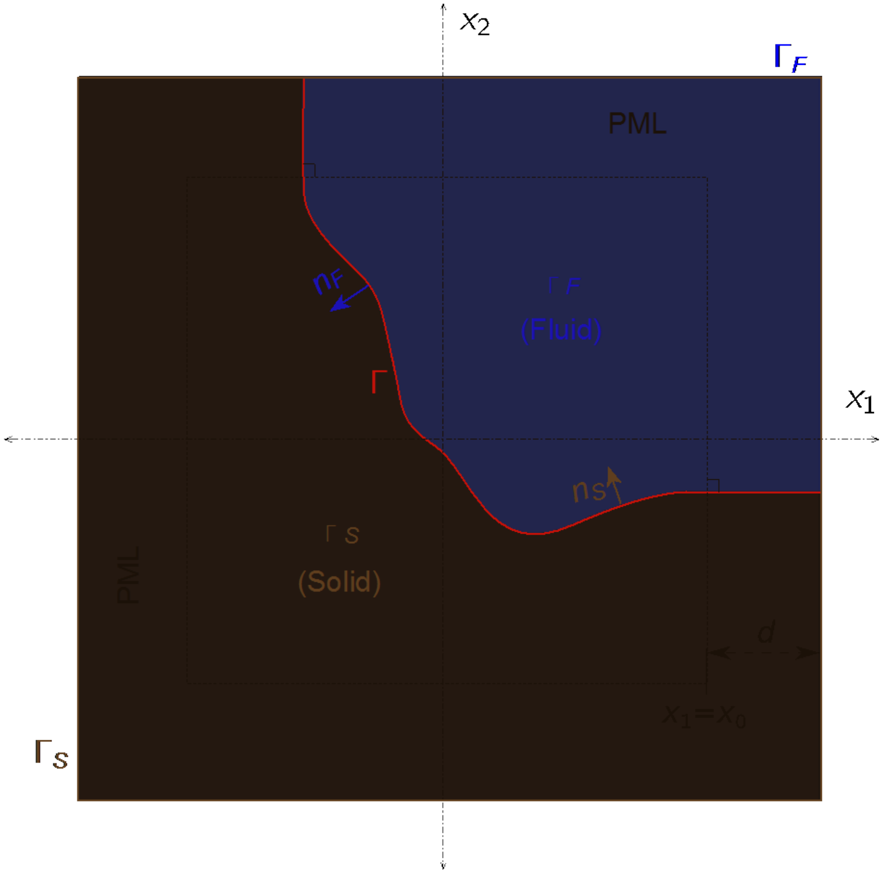
Geometric stability (Bécache *et al*, 2003): *A* necessary condition for the stability of the PML in x_j direction is:

$$S_j \times (V_g)_j \geqslant 0$$

for all points on the slowness curve.

We might have troubles in metamaterials

PML FORMULATION FOR FLUID-SOLID MEDIUM



$$
\begin{cases}
\frac{1}{\tilde{K}}\left(\frac{\partial^2 p}{\partial t^2} + b\,\frac{\partial p}{\partial t} + c\,p\right) = \sum_{j=1}^{2} \frac{\partial}{\partial x_j}\left(\frac{1}{\rho_{F_j}}\frac{\partial p}{\partial x_j} - a_j v_j\right) + F & \mathbf{x} \in \Omega_F \\
\frac{\partial v_j}{\partial t} + \beta_j v_j = \frac{-1}{\rho_F\,\alpha_j}\frac{\partial p}{\partial x_j} & \mathbf{x} \in \Omega_F \\
\tilde{\rho}_S\left(\frac{\partial^2 u_i}{\partial t^2} + b\,\frac{\partial u_i}{\partial t} + c\,u_i\right) = \sum_{j=1}^{2}\frac{\partial}{\partial x_j}\left(\sum_{k,l=1}^{2}\tilde{C}_{ijkl}\frac{\partial u_k}{\partial x_l} + a_j w_{ij}\right) & \mathbf{x} \in \Omega_S \\
\frac{\partial w_{ij}}{\partial t} + \beta_j\,w_{ij} = \sum_{k=1}^{2}\frac{C_{ijkj}}{\alpha_j}\frac{\partial u_k}{\partial x_j} & \mathbf{x} \in \Omega_S \\
\sum_{j=1}^{2} n_{F_j}\left(\frac{1}{\rho_{F_j}}\frac{\partial p}{\partial x_j} - a_j v_j\right) = -\sum_{j=1}^{2} n_{F_j}\frac{\alpha_1\alpha_2}{\alpha_j}\left(\frac{\partial^2 u_j}{\partial t^2} + \frac{\beta_1\beta_2}{\beta_j}\frac{\partial u_j}{\partial t}\right) & \mathbf{x} \in \Gamma \\
\sum_{j,k,l=1}^{2} n_{S_j}\left(\sum_{k,l=1}^{2}\tilde{C}_{ijkl}\frac{\partial u_k}{\partial x_l} + a_j w_{ij}\right) = -n_{S_i}\,\alpha_1\alpha_2\,(p + b\,P) & \mathbf{x} \in \Gamma \\
p\,(\mathbf{x}, t) = 0 & \mathbf{x} \in \Gamma_F \\
u_i\,(\mathbf{x}, t) = 0 & \mathbf{x} \in \Gamma_S.
\end{cases}
$$

Assi and Cobbold, *JASA*, (in second revsion)

...AND THE WEAK FORM

$$\int_{\Omega_F} \left[\sum_{j=1}^{2} \left(\frac{1}{\rho_{F_j}} \frac{\partial p}{\partial x_j} - a_j v_j \right) \frac{\partial \phi}{\partial x_j} + \frac{1}{\tilde{K}} \left(\frac{\partial^2 p}{\partial t^2} + b \frac{\partial p}{\partial t} + c\, p \right) \phi - F \phi \right] \mathrm{d}\Omega_F$$

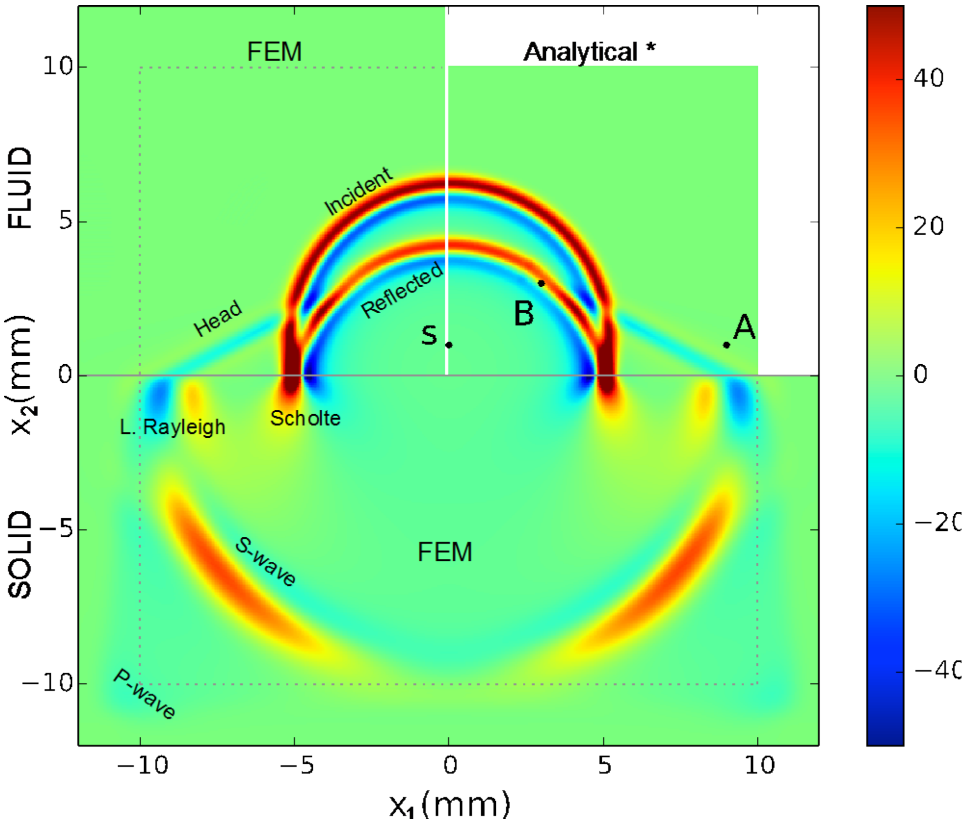
$$+ \int_{\Gamma} \sum_{j=1}^{2} n_{F_j} \frac{\alpha_1 \alpha_2}{\alpha_j} \left(\frac{\partial^2 u_j}{\partial t^2} + \frac{\beta_1 \beta_2}{\beta_j} \frac{\partial u_j}{\partial t} \right) \phi \, \mathrm{d}\Gamma = 0,$$

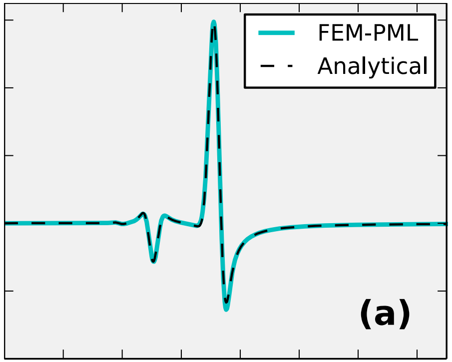
$$\int_{\Omega_S} \left[\sum_{j=1}^{2} \left(\sum_{k,l=1}^{2} \tilde{C}_{ijkl} \frac{\partial u_k}{\partial x_l} + a_j w_{ij} \right) \frac{\partial \phi_i}{\partial x_j} + \tilde{\rho}_S \left(\frac{\partial^2 u_i}{\partial t^2} + b \frac{\partial u_i}{\partial t} + c\, u_i \right) \phi_i \right] \mathrm{d}\Omega_S$$

$$+ \int_{\Gamma} n_{S_i} \alpha_1 \alpha_2 \left(p + b\, P \right) \phi_i \, \mathrm{d}\Gamma = 0,$$

\+ The auxiliary equations

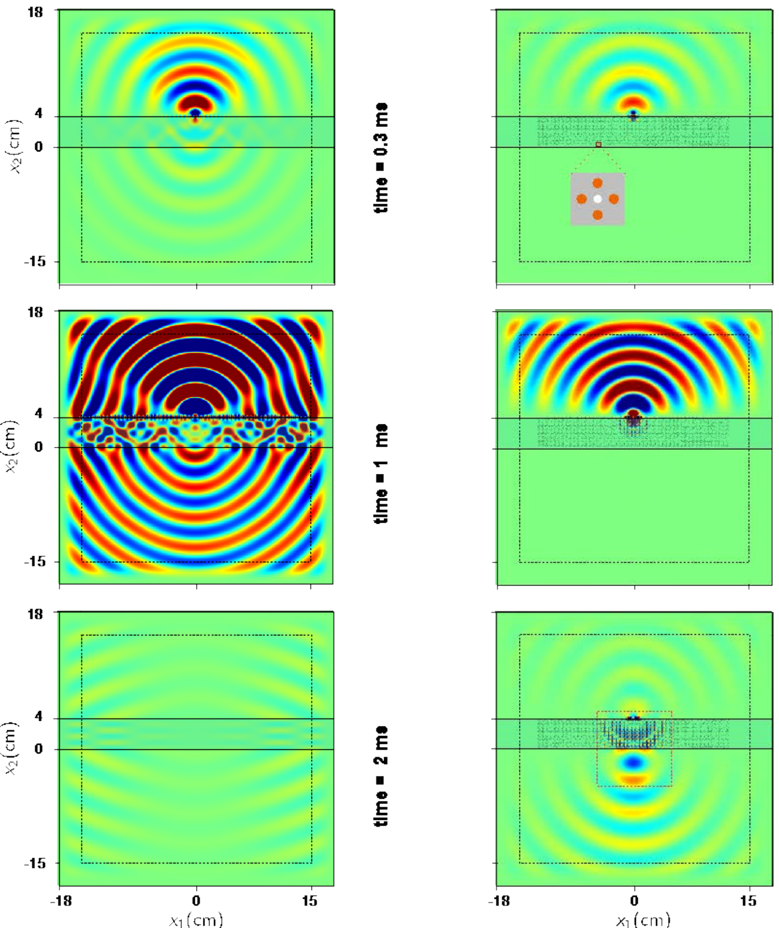
MODEL VALIDATION

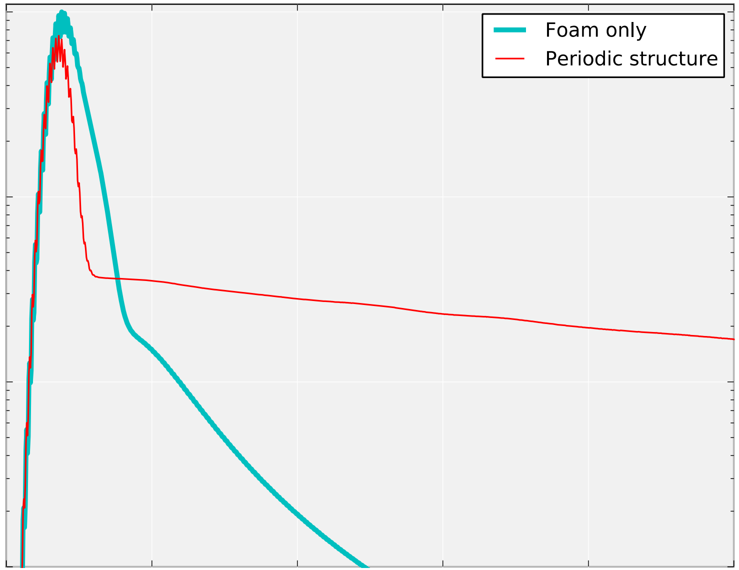




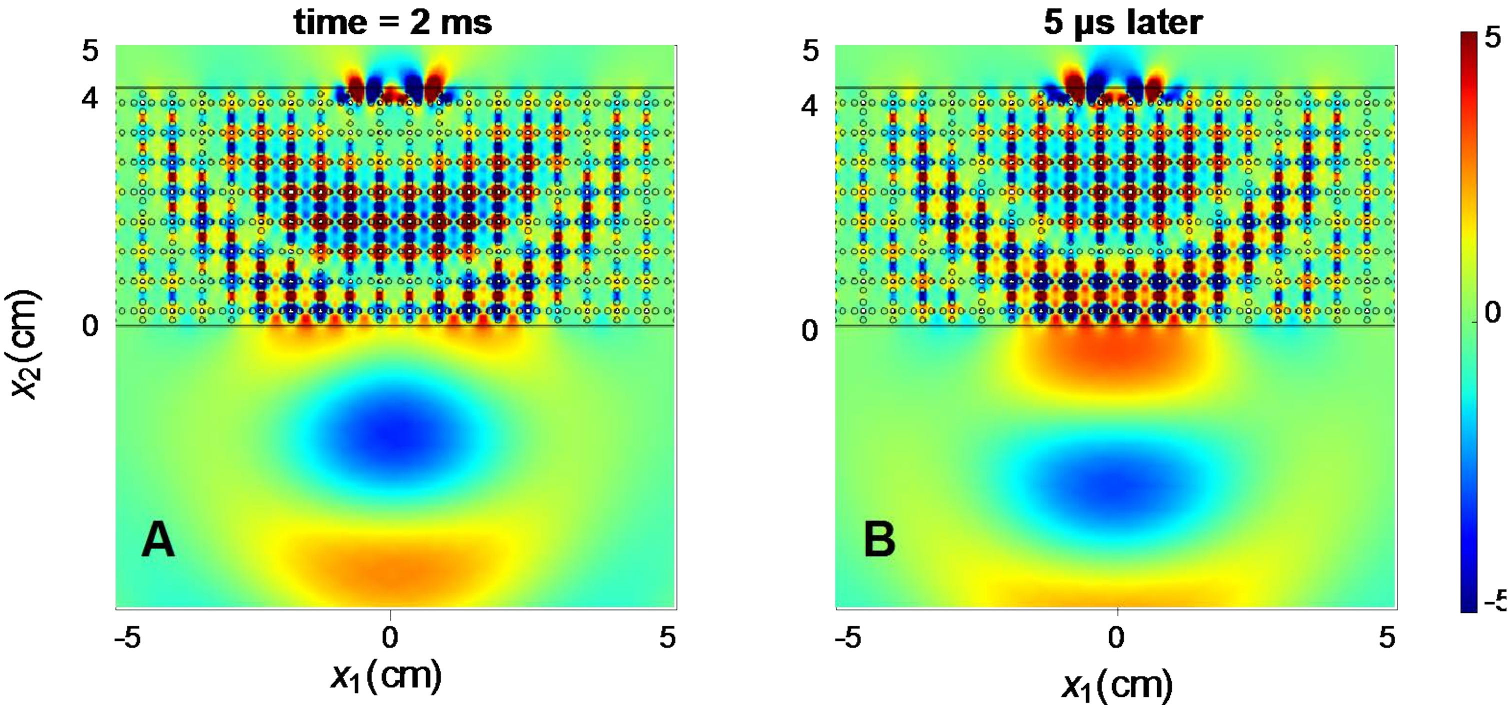
* de Hoop *et al.* (1983). *JASA*, *74*(1), 333–342.

INFINITE SOLID SLAB IN WAVER: METAMATERIALS LENS



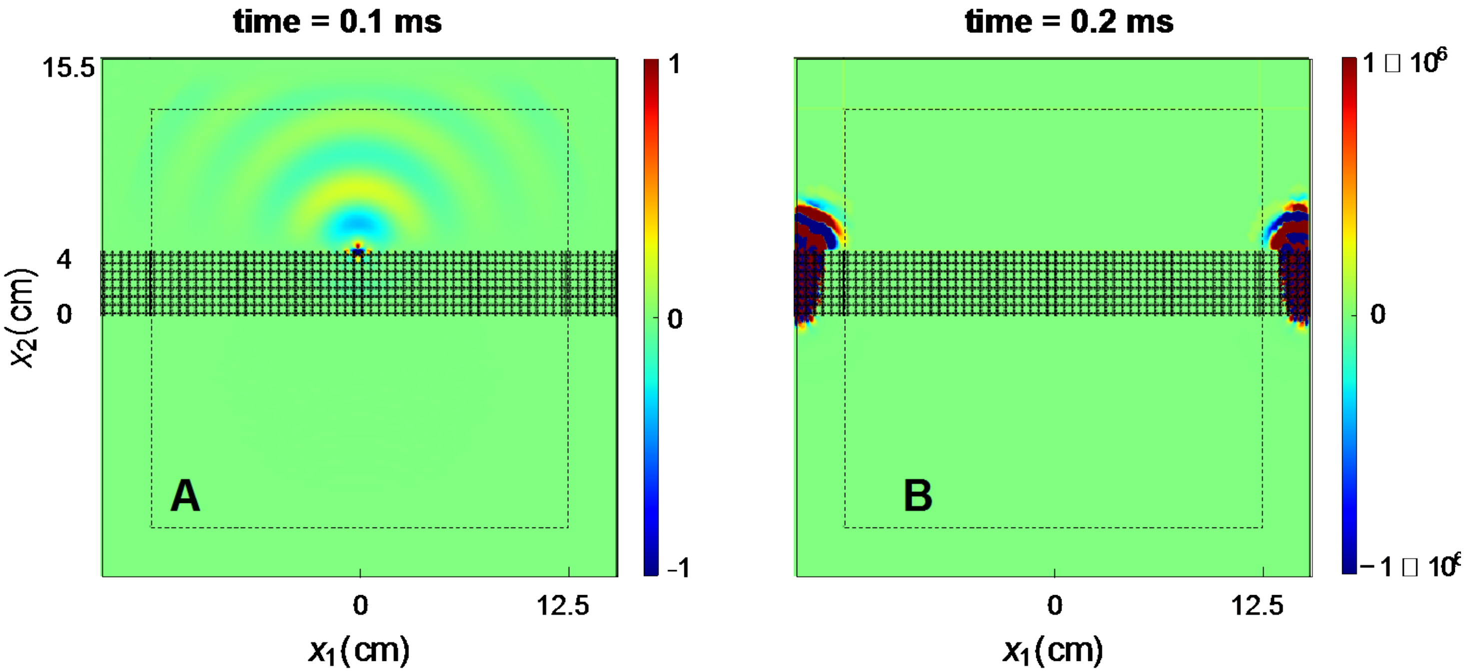


... AND ZOOM IN SPACE AND TIME

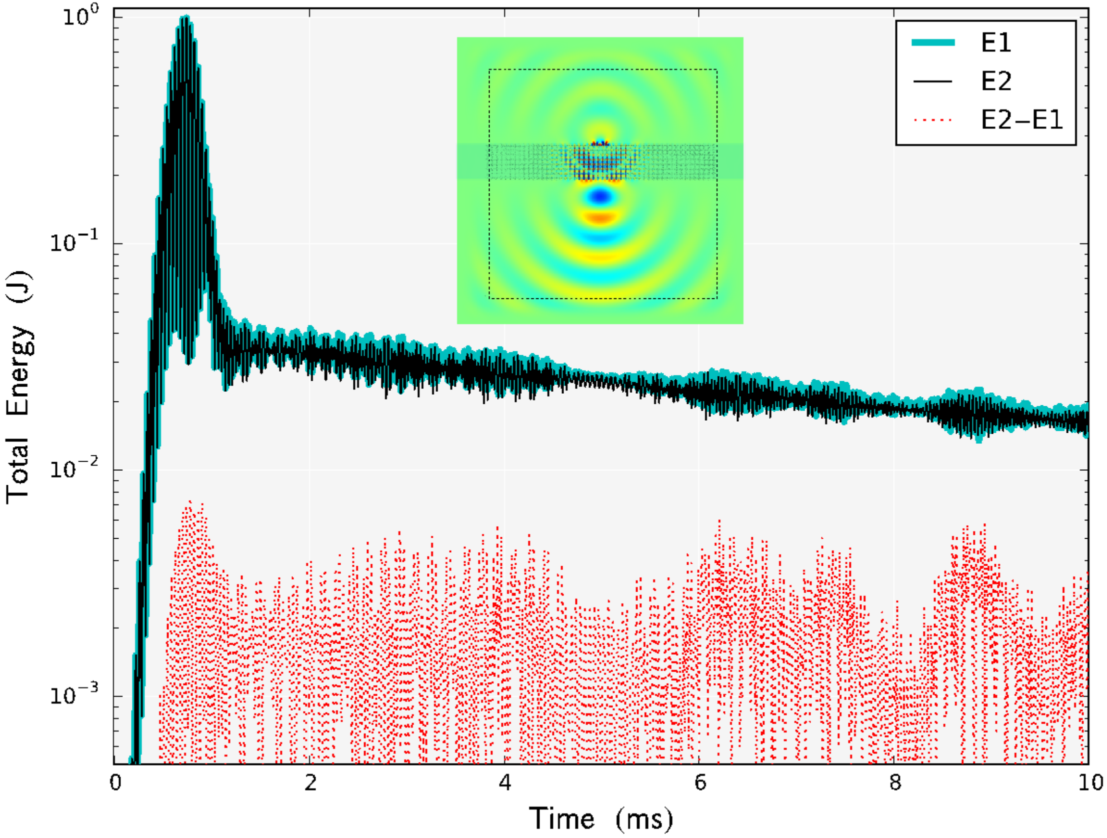


We observe one of the interesting characteristics of metamaterial: the wavevector and the group velocity have opposite directions, leading to the negative refraction and focusing.

PERIODIC STRUCTURE WITHIN PML: LIMITATION



CAN WE PUT IT ON THE EDGE ?

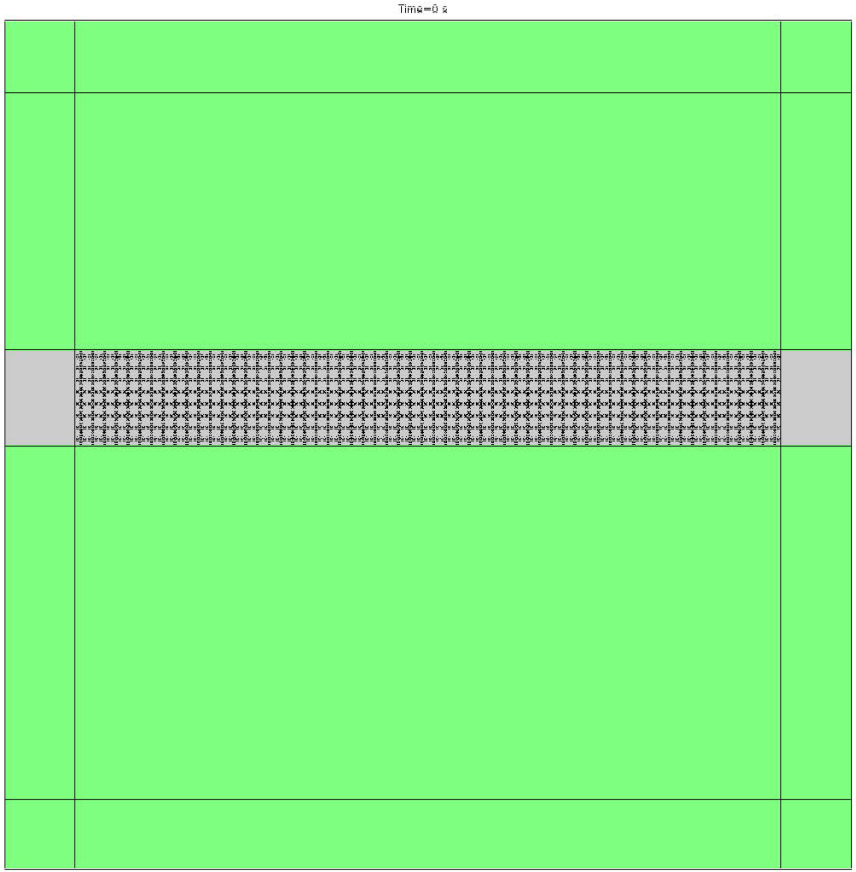


YES, we save in computational domain and we pay only (E2-E1)

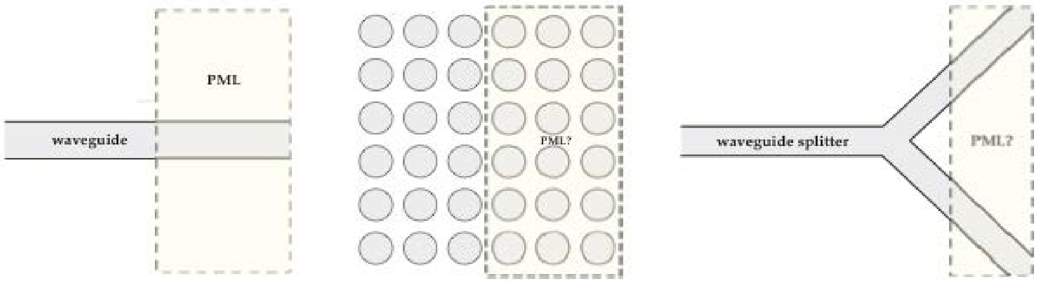
SUMMARY

We have developed second-order time-domain PML formulations in order to simulate wave propagation in unbounded solid, fluid, coupled fluid-solid, that are numerically efficient and easy to implement. We used them to simulate the transient response of acoustic metamaterials.

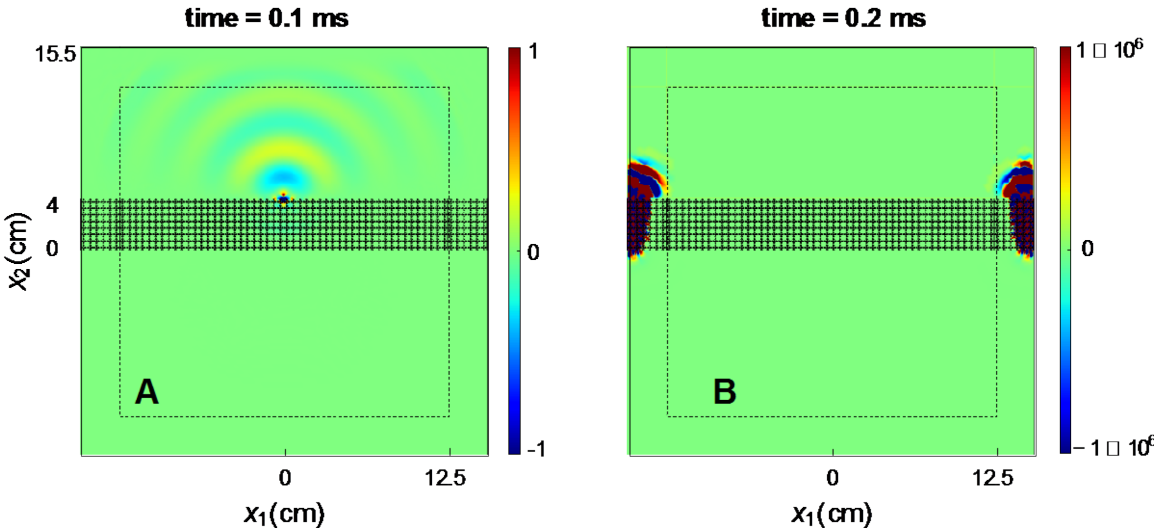
THANK YOU



PERIODIC STRUCTURE WITHIN PML: LIMITATION



Oskooi *et al* (2008). *Optics Express, 16*(15)



Future directions: PML & metamaterials

Periodic Structure

- Would PML works for low frequency with only forward wave ?
- Would PML work for fluid metamaterials ?
- Would PML work in other numerical schemes?

Homogenized Metamaterials

- Materials properties are homogenous but frequency dependent.
- What is the shape of complex stretch function?
- Can complex stretch function parameters be used to stabilize the problem?

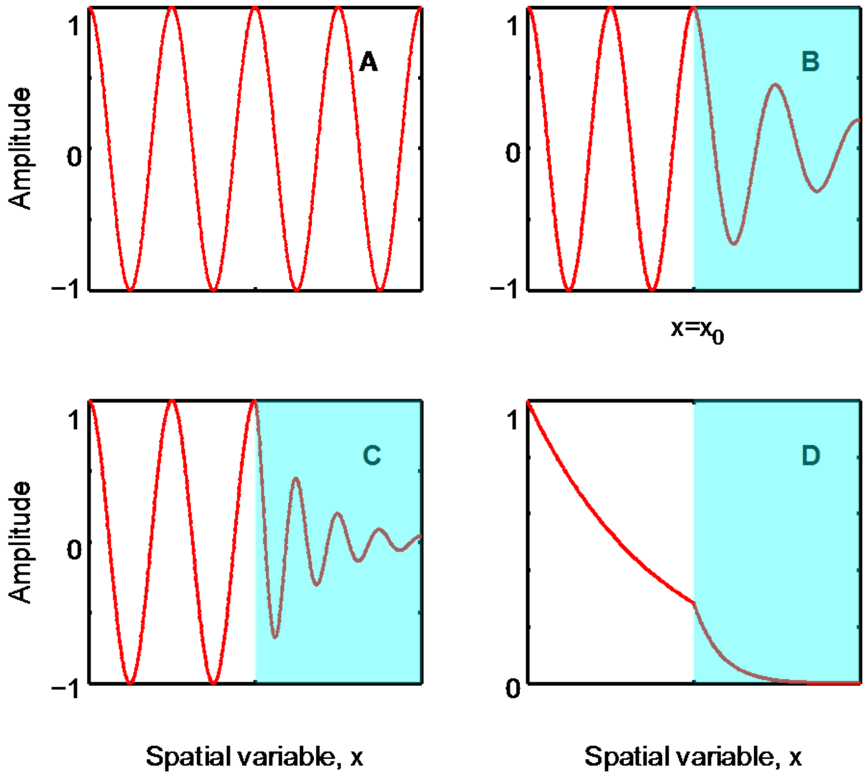
Complex coordinates stretching

$$\tilde{x} = f(x) : \mathbb{R} \to \mathbb{C}$$

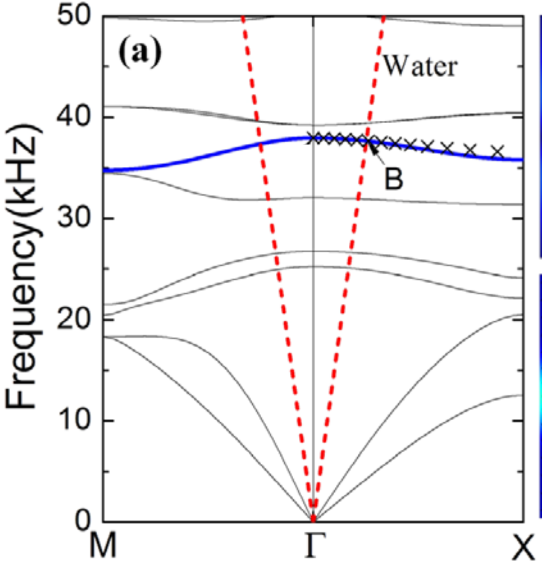
$$\Rightarrow \frac{1}{\partial \tilde{x}} = \frac{1}{\dot{f}(x)} \frac{1}{\partial x}$$

$$\dot{f}(x) = \alpha \left(1 + i \frac{\beta}{\omega}\right)$$

$$u = e^{ikx}$$



BAND STRUCTURE



k_1a/π

Zhou *et al.,* Appl. Phys. Lett. 105, 233506 (2014)

Plane wave analysis

$$\mathbf{u} = \mathbf{u}_0 e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}, \ \mathbf{k} \in \mathbb{R}^2 \text{ and } \omega \in \mathbb{C}$$

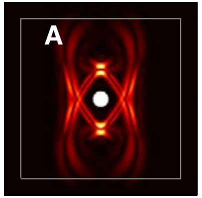
Substituting it in the elastic wave equation we obtain the dispersion relation

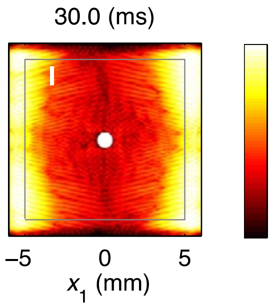
$$F_0(\omega, \mathbf{k}) = \det\left(\omega^2 \delta_{ik} - \sum_{j,l=1}^{2} C_{ijkl} k_j k_l\right) = 0$$

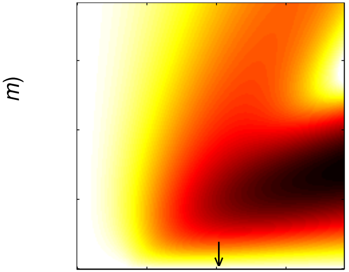
with conditions on C_{ijkl} , the four roots, $\omega(\mathbf{k})$ are real and distinct, and a group velocity can be defined

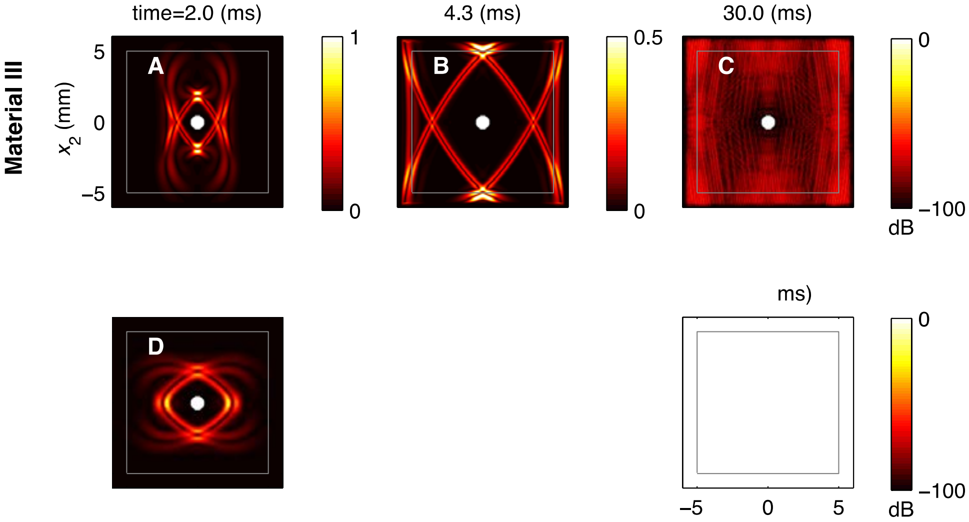
$$\mathbf{V}_g = \nabla_{\mathbf{k}} \omega = -\frac{\nabla_{\mathbf{k}} F_0(\omega, \mathbf{k})}{\partial F_0(\omega, \mathbf{k}) / \partial \omega}$$

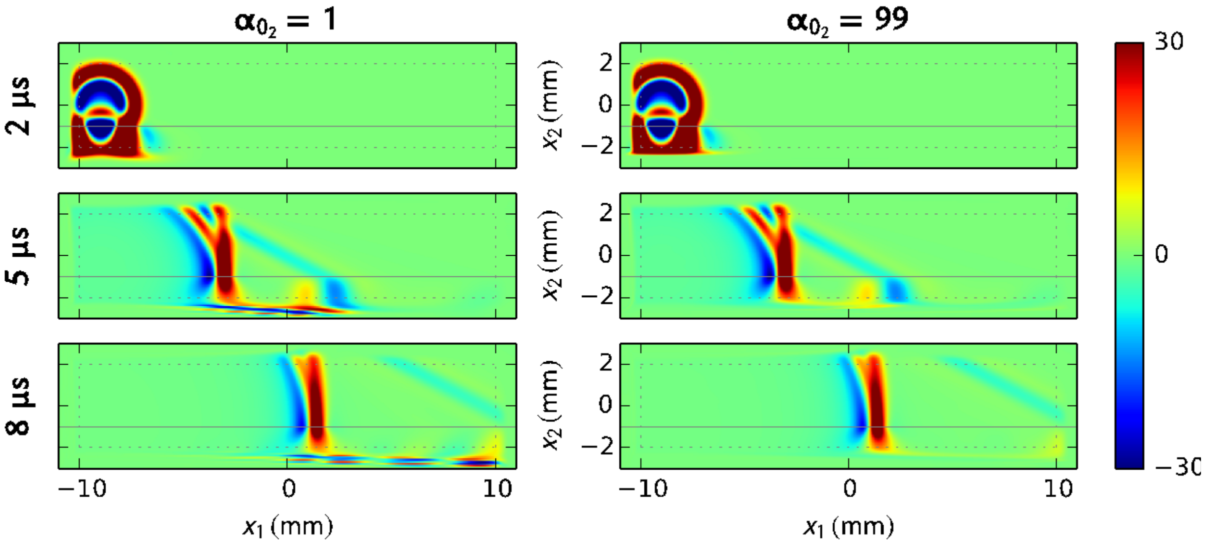
Slowness vector is defined as $S = \mathbf{k}/\omega$, then $F_0(1, \mathbf{S}) = 0$


A

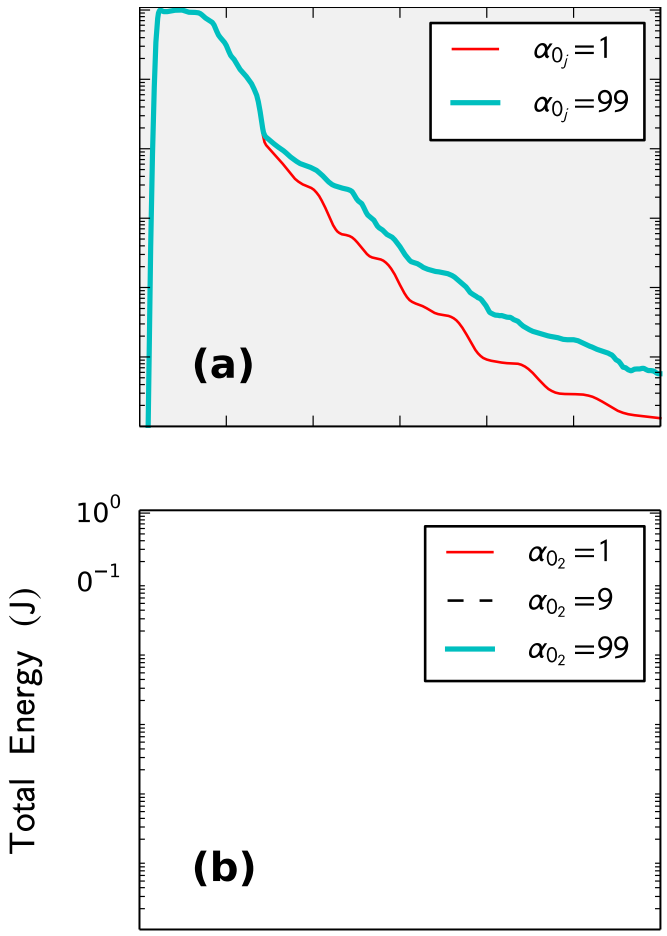

30.0 (ms)
I
–5
0
5
x_1 (mm)


m)


time=2.0 (ms)
4.3 (ms)
30.0 (ms)
Material III
x_2 (mm)
5
0
−5
A
B
C
D
1
0
0.5
0
0
−100
dB
ms)
0
−100
dB
−5
0
5



α02 = 1
α02 = 99
2 μs
5 μs
8 μs
x2 (mm)
2
0
−2
−10
0
10
x1 (mm)
30
0
−30



α0j =1
α0j =99
(a)
10^0
0^−1
Total Energy (J)
α02 =1
α02 =9
α02 =99
(b)