COMSOL CONFERENCE
2017 ROTTERDAM

Topology Optimization of a 3D-printed Acoustic Chamber For Photoacoustic Spectroscopy with COMSOL Multiphysics®

by RACHID HAOUARI
PhD Candidate

imec

KU LEUVEN

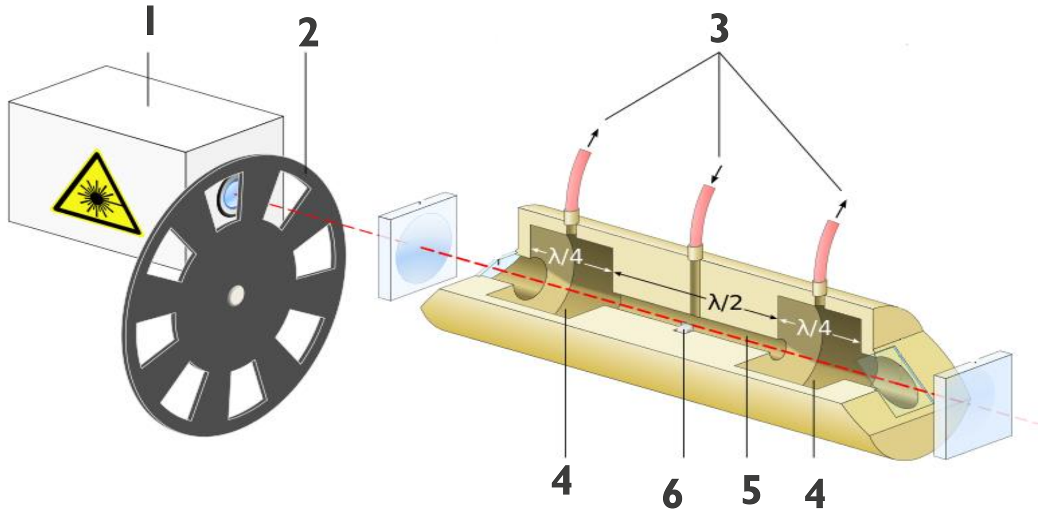
OVERVIEW

STRUCTURE OF THIS PRESENTATION

- Principles of photoacoustic spectroscopy
- What is topology optimization ?
- Problem definition and simulation set up
- Results, comparison and confirmation
- Conclusion

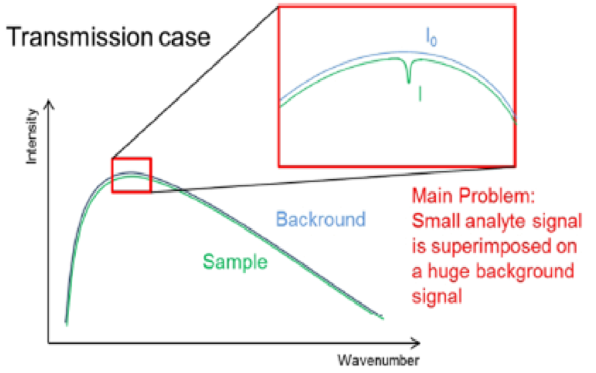
PHOTOACOUSTIC SPECTROSCOPY

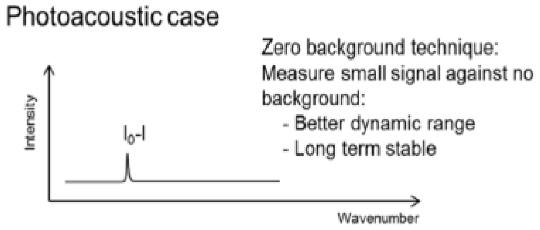
BASIC PRINCIPLES OF GASEOUS PHOTOACOUSTIC SPECTROSCOPY AND MAIN ADVANTAGE



1. Laser emitter
2. Chopper (amplitude modulation)
3. Gas with analyte inlet/outlet
4. Buffer
5. Resonator
6. Microphone

(4.–6.) } Gas chamber = cell





SIGNAL IMPROVEMENT

DESIGN CONSIDERATIONS TO PUSH FURTHER THE DETECTION LIMIT

COMSOL CONFERENCE
2017 ROTTERDAM

Pressure response of a PAS cell

$$p = K_{geom} \frac{(\gamma - 1)\, L\, Q}{\omega\, V} \alpha P_L$$

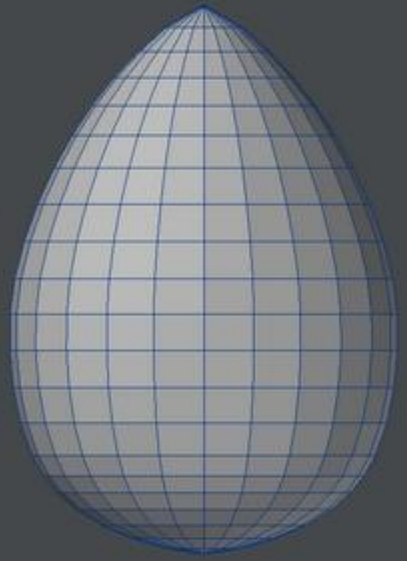
p	Pressure @ microphone
L	Laser path length
V	Cell volume
Q	Quality factor of the cell
ω	Frequency of operation
α	Analyte absorption coefficient
P_L	Laser power
γ	Buffer gas constant ratio

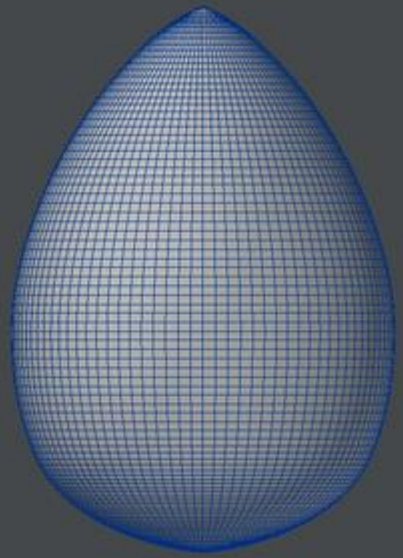
Ways for improvement

- Downsizing (V)
- Multiple laser beam crossing (mirrors) (L)
- Noble gas as a buffer (γ)
- Higher laser power (P_L)

K_{geom}
Geometry of the cell ?

CAN WE SIGNIFICANTLY IMPROVE THE RETRIEVED SIGNAL BY JUST TAILORING THE CELL SHAPE ?





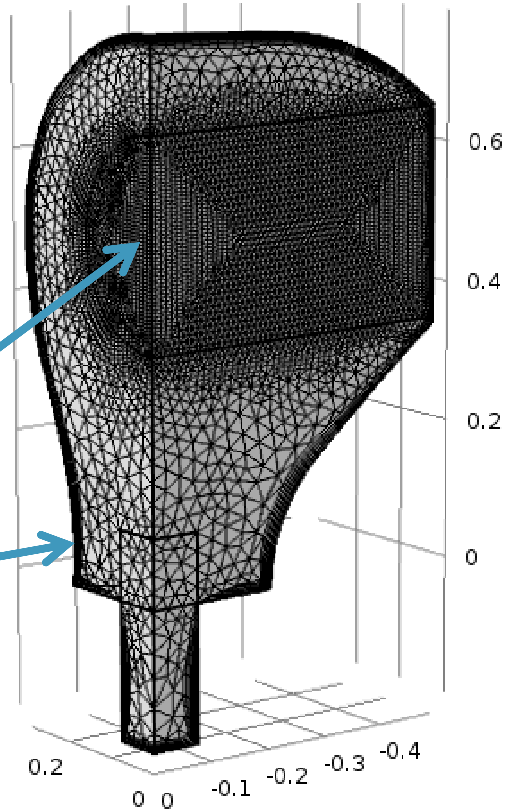
SIMULATION OF THE PHOTOACOUSTIC EFFECT

DESCRIPTION OF BOUNDARY CONDITIONS

Use Thermoacoustic module to take into account thermal and viscous losses

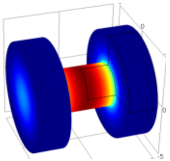
Harmonic excitation $\Rightarrow$ Frequency domain study

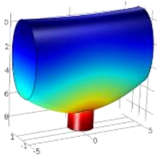
- Gaussian radial repartition of heat power = laser heating
- Air bulk modulus : 17 µPoise
- Boundary layer = $max(d_{th}, d_{visc})$



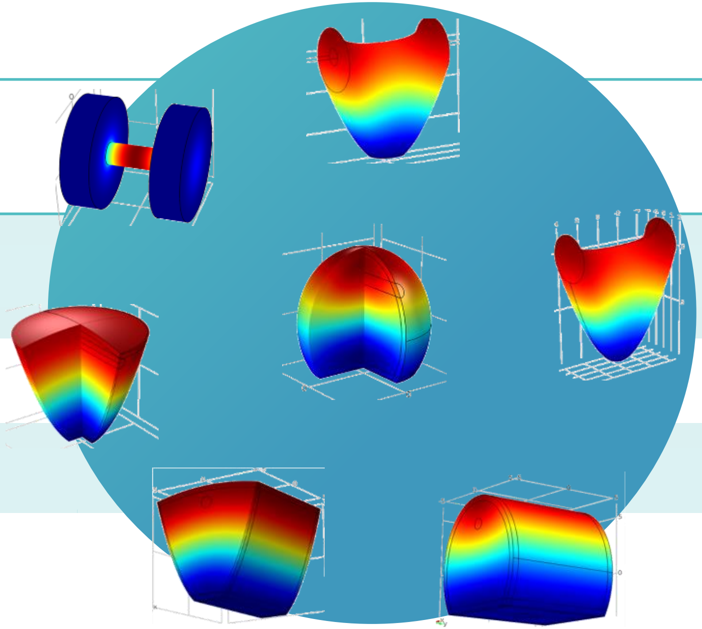
IMPACT OF THE CELL SHAPE

ALL SHAPES FIT A 1CM³ VOLUME





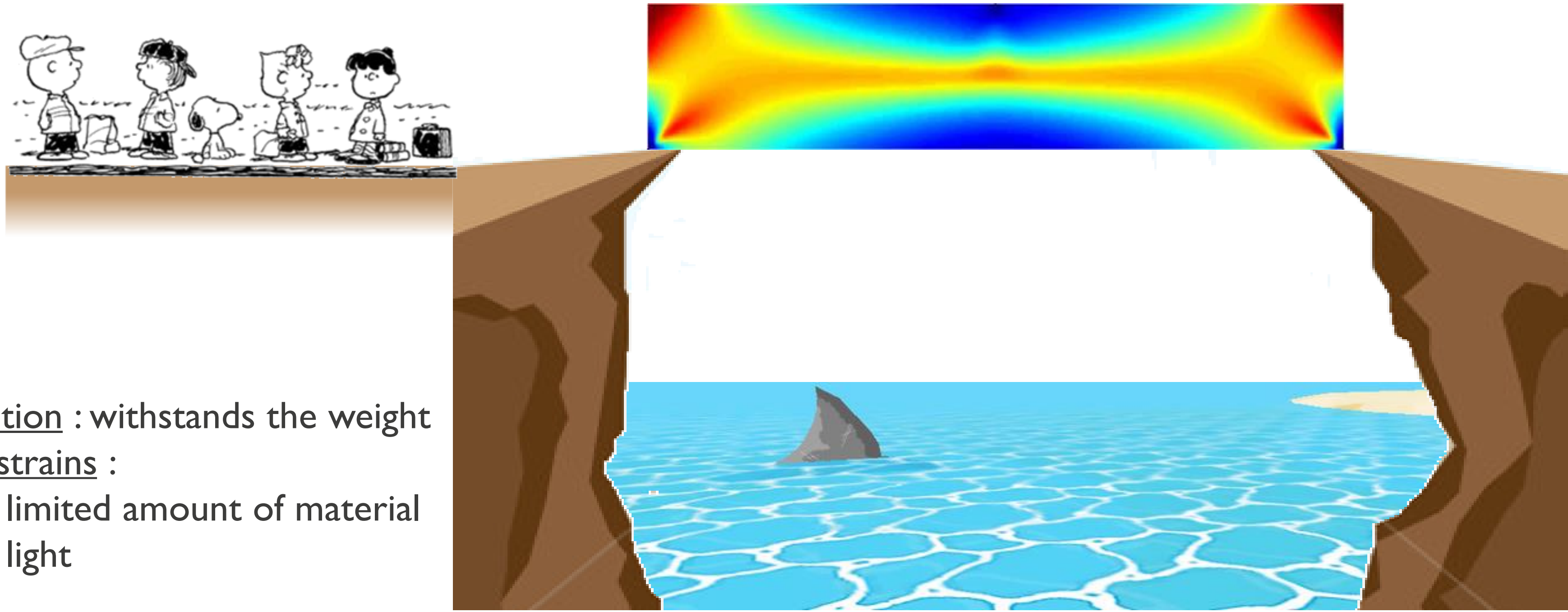
	Buffered cylinder Ø 4 mm	Heart + res.
Target eigenfrequency (kHz)	26	24,7
Q factor	67,877	95
Cell constant (Pa.cm/W)	6100,9	17062
Average pressure at mic's location (Pa)	4,0266	11,26



PURPOSE OF TOPOLOGY OPTIMIZATION

COMSOL CONFERENCE
2017 ROTTERDAM

FIND THE BEST SHAPE OPTIMIZING ITS FUNCTION WHILE COMPLYING TO A SET OF CONSTRAINS



Bridge

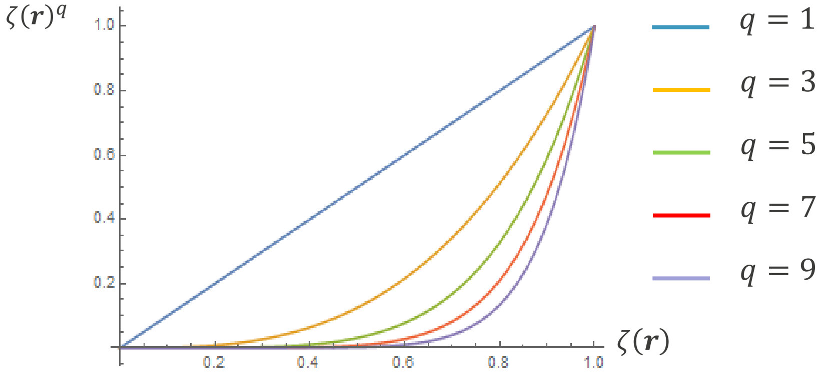
- Function : withstands the weight
- Constrains :
  - limited amount of material
  - light

MATERIAL DEFINITION

THE OPTIMIZED SHAPE IS AN OPTIMISED DISTRIBUTION OF A MATERIAL PROPERTY

We are looking for material distribution $\zeta(\boldsymbol{r}) = \begin{cases} 1 & if \;\; material\ 1 \\ 0 & if \;\; material\ 2 \end{cases}$ $\zeta(\boldsymbol{r}) \in C_2([0;1])$ over Ω

q penalization parameter :
pushes toward 0 or 1 $\zeta(\boldsymbol{r})^q$



Material property will depend on the position

SIMP model

(Solid Isotropic Material with Penalization)

$$\rho(\boldsymbol{r}) = \rho_{mat1} + \zeta(\boldsymbol{r})^q \left(\rho_{mat2} - \rho_{mat1}\right)$$

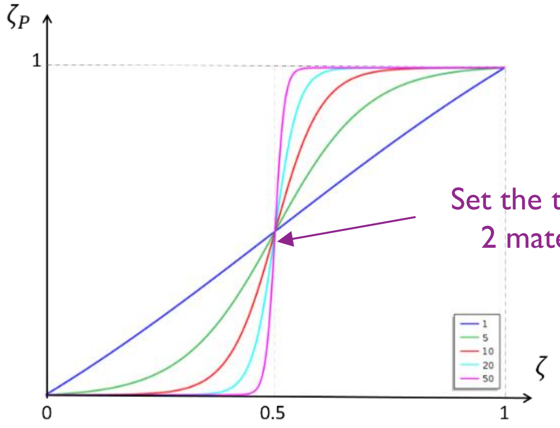
PENALIZATION FUNCTIONS

SET OF FUNCTIONS TO FORCE THE CONVERGENCE TOWARD DESIRED SOLUTIONS

Heaviside projection

- Slow convergence of ζ values toward 0 & 1
- Gradient based optimization techniques

  $\Rightarrow$ continuous function $\zeta_P = P(\zeta)$

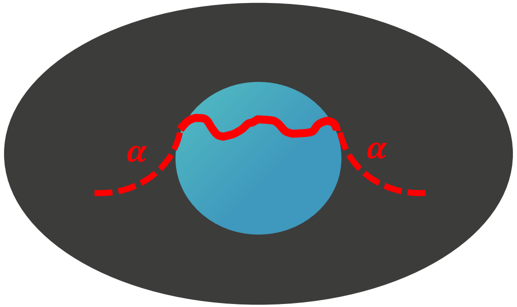


Set the threshold between 2 materials @ $\zeta = 0{,}5$

Penalized damping = Pamping

- $\sim$ no sound in the solid (impedance mismatch)
- $\Rightarrow$ artificial damping
- damping coefficient

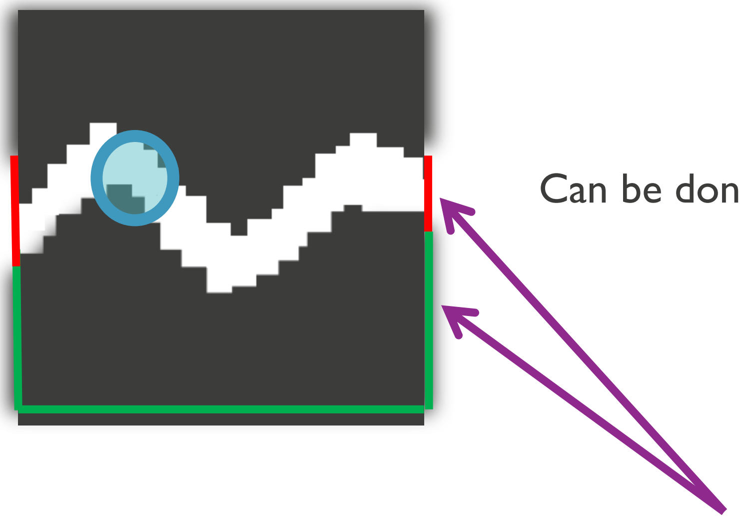
$$\alpha\Big(P\big(\zeta(\boldsymbol{r})\big)\Big) = \begin{cases} 0 & \text{if air} \\ K \gg 1 & \text{if solid} \end{cases}$$



REGULARIZATION

SMOOTHING TECHNIQUE OF THE SOLUTION

Solution presents a checkerboard pattern



Averaging ζ the over an r_0 radius circle

Typical value for $r_0 \approx 1.5\, mesh\ size$

Can be done by solving $$-{r_0}^2 \nabla^2 \tilde{\zeta} + \tilde{\zeta} = \zeta$$

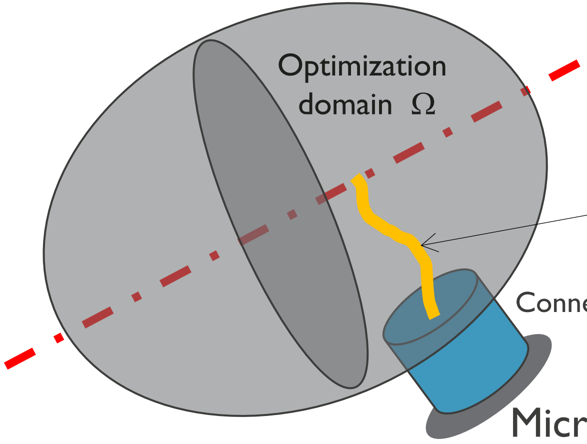
→ Smoothed solution $\tilde{\zeta}$

! destructive process

BC : convenient to set material on desired boundaries

OBJECTIVE AND CONSTRAINS DEFINITION

SETTING UP THE GEOMETRY AND OBJECTIVES FOR OPTIMIZATION



Constrains

- Relative positioning
- Guaranteed acoustical path
- Amount solid in Ω

$$0 < k_{down} \leq \frac{\int_{\Omega} \zeta \, dV}{V} \leq k_{up} < 1$$

Maximize the average pressure retrieved @ microphone

Objective

$$\max! \int_{mic} |p|^2 \, dS$$

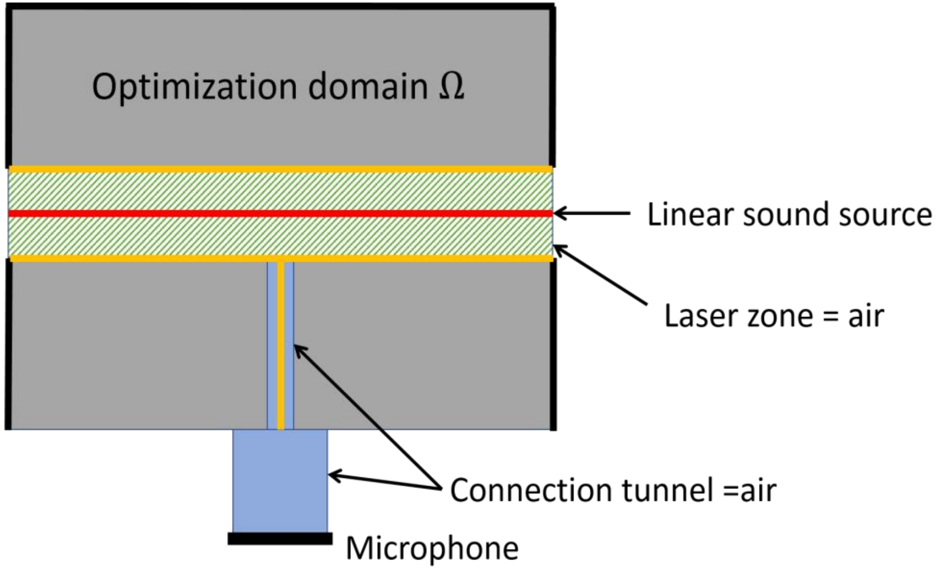
BOUNDARY CONDITIONS

SCHEMATIC VIEW AND PARALLEL BETWEEN BC AND MATERIAL TOPOLOGY

- Dirichlet BC for air : $\tilde{\zeta} = 0$
- Dirichlet BC for solid : $\tilde{\zeta} = 1$
- Linear sound source $p_0 e^{j\omega t}$
- laser volume
- sound connection
- Topo opt SIMP material

Lossless sound propagation

Pamping
Lossy sound propagation



COMSOL® IMPLEMENTATION

KEY VARIABLES AND PARAMETERS TO BE IMPLEMENTED

Heaviside projection

SIMP model

Topo Opt

ζ def

ζ bounds

Objective

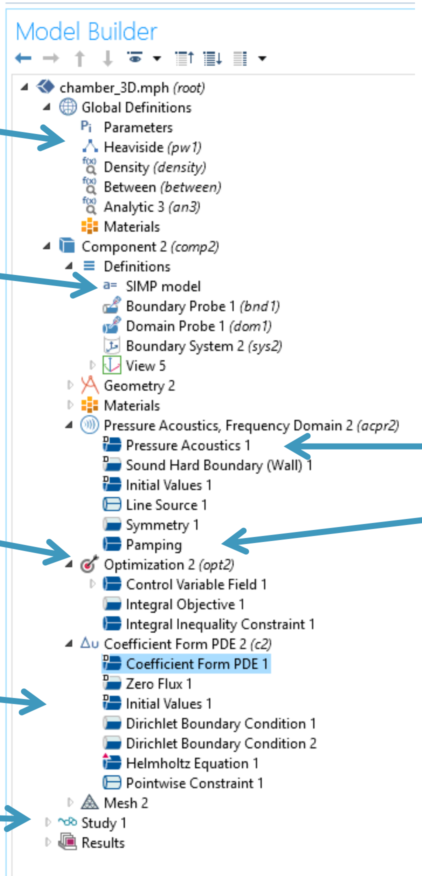
Constrains

Regularization $\tilde{\zeta}$

$\tilde{\zeta}$ BC

Solvers available :

- SNOPT
- MMA

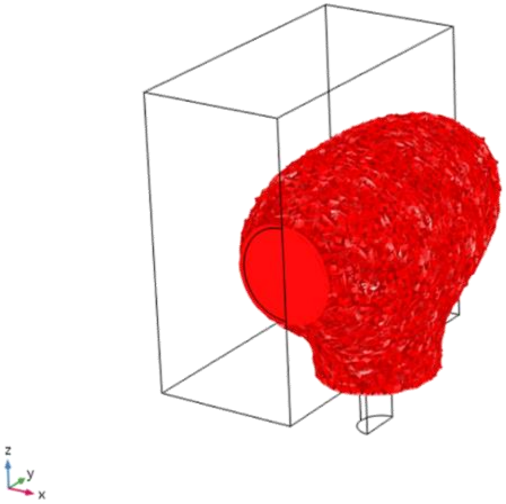


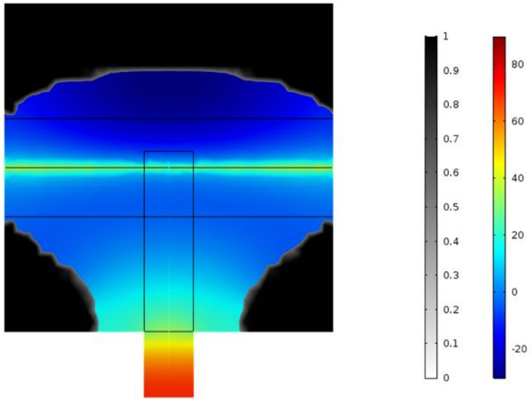
No damping

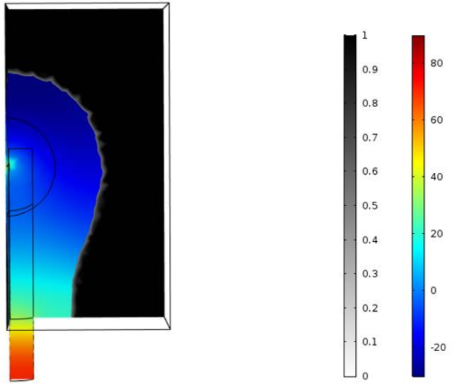
Pamping

OPTIMIZED CHAMBER @ 25 kHz

MICROPHONE LOCATION SET @ THE CENTRE

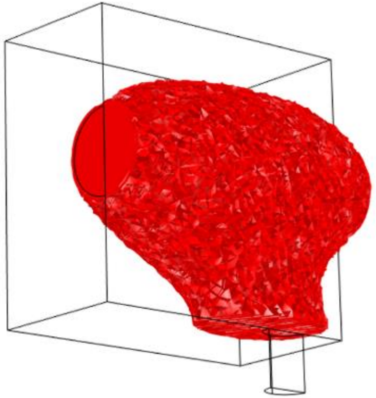


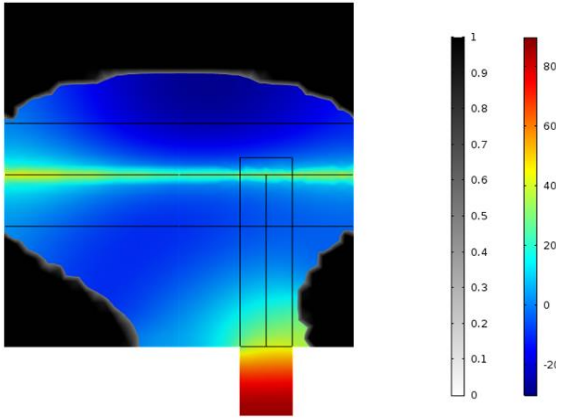


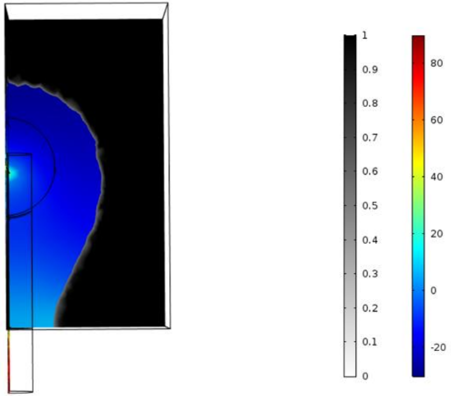


OPTIMIZED CHAMBER @ 25 kHz

MICROPHONE LOCATION SHIFTED FROM THE CENTRE







COMPARISON BETWEEN PAS CELLS

CRITERIONS TO COMPLY TO MAKE CORRECT COMPARISONS OF TWO CELLS

Pressure response of a PAS cell

$$p = K_{geom} \frac{(\gamma - 1)\, L\, Q}{\omega W} \alpha P_L \qquad \frac{p}{Q K_{geom}} = \frac{(\gamma - 1)\, L}{\omega W} \alpha P_L$$

2 PAS cells are equivalent if they have the same

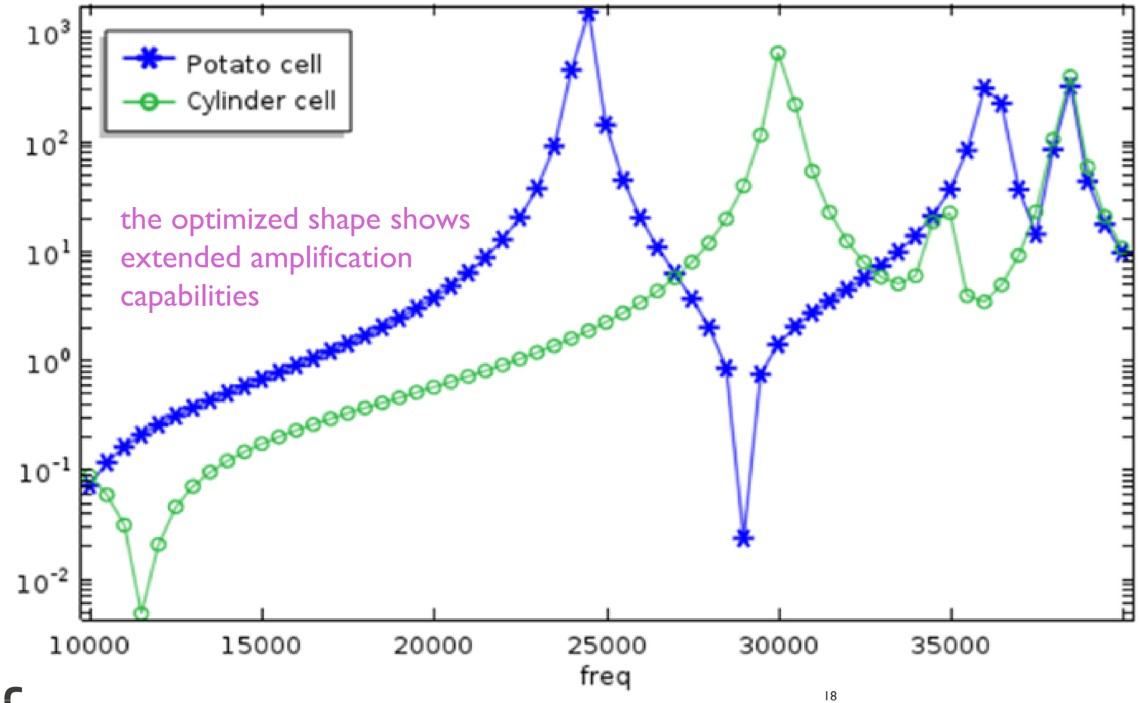
- Volume V
- Laser path length L
- Buffer gas γ
- Absorbed laser power αP_L

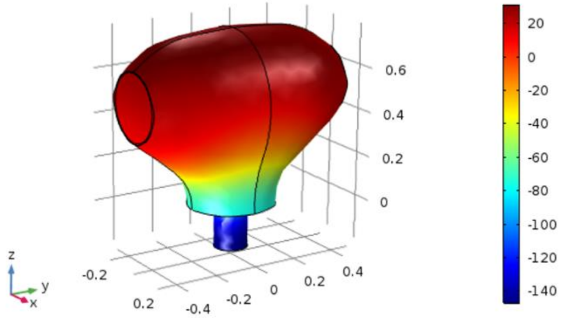
The rest is shape dependent

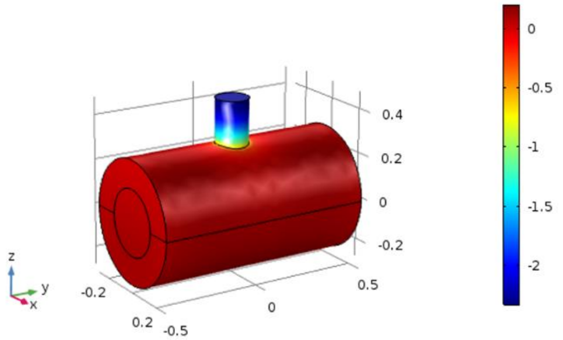
CONFIRMATION OF SIGNAL IMPROVEMENT THANKS TO TOPOLOGY OPTIMIZATION

COMPARISON OF SIMULATED PHOTOACOUSTIC SIGNAL FROM TWO CELLS

Frequency domain analysis







CONCLUSION

CONCLUSION

- Topology optimization of PAS cell was undertaken
- Building and setting up the COMSOL model
- Definition of equivalency between cells for improvement signal assessment
- Comparison and confirmation of improved signal simulated

imec
embracing a better life

KU LEUVEN

COMSOL MULTIPHYSICS®

COMSOL CONFERENCE
2017 ROTTERDAM