Advanced computational tools for the analysis and design of metamaterials

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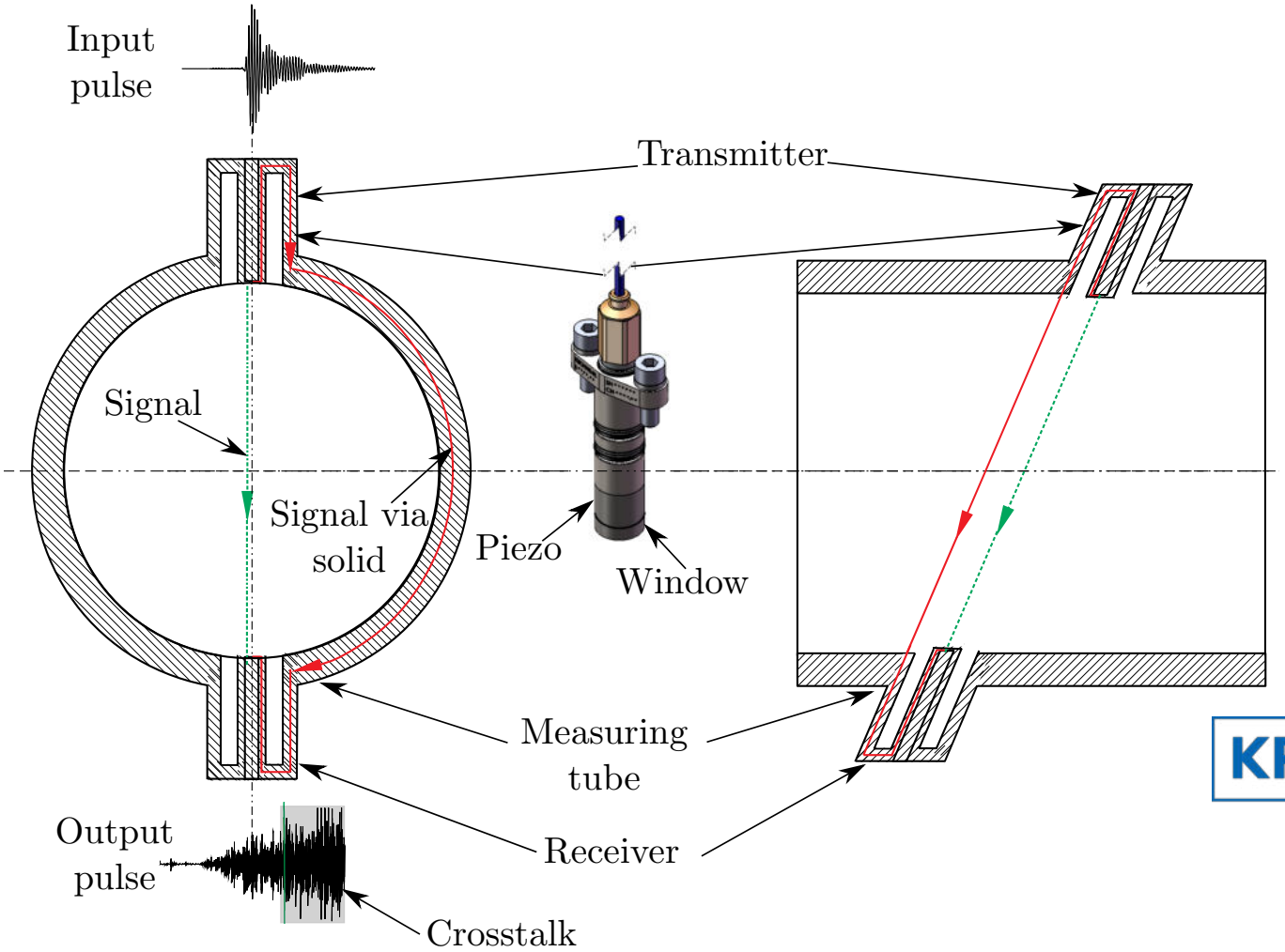
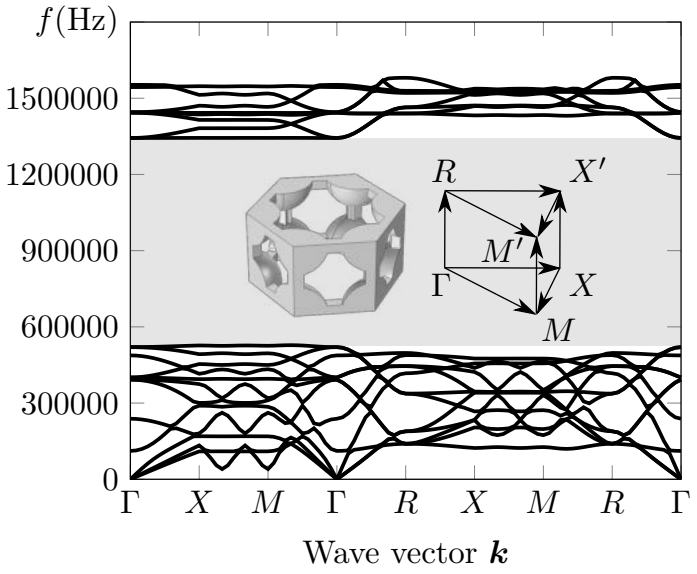
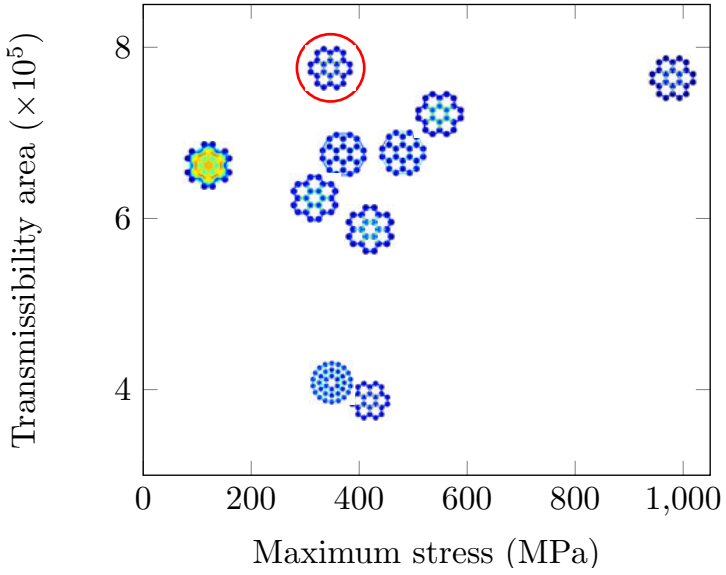
Test case: Design a waveguide to eliminate crosstalk in ultrasound flowmeters



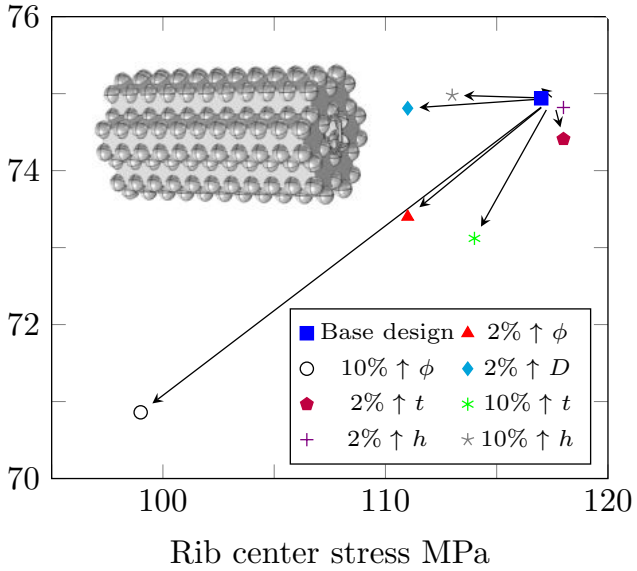
KROHNE

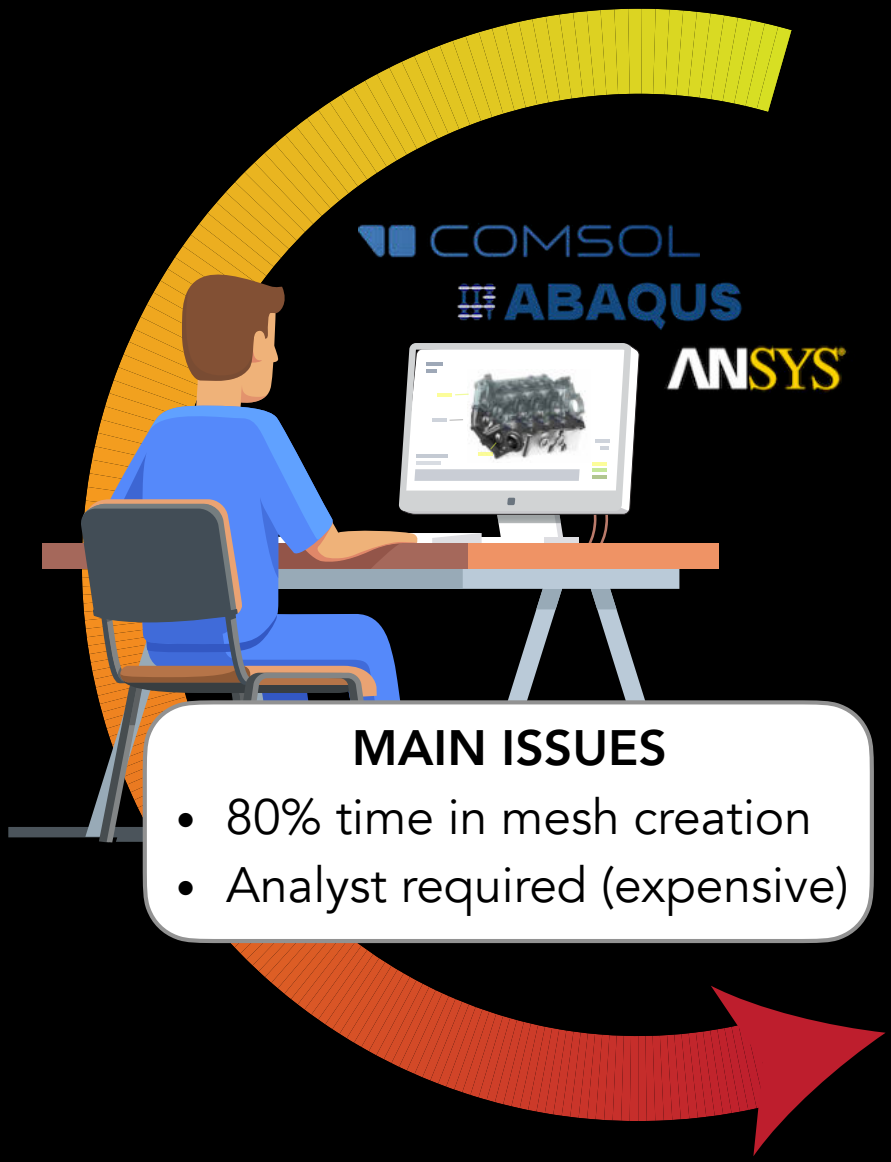
Crosstalk is mitigated by a phononic crystal waveguide with large bandgap at 1 MHz





Patent pending: Ultrasonic Transducer and Ultrasonic Flowmeter



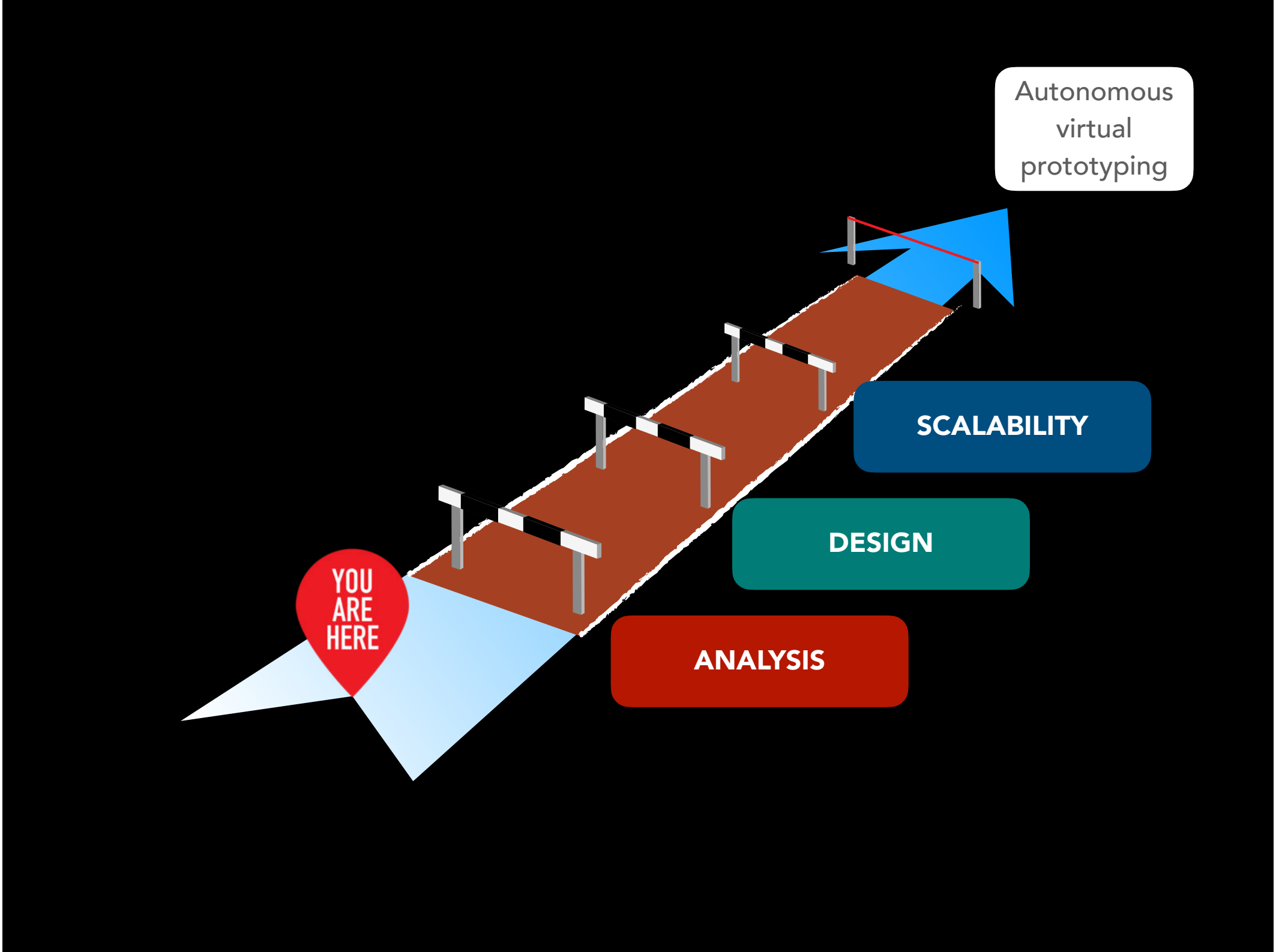


MAIN ISSUES

- 80% time in mesh creation
- Analyst required (expensive)

Phononic crystal waveguide

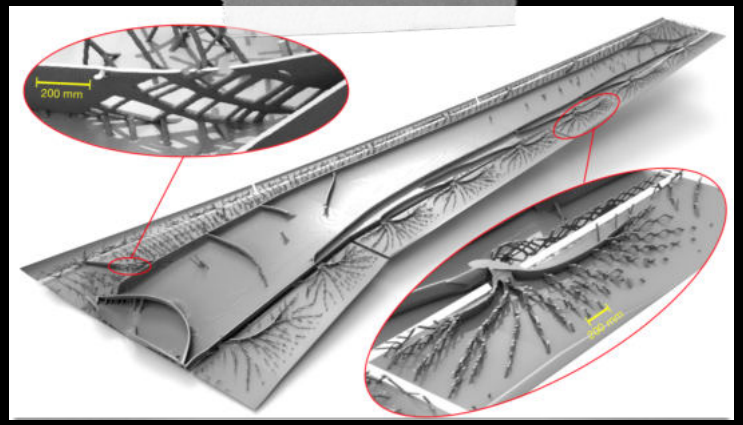
- Multiple objectives;
- Heavy mesh burden;
- Even heavier *trial-and-error* optimization.


Autonomous virtual prototyping
SCALABILITY
DESIGN
ANALYSIS
YOU ARE HERE

ANALYSIS

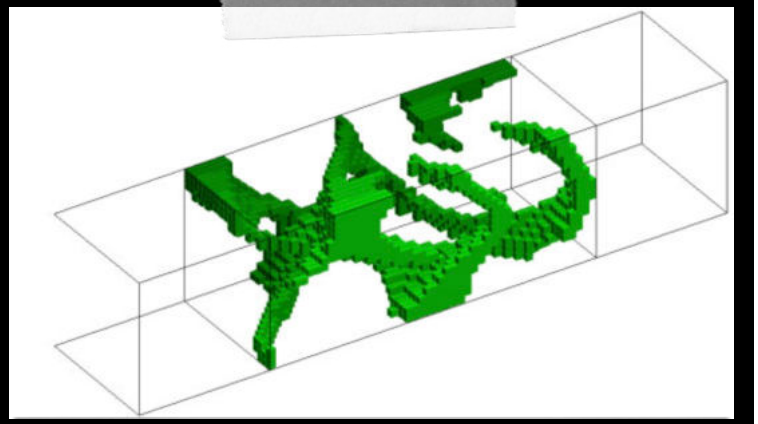
DESIGN

SCALABILITY



Giga-voxel resolution topology optimization
Aage *et al.*, Nature (2017)

Topology optimization of microfluidic mixers
Andreasen and Sigmund, *Int J Numer Meth Eng* (2009)



problem size

large

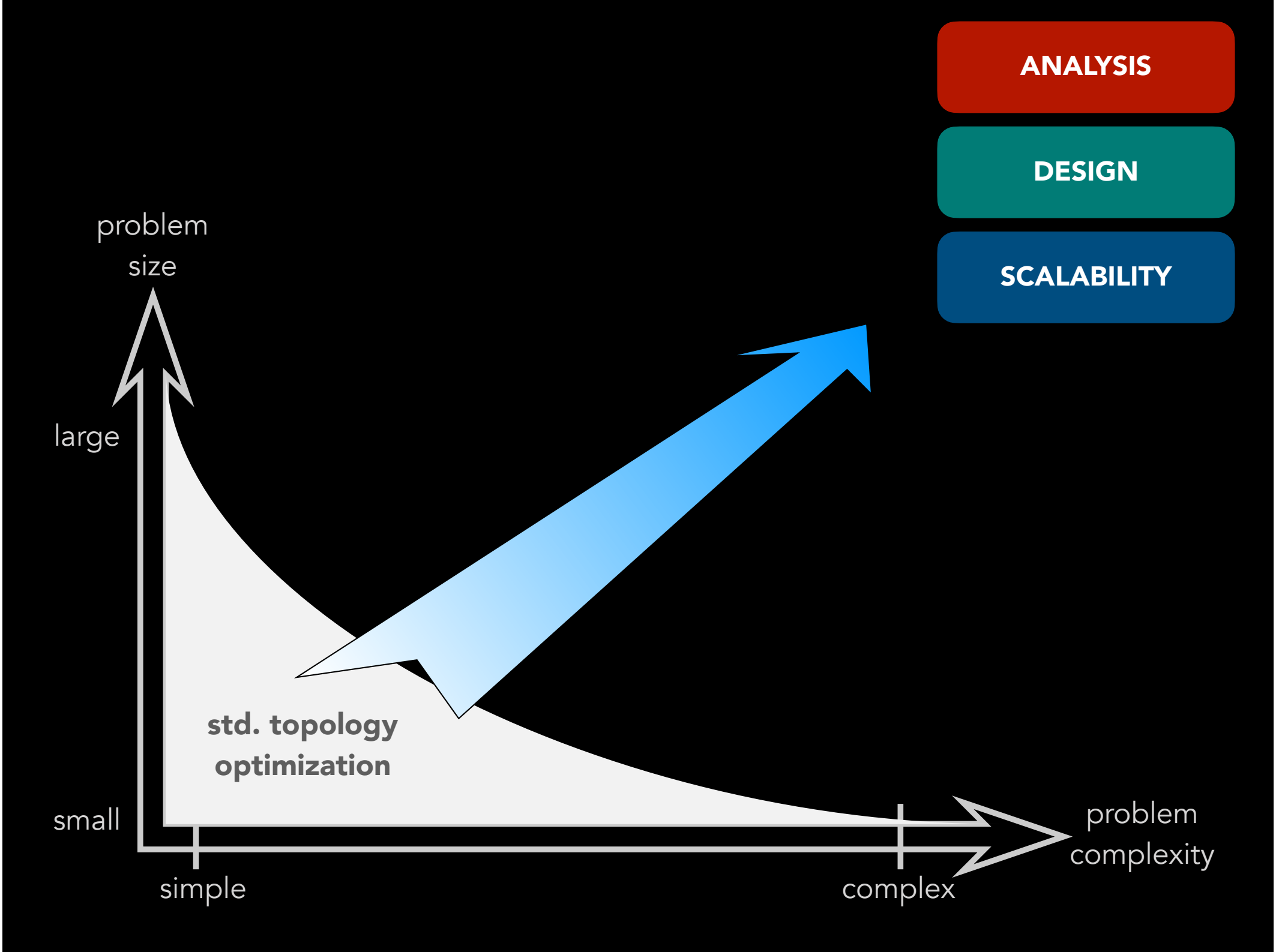
small

std. topology optimization

simple

complex

problem complexity


ANALYSIS
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std. topology
optimization
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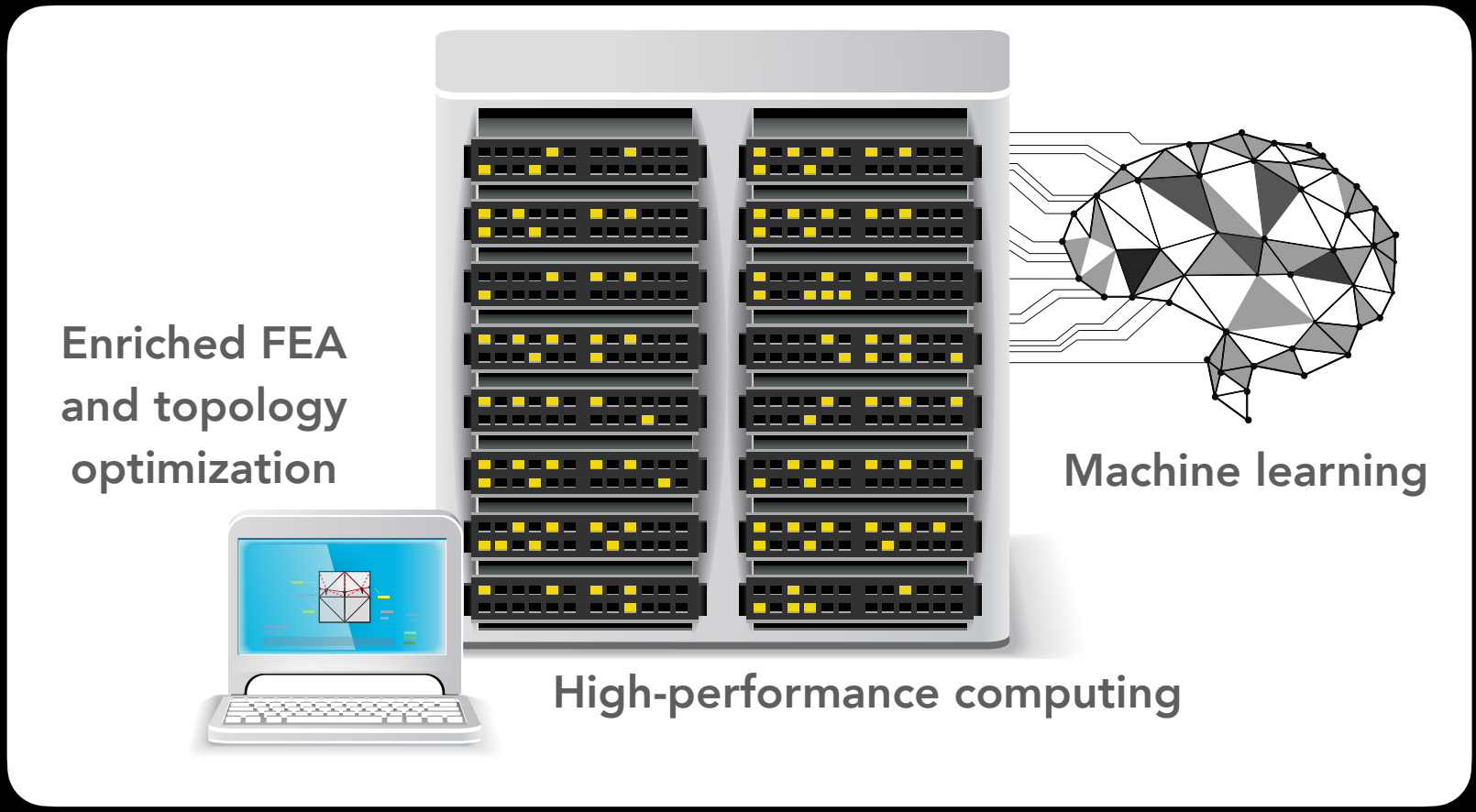
complex
problem
complexity

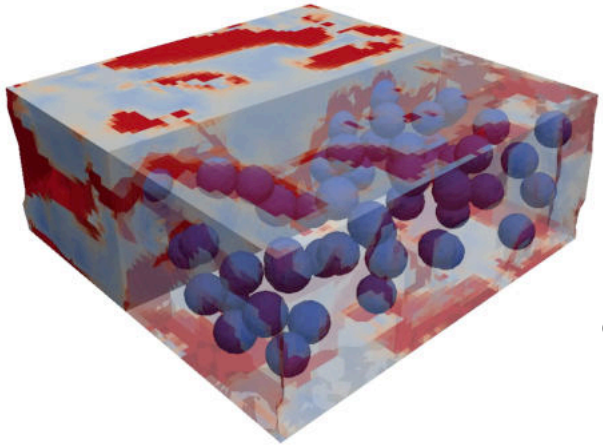
DESIGN

SCALABILITY

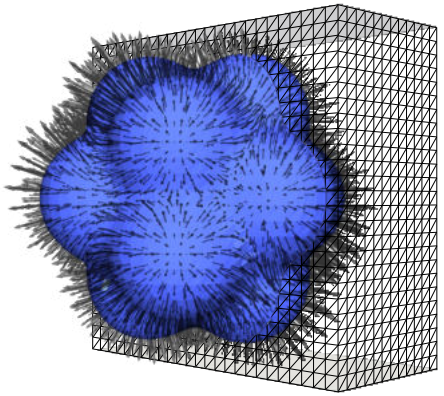
ANALYSIS



Enriched FEA has been developed for many problems with discontinuities

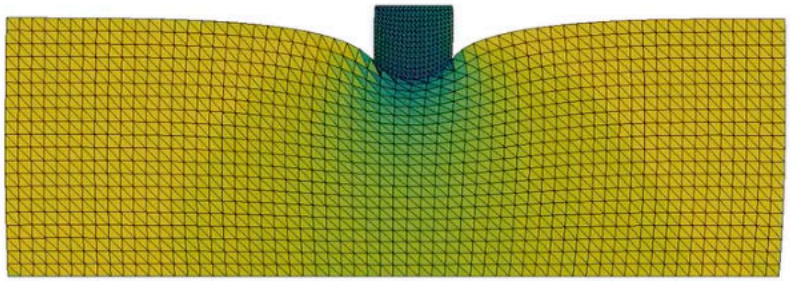


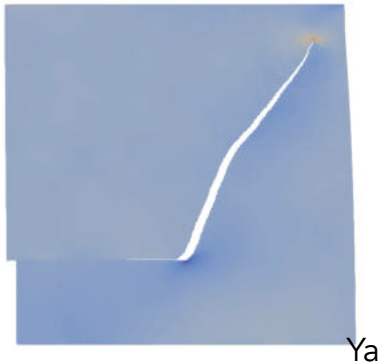
Interface and damage mechanics
Aragón *et al.*, *J Mech Phys Solids* (2013)



Immersed boundaries (fictitious domains)
van den Boom *et al.*
Int J Numer Meth Eng (2019)

Contact mechanics
Liu *et al.*, *Comput Mech* (In Press)

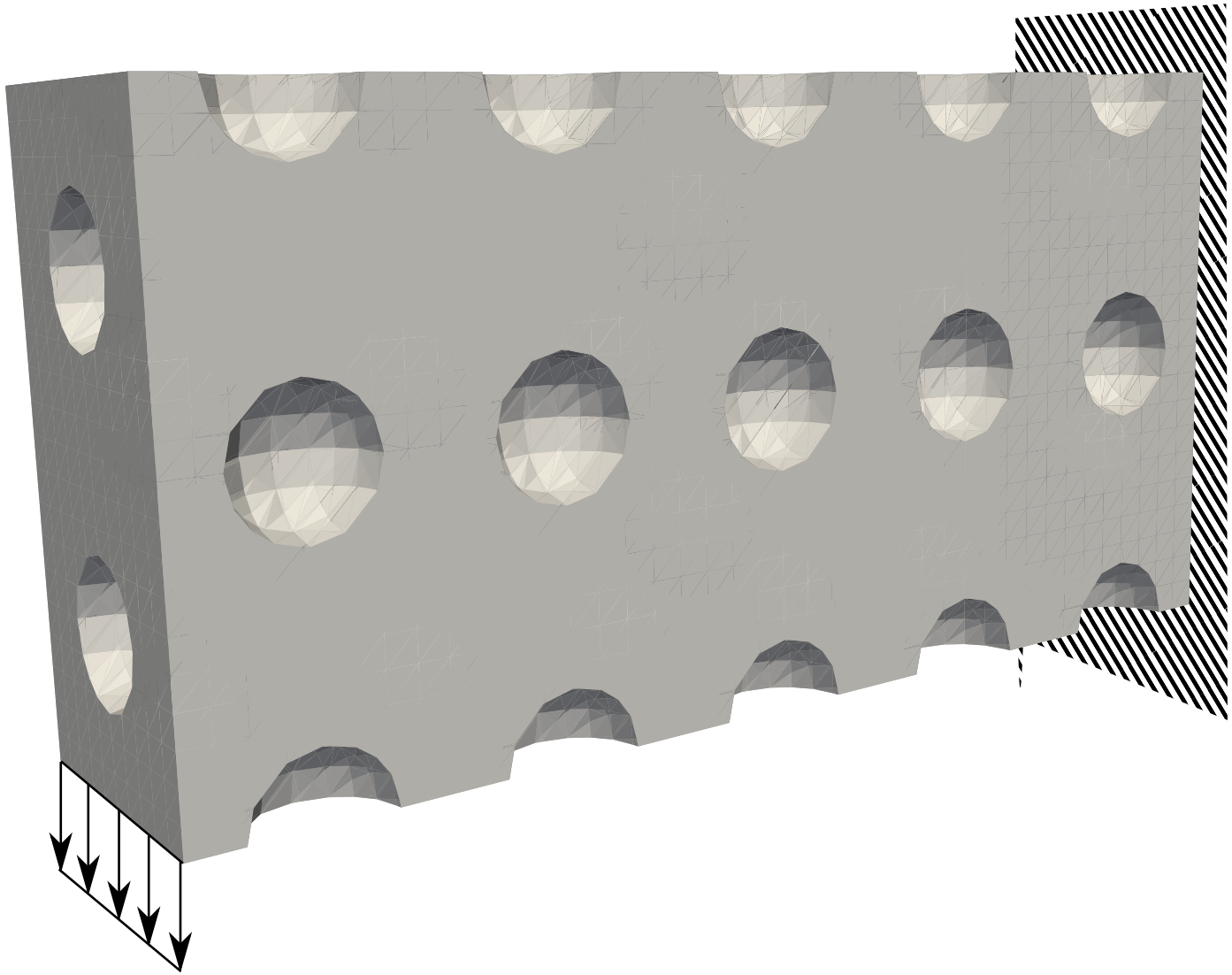




Fracture mechanics
Yang and Aragón, *Int J Numer Meth Eng* (In Preparation)

ANALYSIS

Enriched topology optimization was first used to minimize compliance



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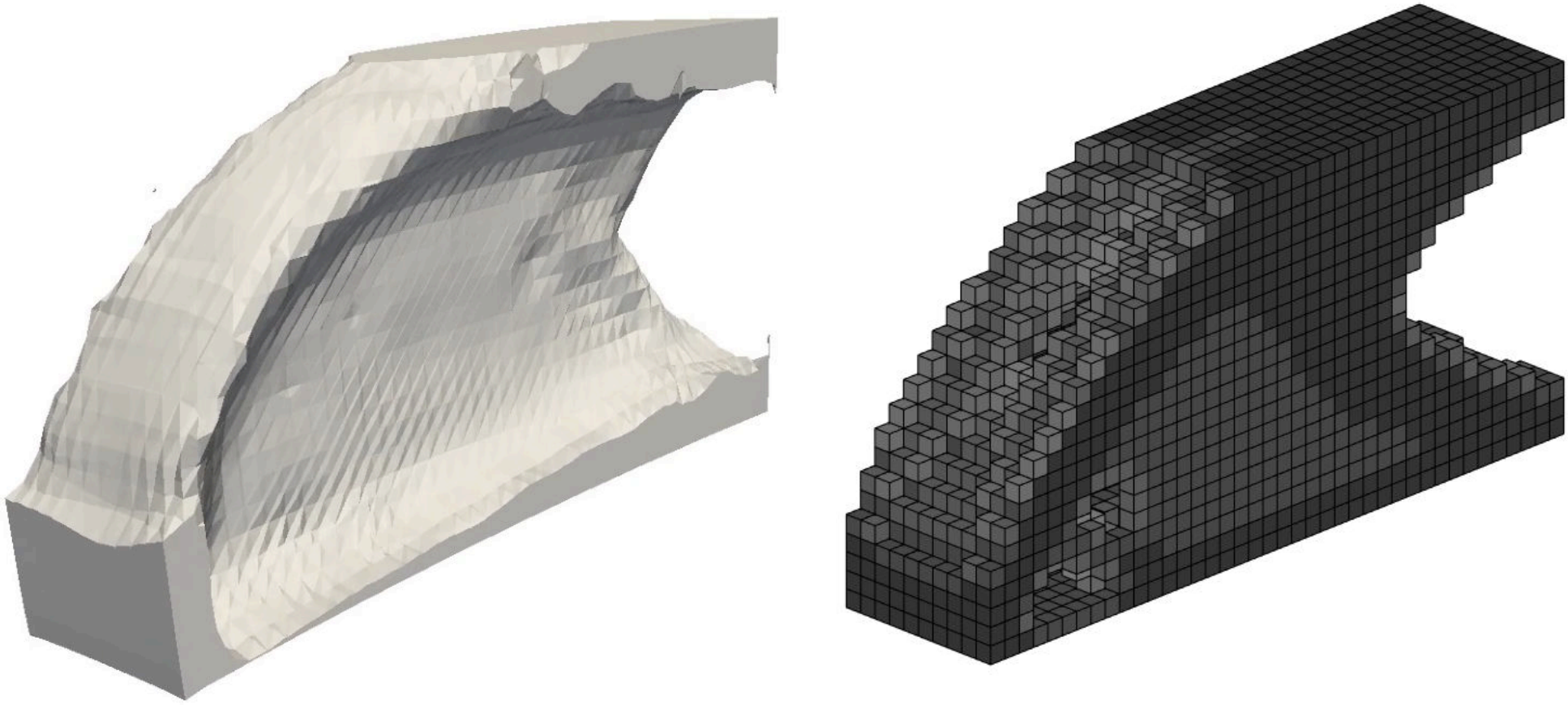
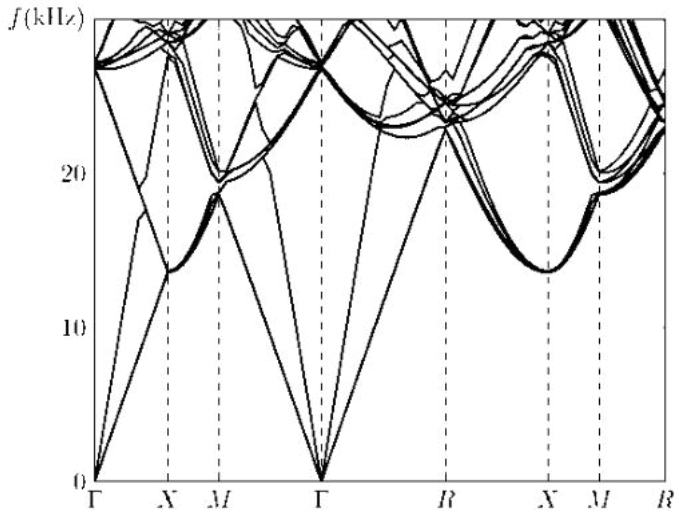
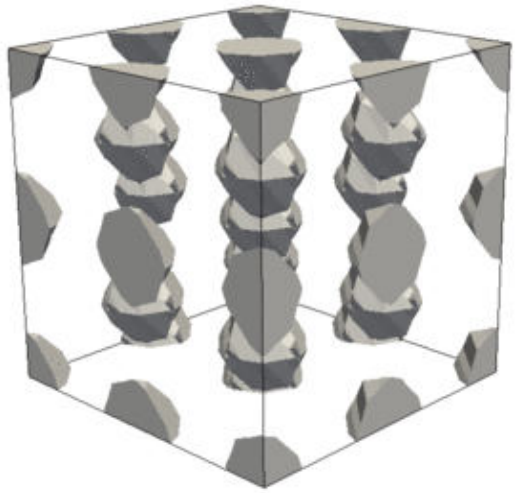


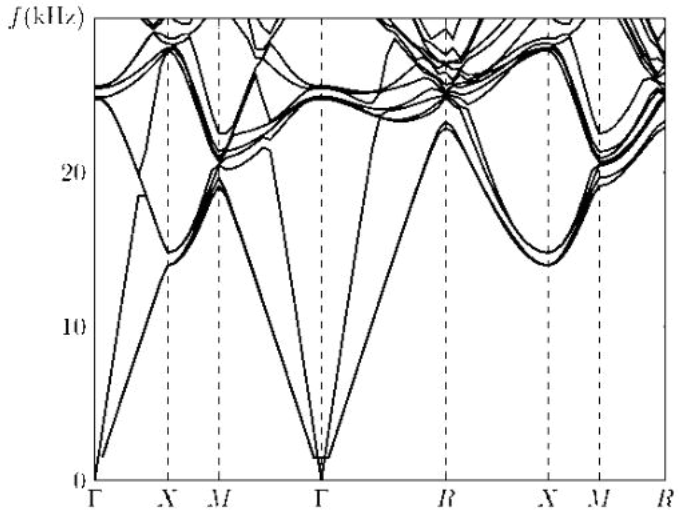
- van den Boom *et al.*, *Struct Multidiscipl Optim* (2020)

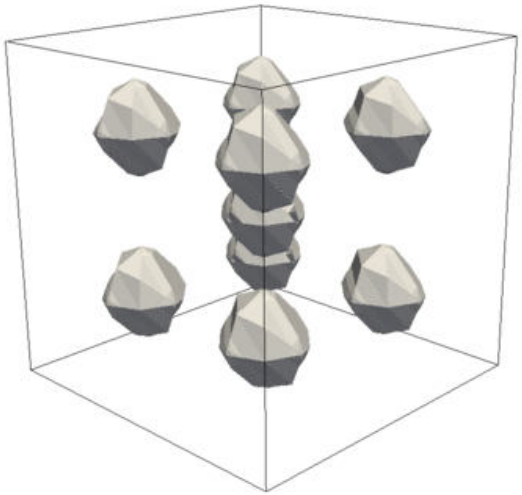
Phononic crystals (PnCs) and acoustic/elastic metamaterials (A/E MMs)

Level set optimization with an initial hole seed is sensitive to initial design









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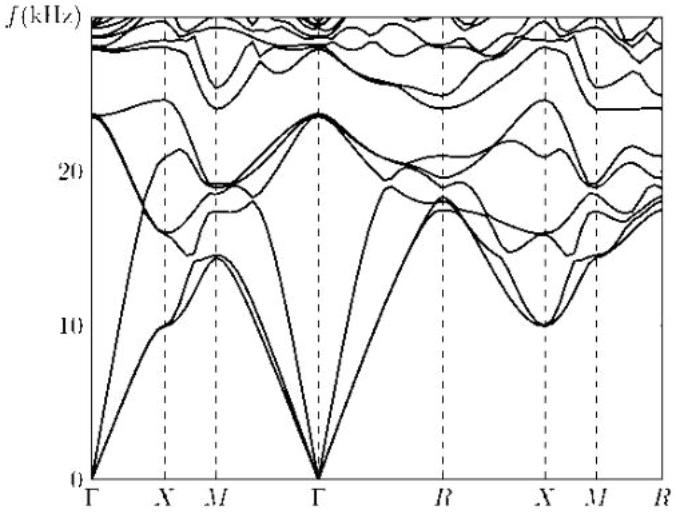
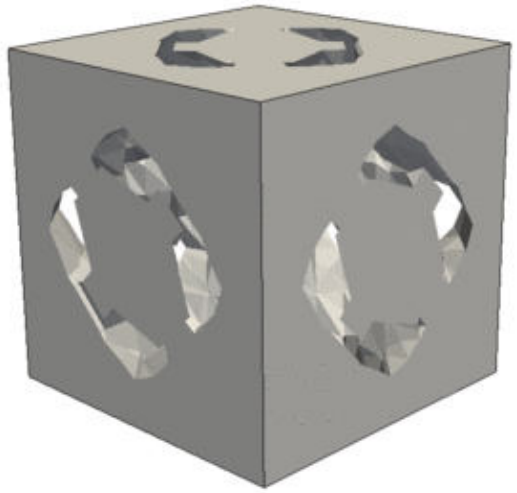
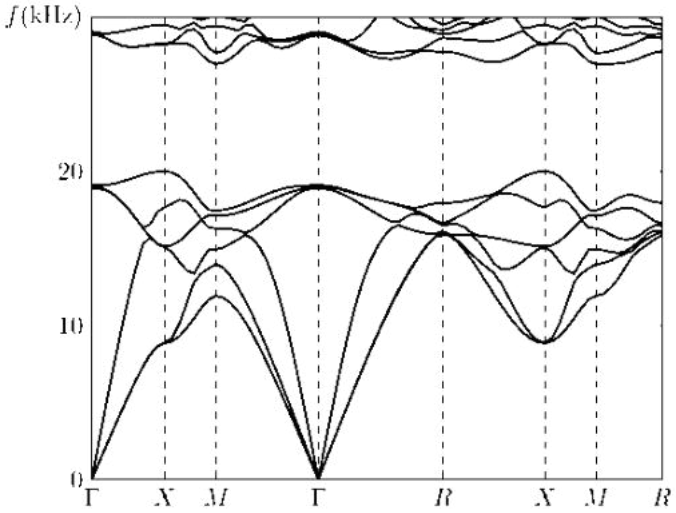
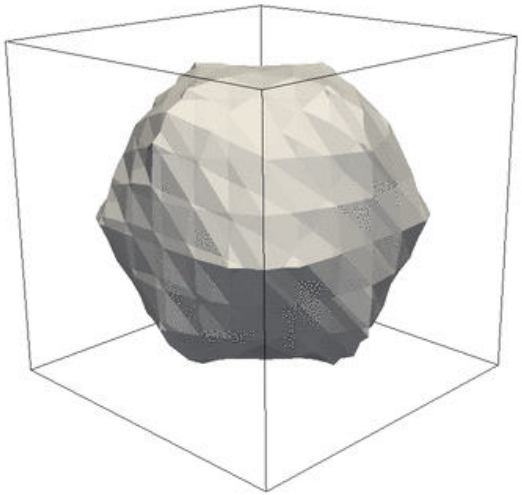
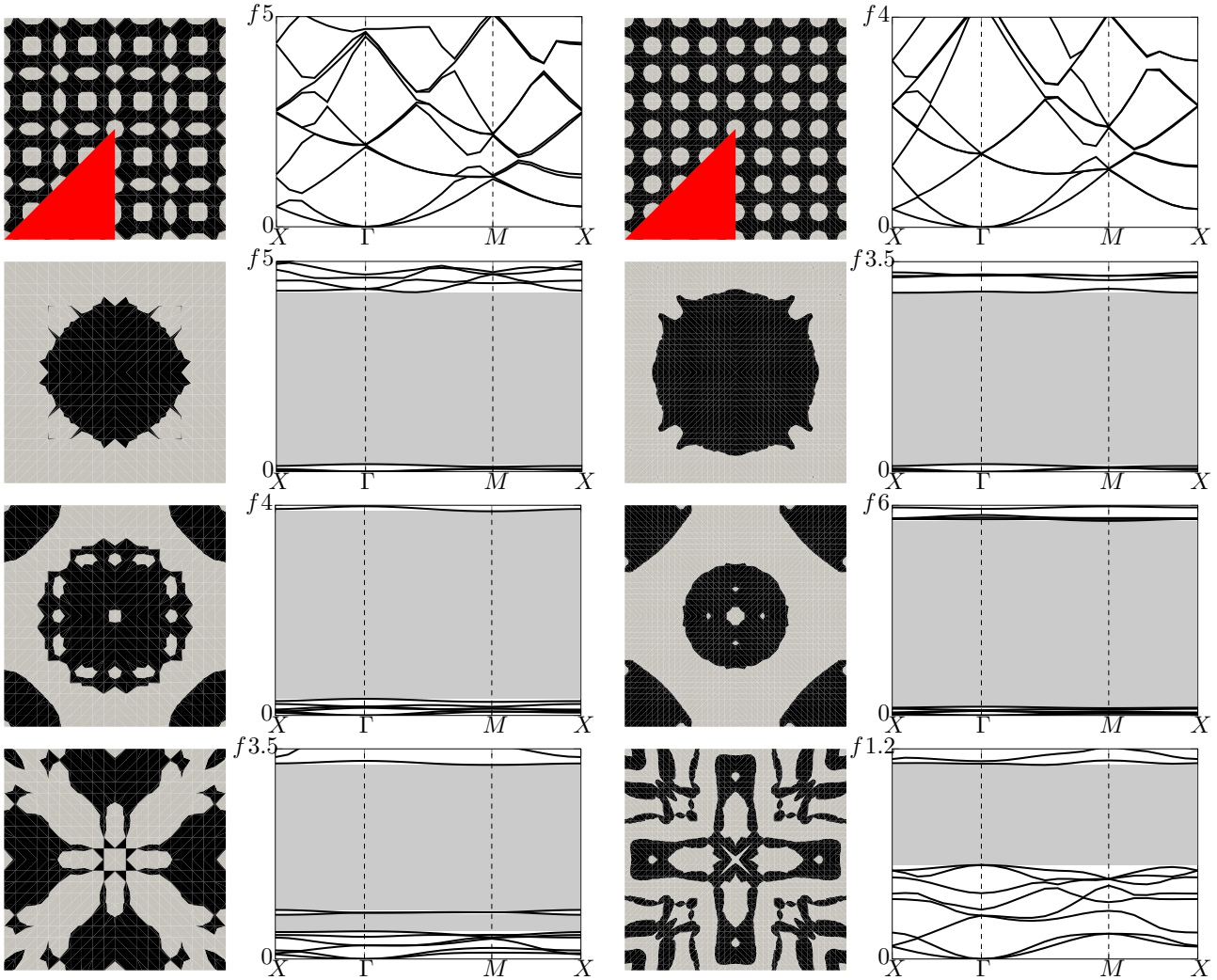








We used the technique to create bandgaps between different bands



initial design
(no bandgap)

bandgap between
3rd and 4th bands

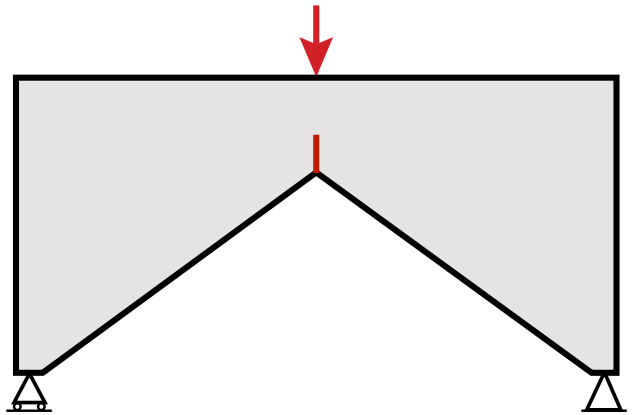
bandgap between
6rd and 7th bands

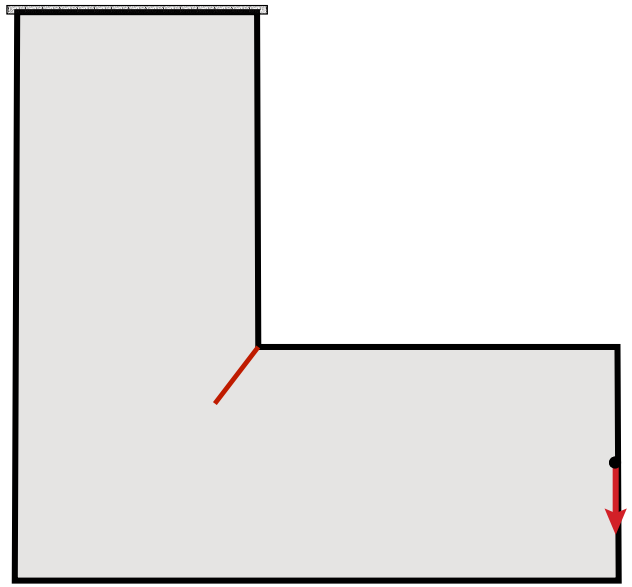
bandgap between
7rd and 8th bands

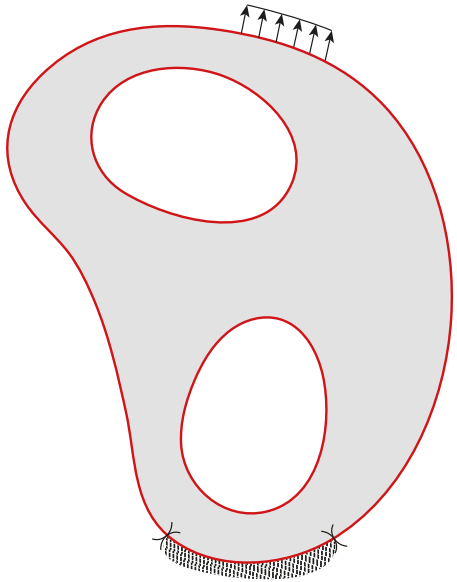
- van den Boom *et al.*, *J Mech Phys Solids* (In Preparation)

Mechanical metamaterials with tailored fracture resistance

Most fracture-based topology optimization mitigate the effect of predefined crack

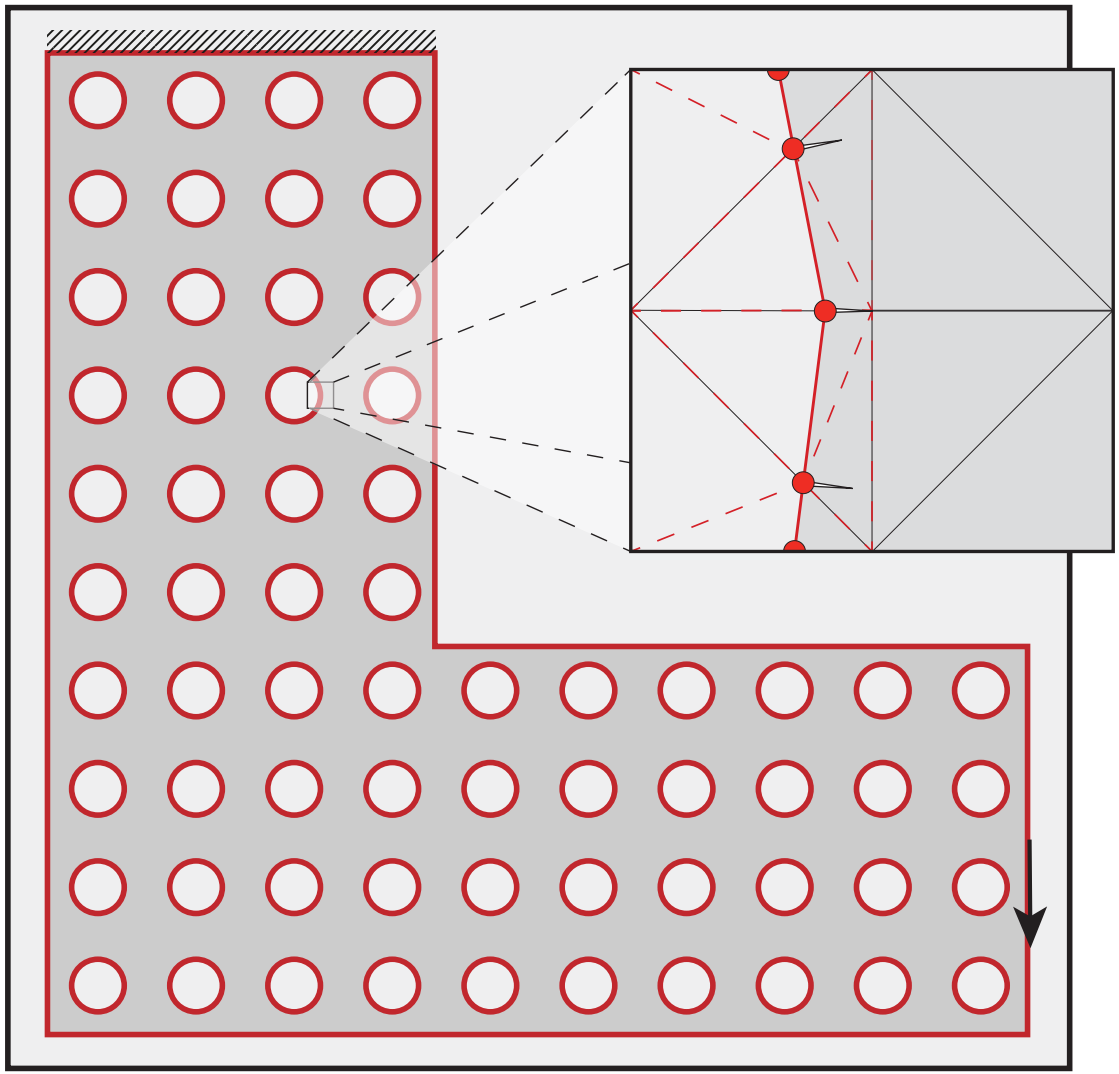






Evaluating energy release rates at along the boundary would require custom-made meshes to capture stress singularities—thus **intractable**!

We proposed a topology optimization that incorporates linear elastic fracture mechanics



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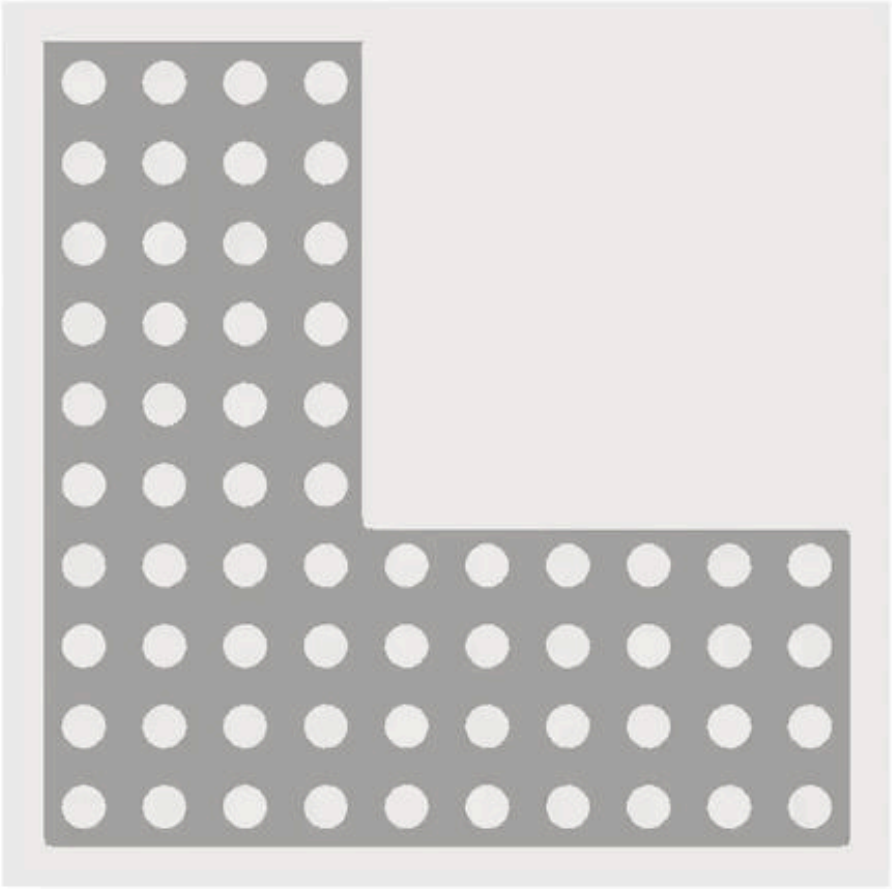
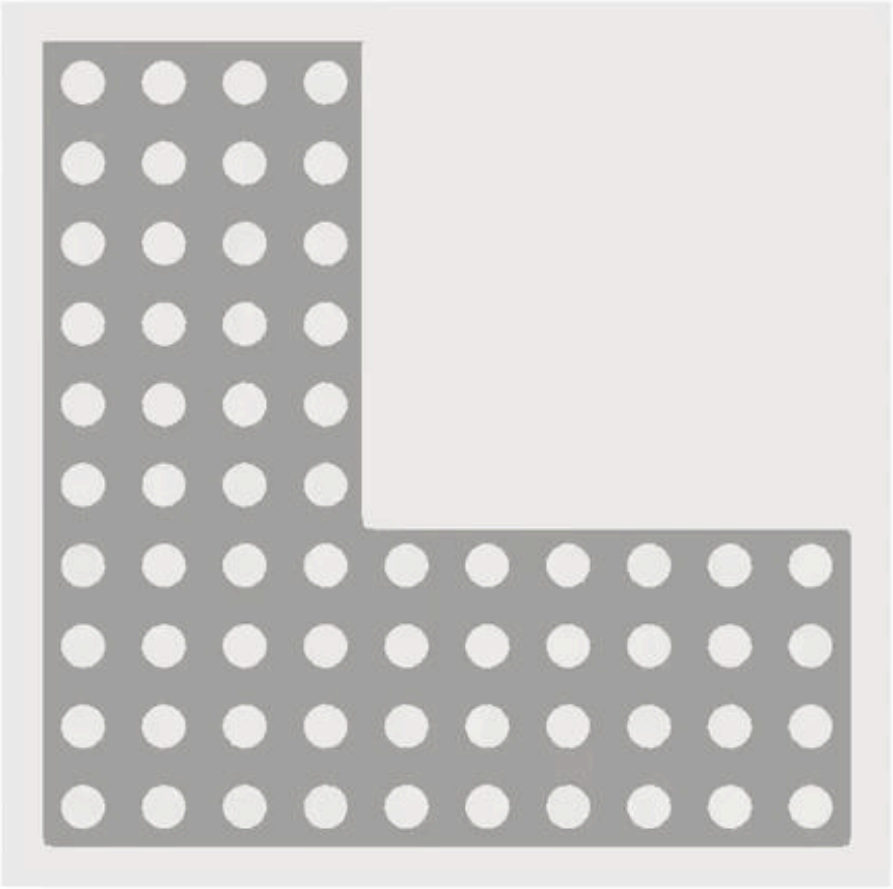


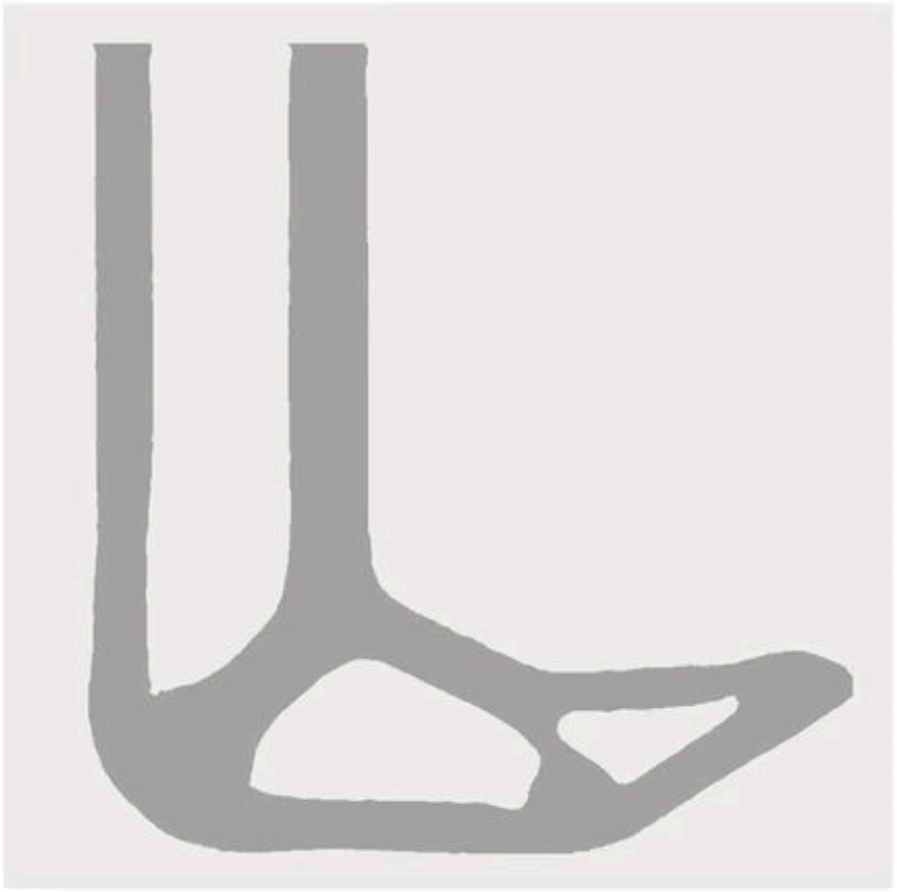
fracture-based



stress-based

We proposed a topology optimization that incorporates linear elastic fracture mechanics

fracture-based



stress-based

- Zhang *et al.*, *Comput Methods Appl Mech Eng* (2022)

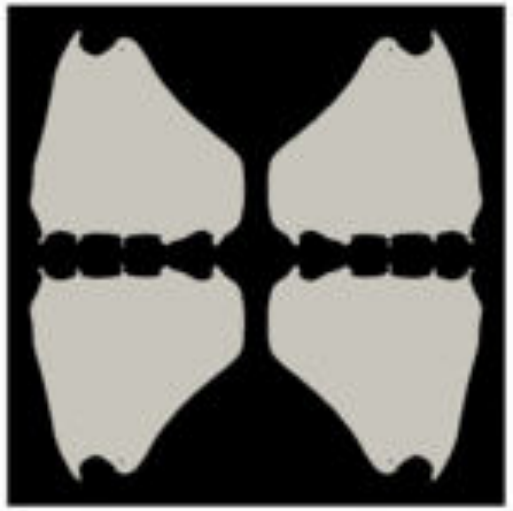
We used topology optimization for fracture anisotropy in chocolate

- Minimize/maximize energy release rate:

$$J = \omega \frac{1}{N} \sum_{i=1}^{N} G_{1i} - (1-\omega) \frac{1}{N} \sum_{i=1}^{N} G_{2i}$$

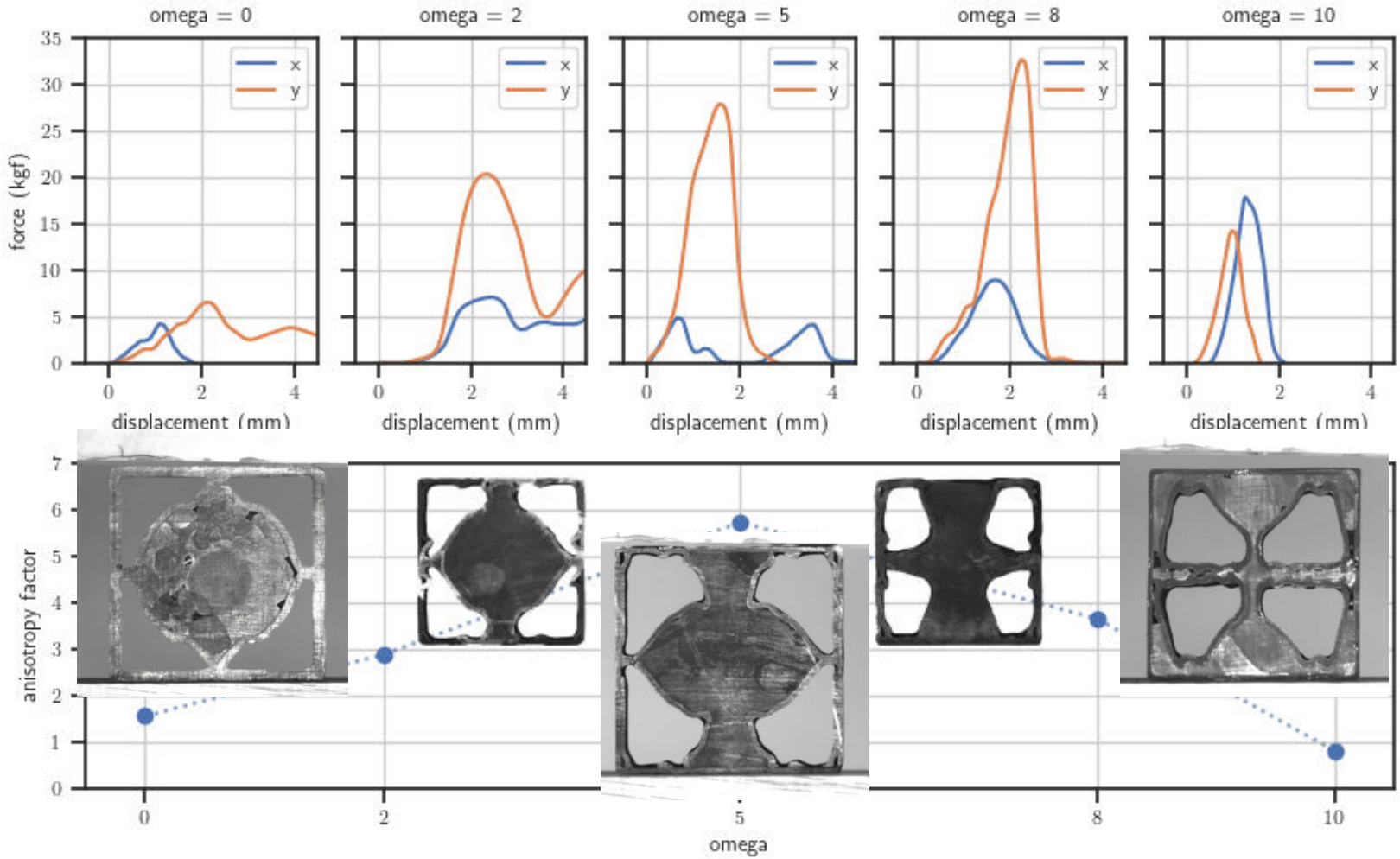
$\omega = 0$

$\omega = 0.5$



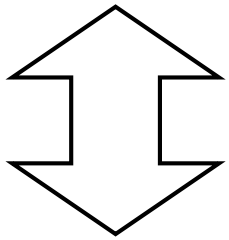
$\omega = 1$

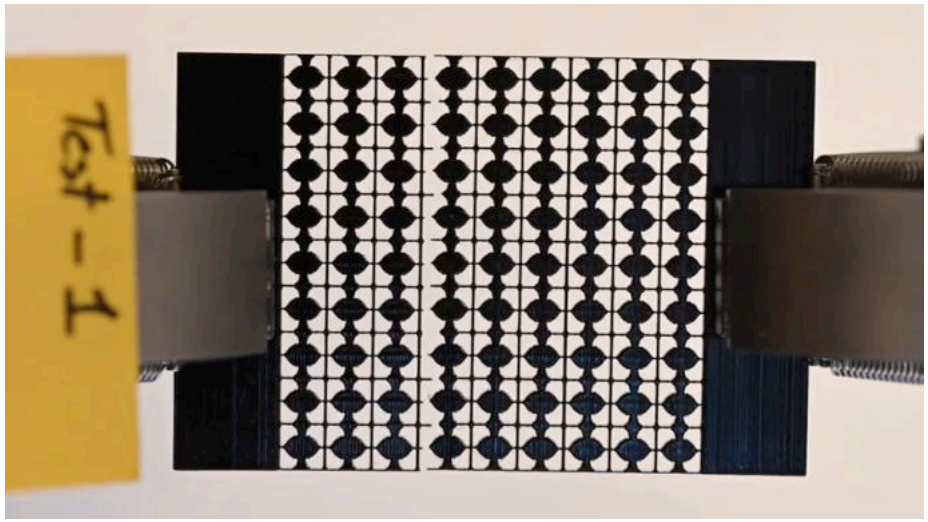
We used this technique to optimize for fracture anisotropy in chocolate

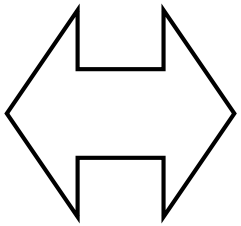


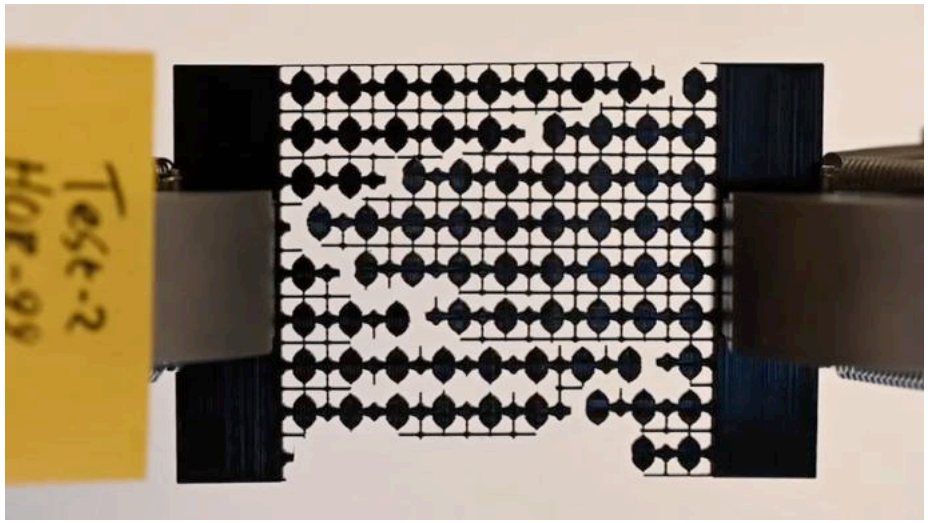
- Souto *et al.*, Edible Edible mechanical metamaterials with designed fracture for mouthfeel control. *Soft Matter (2022).*

Fracture metamaterials are being tested for fracture anisotropy









Conclusions

- Exploring the vast geometry-property design space undoubtedly mandates for efficient computational tools;
- Enriched FEA can effectively be used to analyze challenging problems by decoupling discontinuities from the mesh, saving on 80% of the time;
- Enriched FEA for topology optimization (TO) delivers black-and-white designs that are smoother than standard TO;
- We started using enriched TO for designing metamaterials with promising results;
- Machine learning will further enhance the design capabilities of these procedures.


THANK YOU!

- A. Souto, J. Zhang, A.M. Aragón, K.P. Velikov, and C. Coulais. "Edible Edible mechanical metamaterials with designed fracture for mouthfeel control." *Soft Matter (2022);*
- J. Zhang, F. van Keulen, and A. M. Aragón. "On Tailoring Fracture Resistance of Brittle Structures: A Level set Interface-enriched Topology Optimization Approach." *Comput Methods Appl Mech Eng* (2022);
- S. J. van den Boom, F. van Keulen, and A. M. Aragón. "Fully decoupling geometry from discretization in the Bloch-Floquet finite element analysis of phononic crystals." *Comput Methods Appl Mech Eng* (2021);
- S. J. van den Boom, J. Zhang, F. van Keulen, and A. M. Aragón. "An Interfaced-enriched Generalized Finite Element Method for level set based topology optimization." *Struct Multidiscip Optim* (2020);
- A. M. Aragón, B. Liang, H. Ahmadian, and S. Soghrati. "On the stability and interpolating properties of the Hierarchical Interface-enriched Finite Element Method." *Comput Methods Appl Mech Eng* 362 (2020), pp. 112671;
- S. J. van den Boom, J. Zhang, F. van Keulen, and A. M. Aragón. "A Stable Interface-Enriched Formulation for Immersed Domains with Strong Enforcement of Essential Boundary Conditions." *Int J Numer Meth Eng* 120 (2019), pp. 1163–1183;
- J. Zhang, S. J. van den Boom, F. van Keulen, and A. M. Aragón. "A Stable Discontinuity-Enriched Finite Element Method for the Analysis of 3-D Problems with Weak and Strong Discontinuities." *Comput Methods Appl Mech Eng* 355 (2019), pp. 1097–1123;
- A. M. Aragón and A. Simone. "The Discontinuity-Enriched Finite Element Method." *Int J Numer Meth Eng* 112.11 (2017), pp. 1589–1613;
- S. Soghrati, A. M. Aragón, C. A. Duarte, and P. H. Geubelle. "An interface-enriched GFEM for problems with discontinuous gradient fields." *Int J Numer Meth Eng* 89.8 (2012), pp. 991–1008.

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