SAND2022-2314C

Machine learning of symbolic expressions to model dispersion curves in metamaterials

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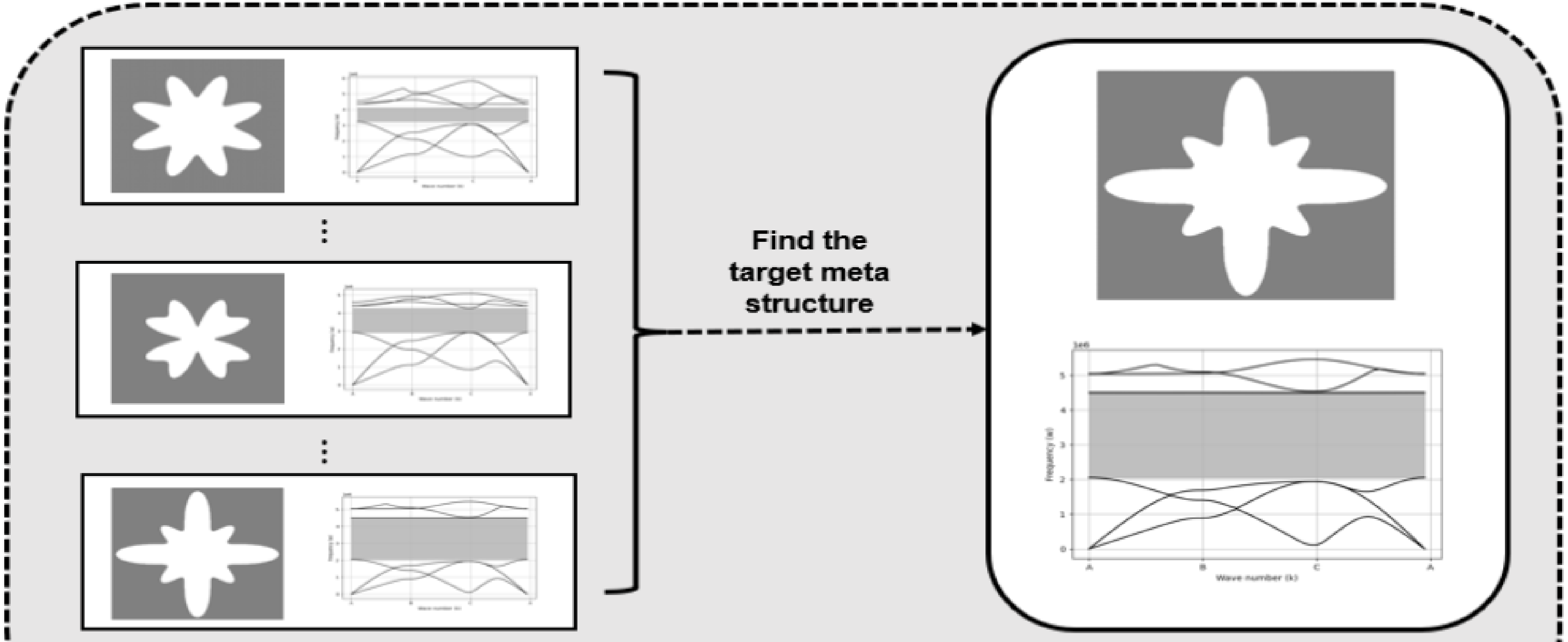
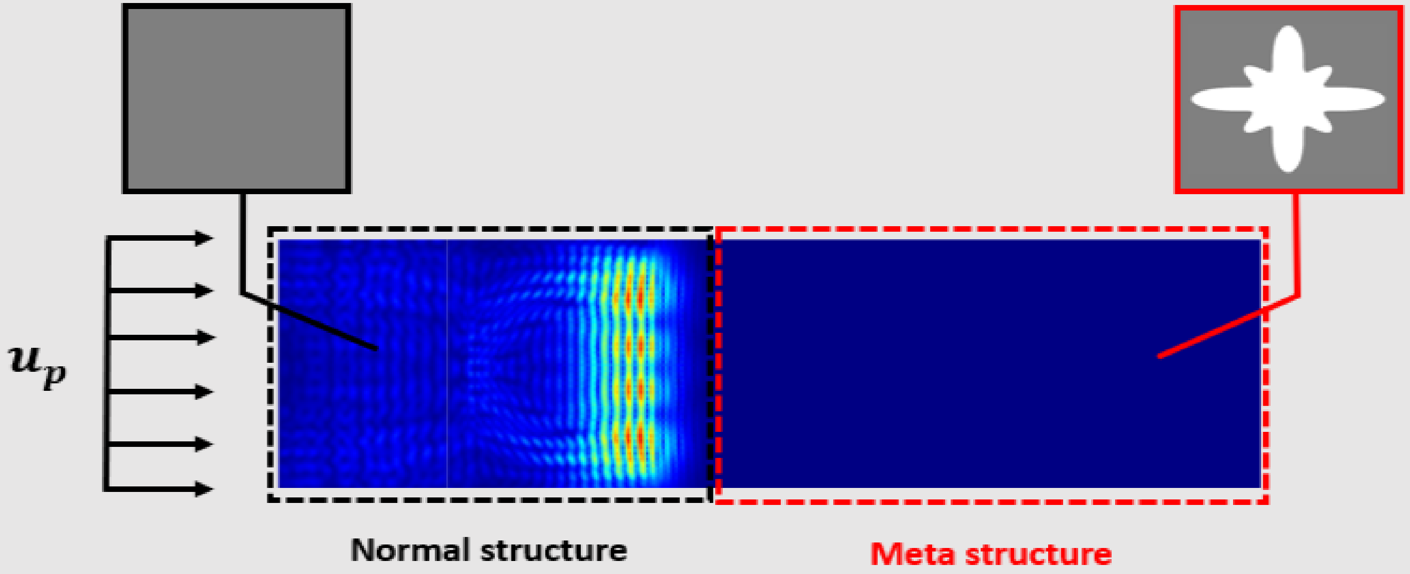
The purpose of the project



The goal of the project is to make the system designing the metamaterial that isolate wave propagation within a specific frequency ranges named band gap.

Application



Wave cannot propagate beyond the section consisting of meta structure unit cell, as there is wave propagation in beam structure.

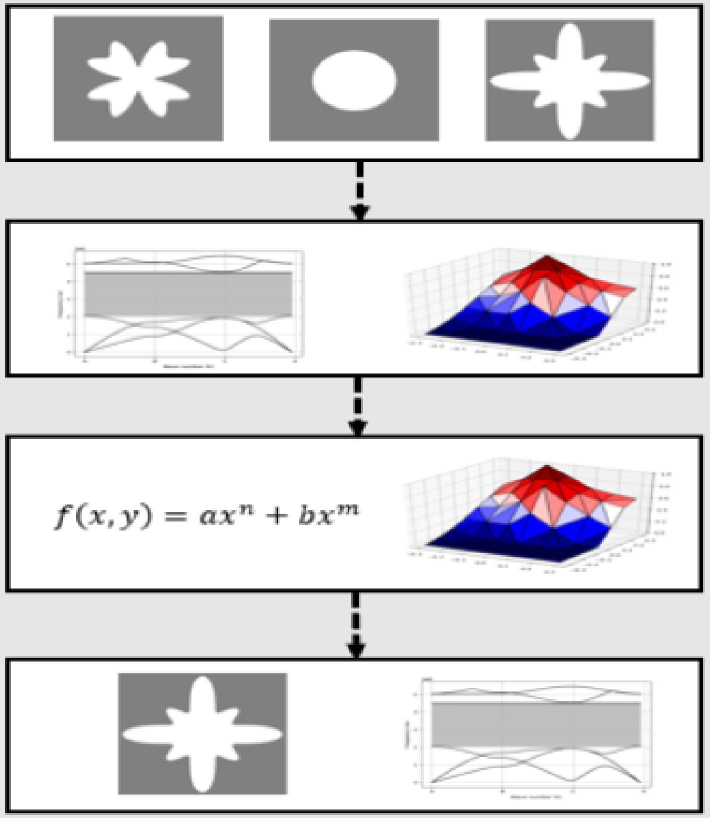
Procedure

1. Periodic structures
Periodic structures defined by trigonometric functions are generated

2. Data collection
The bandgap data on various geometry are collected to generate the bandgap surface

3. Interpretable machine learning
The equations defining the surface are discovered through interpretable machine learning

4. Topology optimization
Optimized metamaterial structures are found through the discovered equations.



Periodic structure

$$r = r_0 \cdot (1 + c_0 \cdot cos(2\theta) + c_1 \cdot cos(4\theta) + c_2 \cdot cos(8\theta))$$

c0 0.00

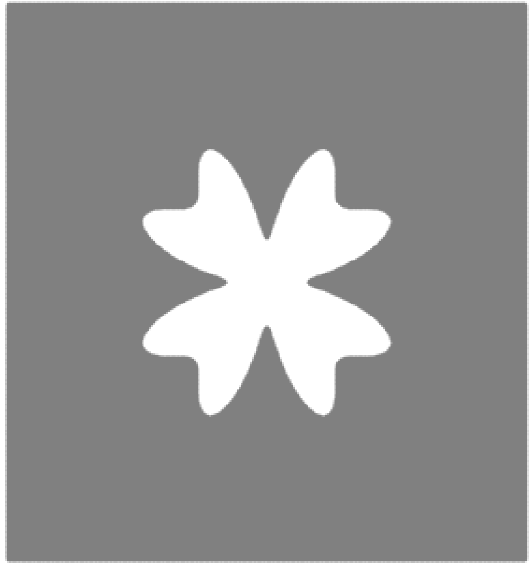
c1 -0.30

c2 -0.30

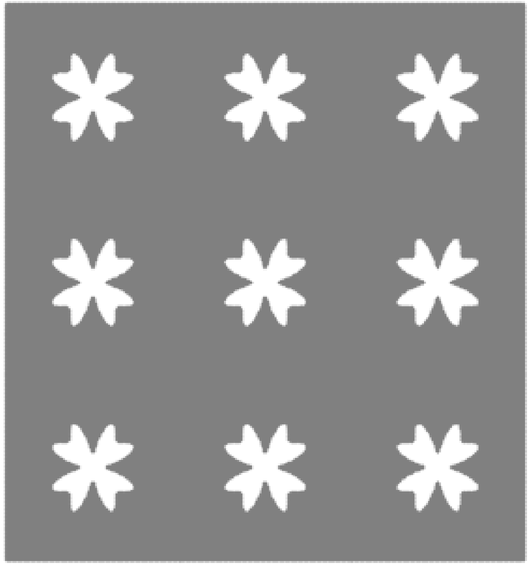
r0 0.20

h : 0.2582582582582582

Unit cell



Periodic structure



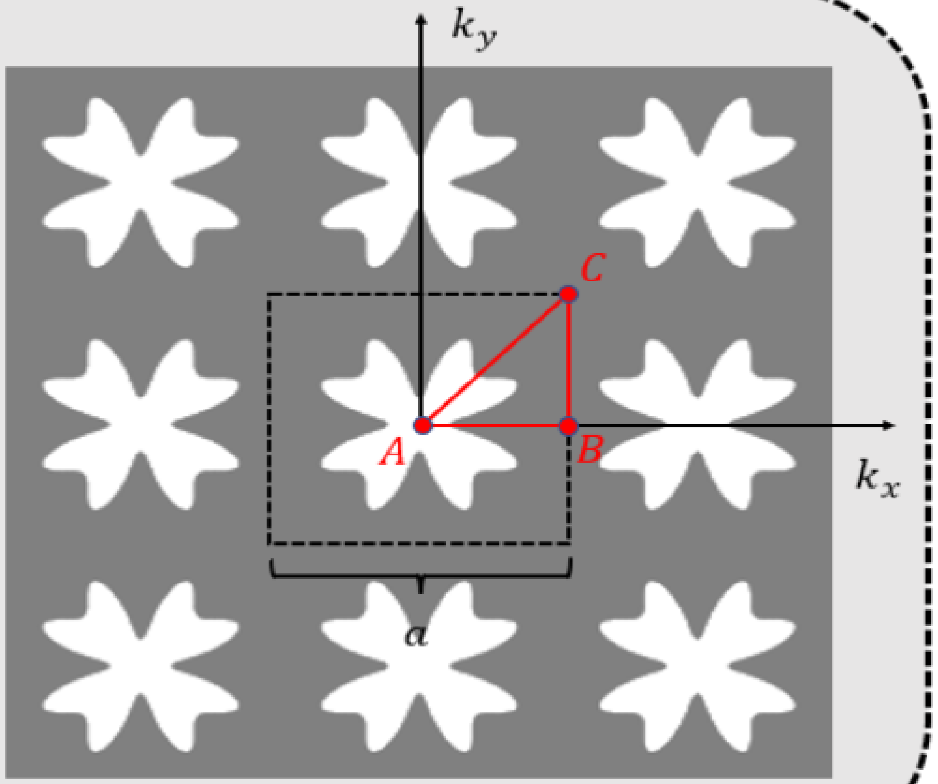
Generate data (Bandgap analysis)

$$(\boldsymbol{K} - \boldsymbol{w}^2\boldsymbol{M}) \cdot \boldsymbol{U} = \boldsymbol{F}$$

The frequencies (w) response of a periodic structures can be simply measured by solving eigen value problem with Bloch periodic boundary conditions within the range of wave vector

$$\boldsymbol{A} = (\boldsymbol{0}, \boldsymbol{0})$$
$$\boldsymbol{B} = (\boldsymbol{\pi}/\boldsymbol{a}, \boldsymbol{0})$$
$$\boldsymbol{C} = (\boldsymbol{\pi}/\boldsymbol{a}, \boldsymbol{\pi}/\boldsymbol{a})$$

It is enough to analyze red triangle edges named irreducible Brillouin zone (IBZ). It spans from A to B to C and then back to A

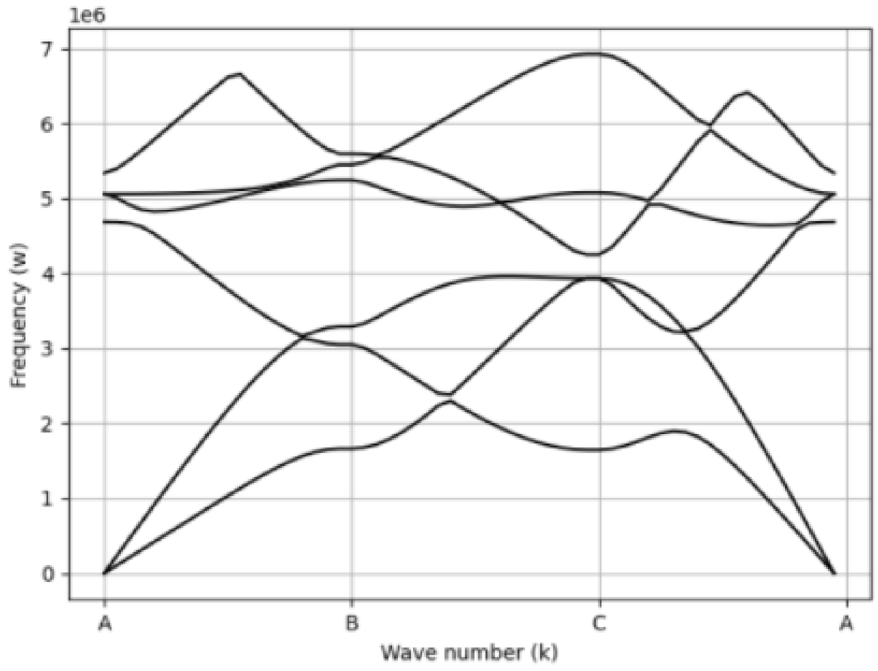


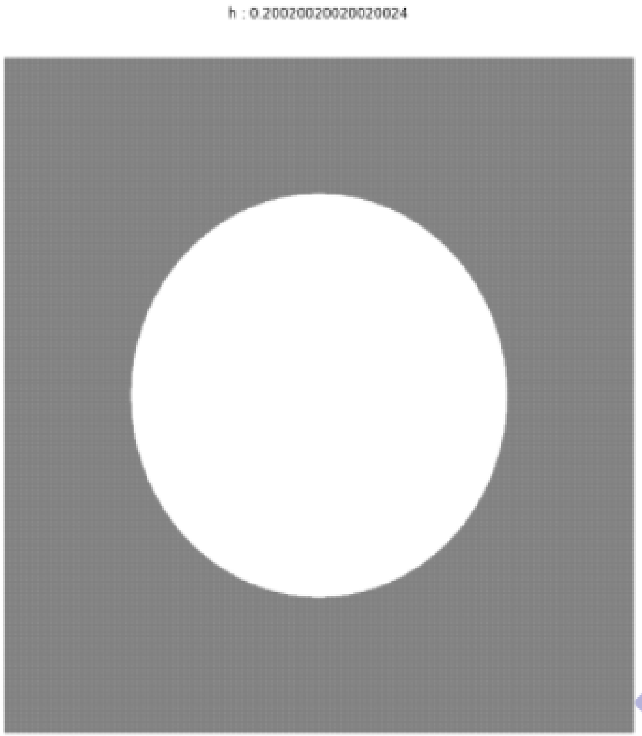
Bandgap equation $f(w_i, w_{i+1})$ is:

$$f(w_i, w_{i+1}) = \begin{cases} min(w_{i+1}) - max(w_i) & \text{if, } min(w_{i+1}) \geq max(w_i) \\ 0 & \text{else} \end{cases}$$

c1_val 0.00

c2_val 0.00



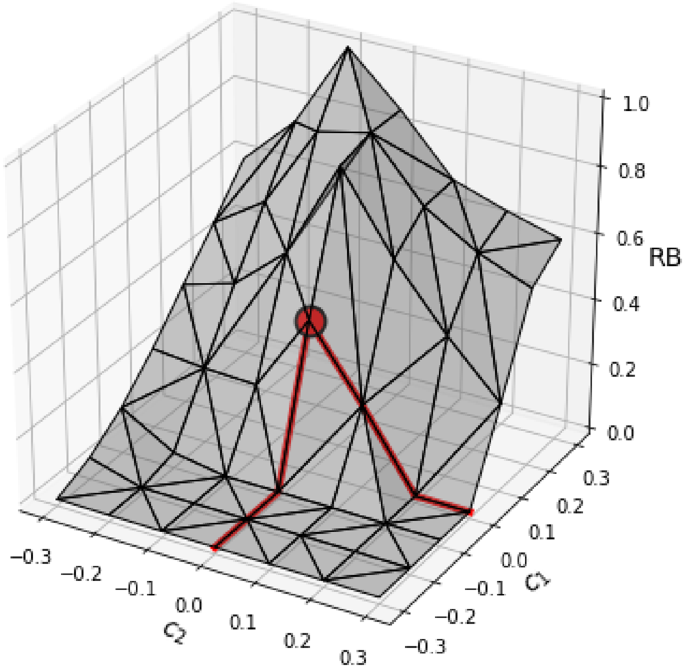


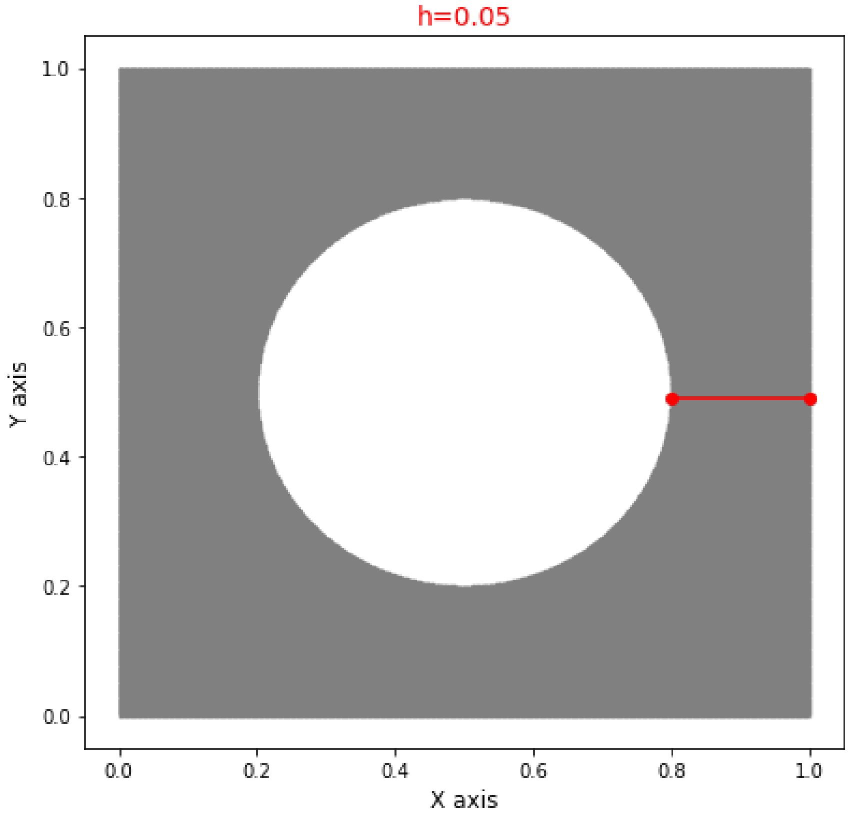
Band gap surface

ind 0.00

c1 0.00

c2 0.00





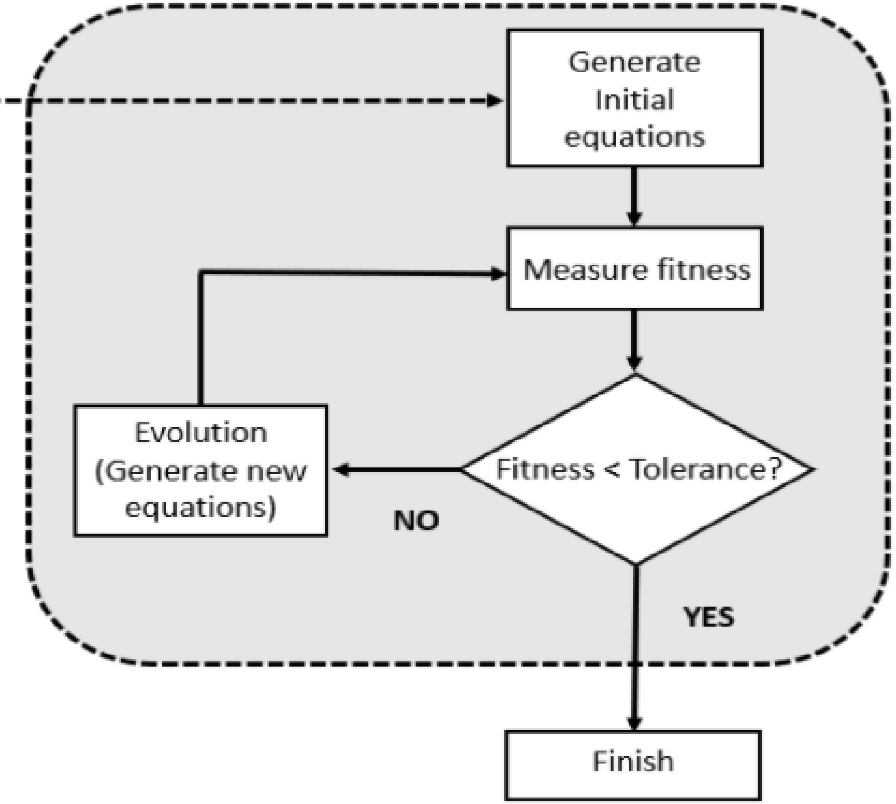
Interpretable machine learning

BINGO
BINGO is an open-source package initially develop at NASA for performing genetic programming symbolic regression.

Genetic programming symbolic regression (GPSR)
It is one of the regression method that search mathematical expression to find the best model based on evolving system similar with natural genetic process.

GPSR algorithm

Input data
(X, Y)

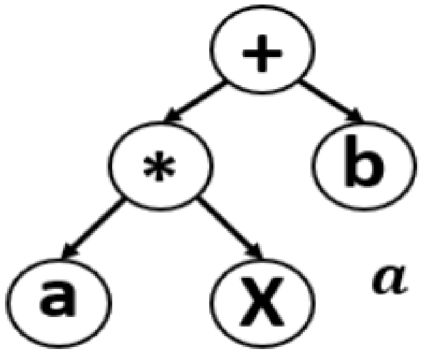


Step 1.
Initial equations are randomly generated

Step 2.
The accuracy of each equation is measured by fitness

Step 3.
The equations will be evolved, based on fitness values and generate next generation equations

Step 4.
Step 1 to 3 will be iterated, until fitness value is lower than tolerance

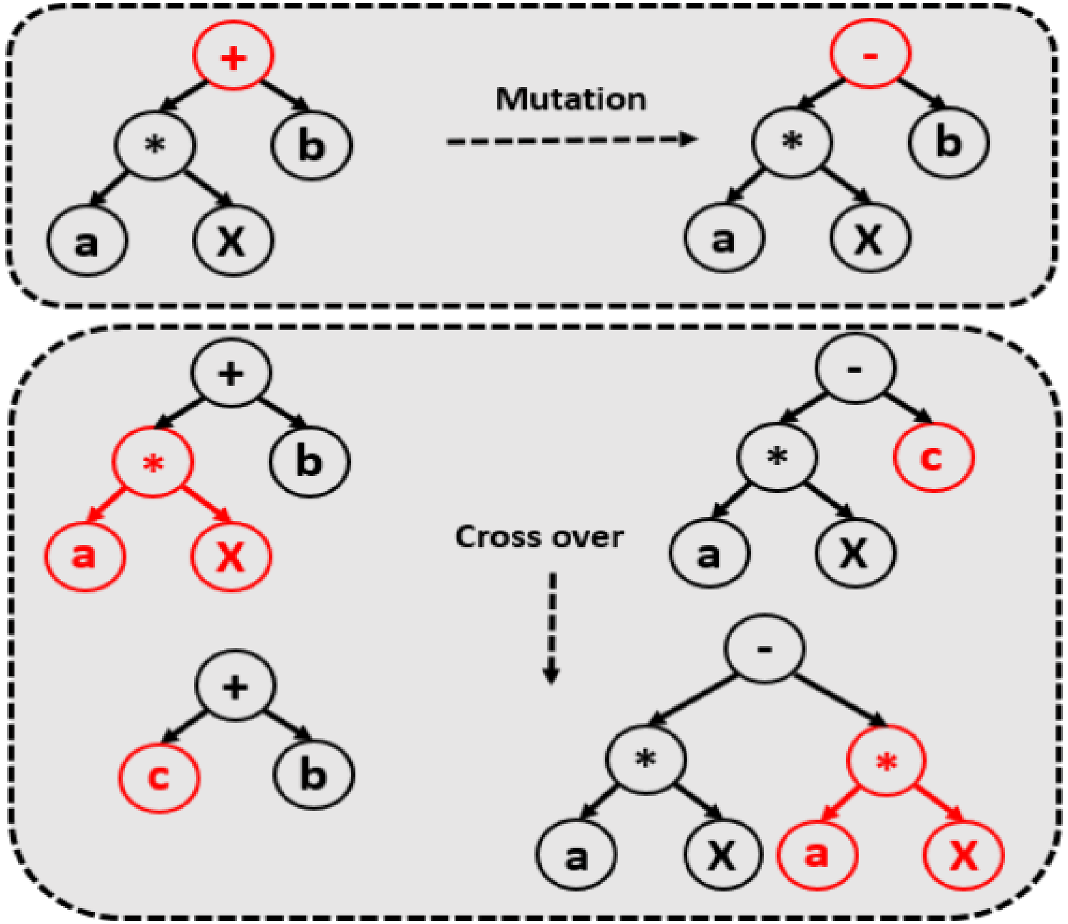


$a * X + b$

1. Equation (Acyclic graph)
Individual equation is expressed as acyclic graph

2. Mutation (Evolution)
Randomly select any node and implement mutation.

3. Cross over (Evolution)
Randomly select sub tree from two equations and implement cross over.



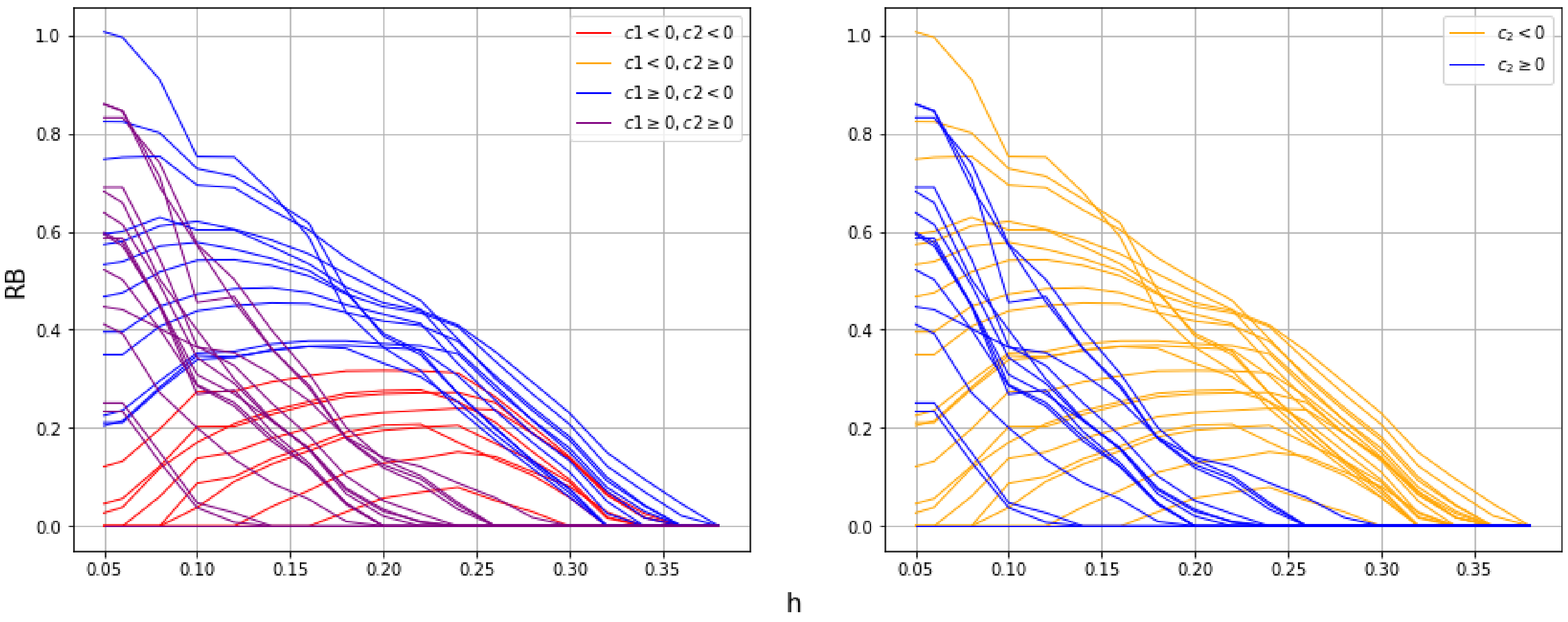
Training data

- We convert negative value of candidate equation as 0 based on bandgap equation.

$$\tilde{u} = \begin{cases} \tilde{u} & \text{if } \tilde{u} \geq 0 \\ 0 & \text{else if } \tilde{u} < 0 \end{cases}$$

- We separate data by geometry parameter c_2.
  - $\text{Group1:}\, c_2 < 0$
  - $\text{Group2:}\, c_2 \geq 0$

ind 1.00

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Out[19]: <function __main__.<lambda>(ind)>
```

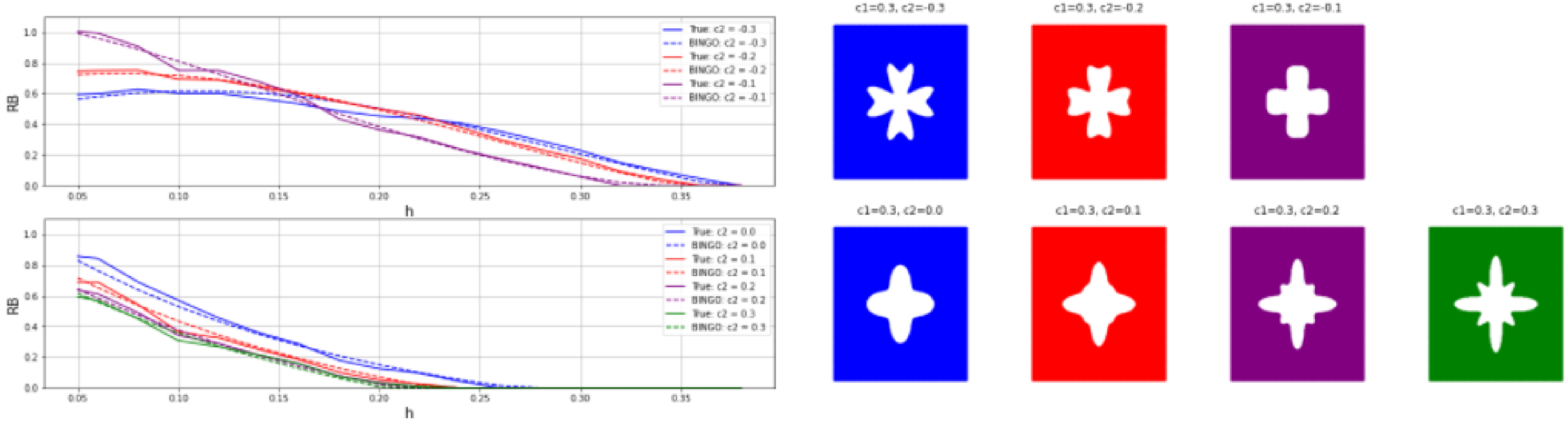
Discovered equations

$$f(c_1, c_2, h) = \begin{cases} (sin(f_1) + 0.33)\,(-0.287 \cdot c_2 \cdot (f_1) - 2.76 \cdot h + 0.84) & \text{if } c_2 < 0 \\ f_4\,(-1.44 \cdot h + (sin\,(f_2 \cdot (f_3 + 0.84)) - 1.63)\,(c_2 \cdot f_3 - f_2 - 0.37) - 0.39) & \text{else if } c_2 \geq 0 \end{cases}$$

where,

- $f_1(h, c_1, c_2) = 5.62h - 0.31 + (-c_1(c_2 \cdot h + 0.49))/c_2$
- $f_2(c_1, c_2) = 2c_1 + c_2$
- $f_3(c_2) = 0.94 - c_2$
- $f_4(h) = 1/(h + 0.27)$

c1 0.30

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Out[20]: <function __main__.<lambda>(c1)>
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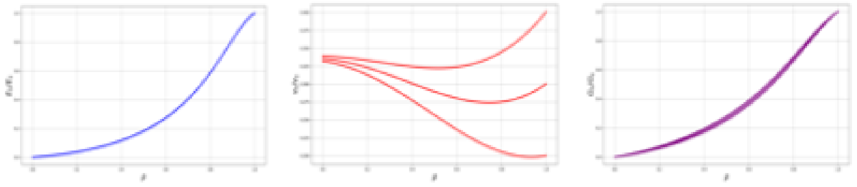
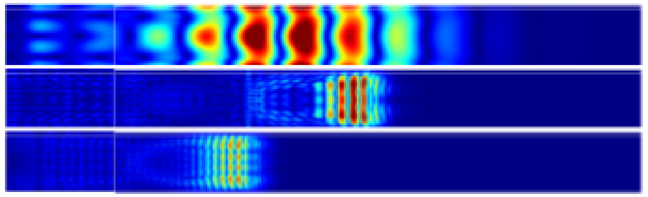
Plato Workflow

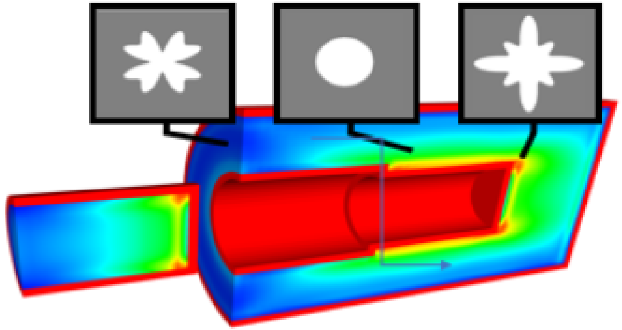
Step1 (BINGO)
Generate functional form of homogenized properties (E_h,v_h,G_h) in terms of relative density



Step2 (PLATO)
Simulate wave propagation in meta-structure



Step3 (PLATO)
Optimize graded meta-structure unit cell layout



Conclusion

- GPSR is able to discover the equation of band gap surface
- Discovered equations are not simple enough

Future plan

- We will regenerate dense band gap data with relaxed micromorphic model to find better equation.
- Geometry variable c_0 will be considered.
- The discovered bandgap equation will be applied to the Plato software to find the optimized metamaterial structure.

Reference

- Bomarito, G., et al., 2018, Bingo. Available: https://github.com/nasa/bingo
- Plato development team, 2022, Plato. Available: https://www.sandia.gov/plato3d/
- Ryan Alberdi, Joshua Robbins, Timothy Walsh, Remi Dingreville, Exploring wave propagation in heterogeneous metastructures using the relaxed micromorphic model

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Thanks! Question?