Design of Viscoelastic Auxetic Materials Through Machine Deep Learning

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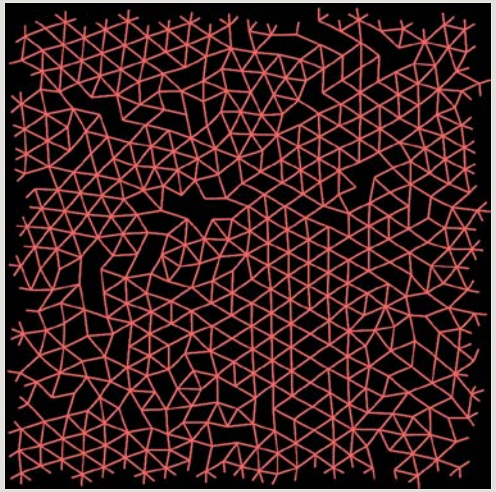
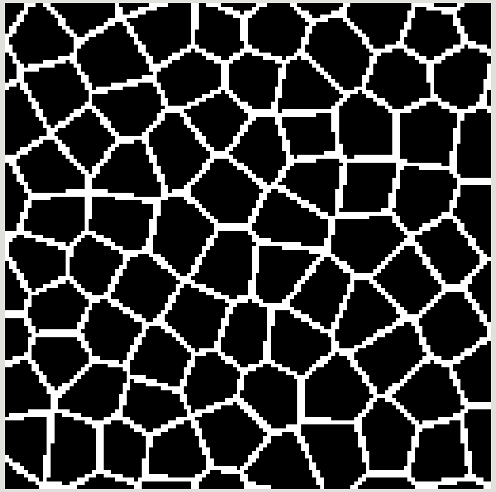
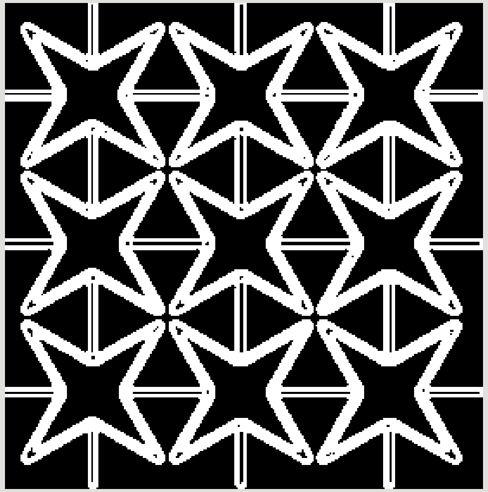
Outline

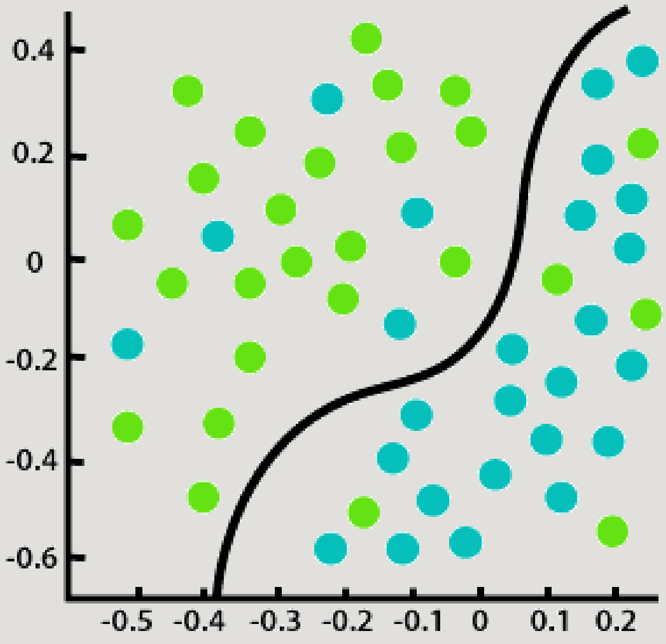
Design the mechanical properties we desire, with constraints.



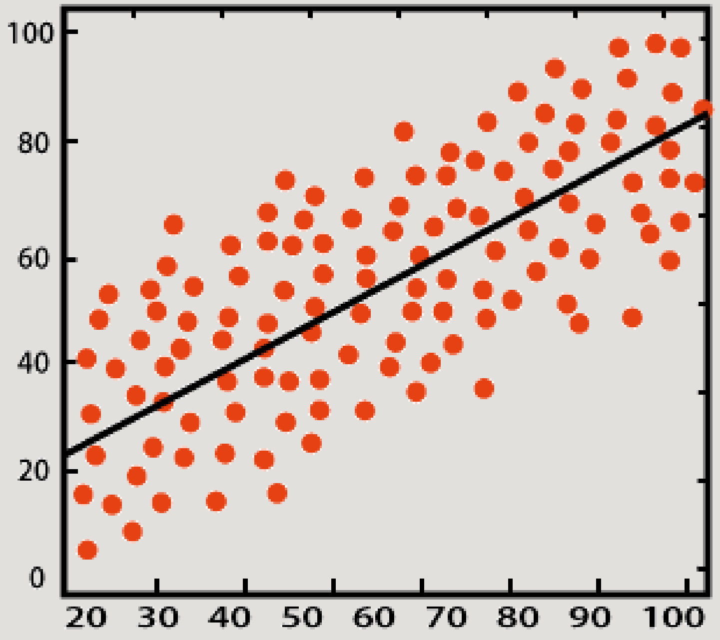




What if we start from random samples?
And let them just evolve, in case we may discover more potential paradigms.

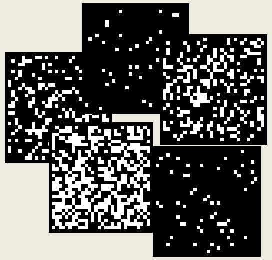


Classification



Regression

The Oracle



Samples

Youngs Modulus

Shear Modulus

Bulk Modulus

Poisson's Ratio

Loss Tangent $\tan\delta$

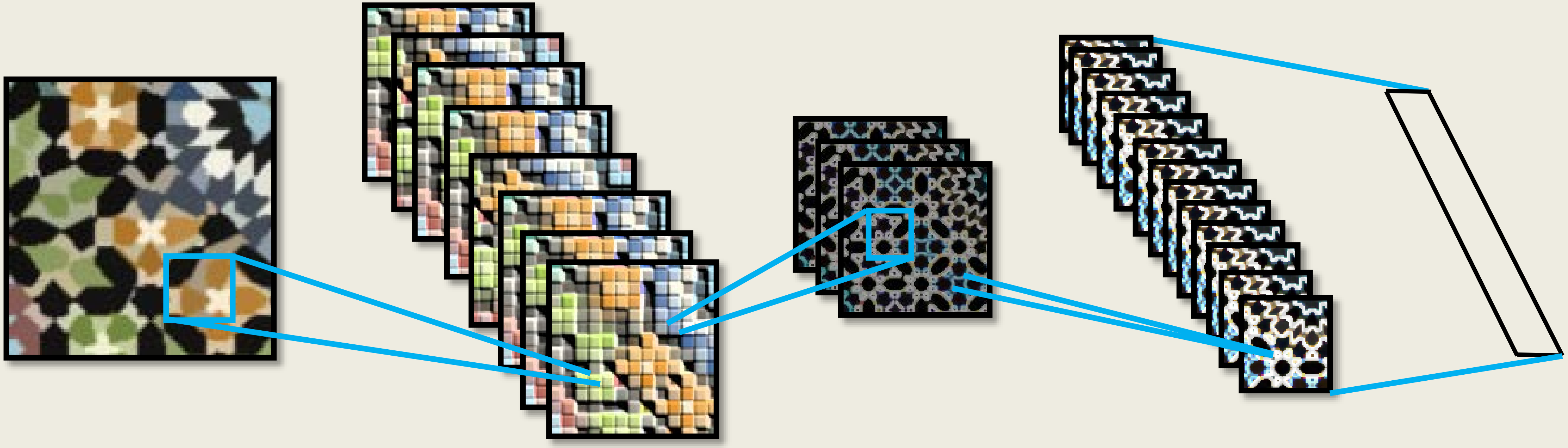
Complex elastic modulus $|E^*|$

Ground Truth Labels

Predicted Labels

$$y = Wx + b$$

Artificial Neural Network



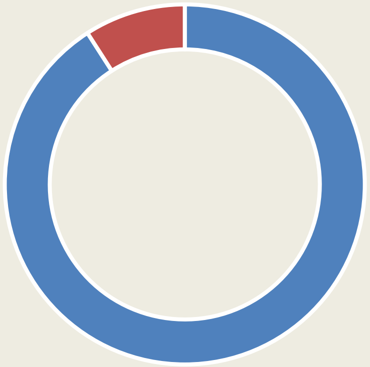
Input Layer

Convolution and Pooling Layers

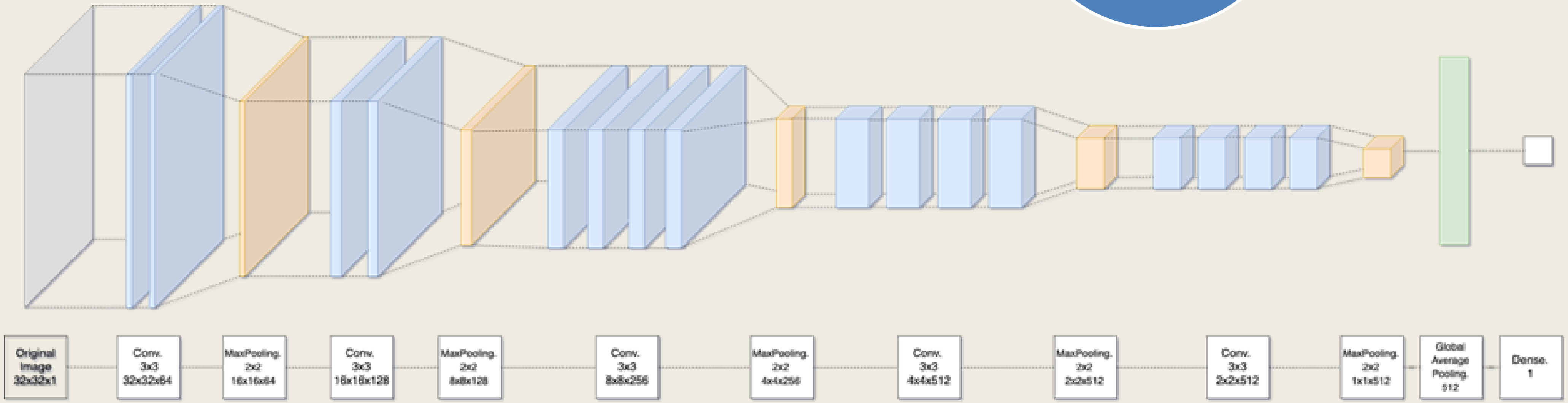
Output and Loss Layer

VGG19

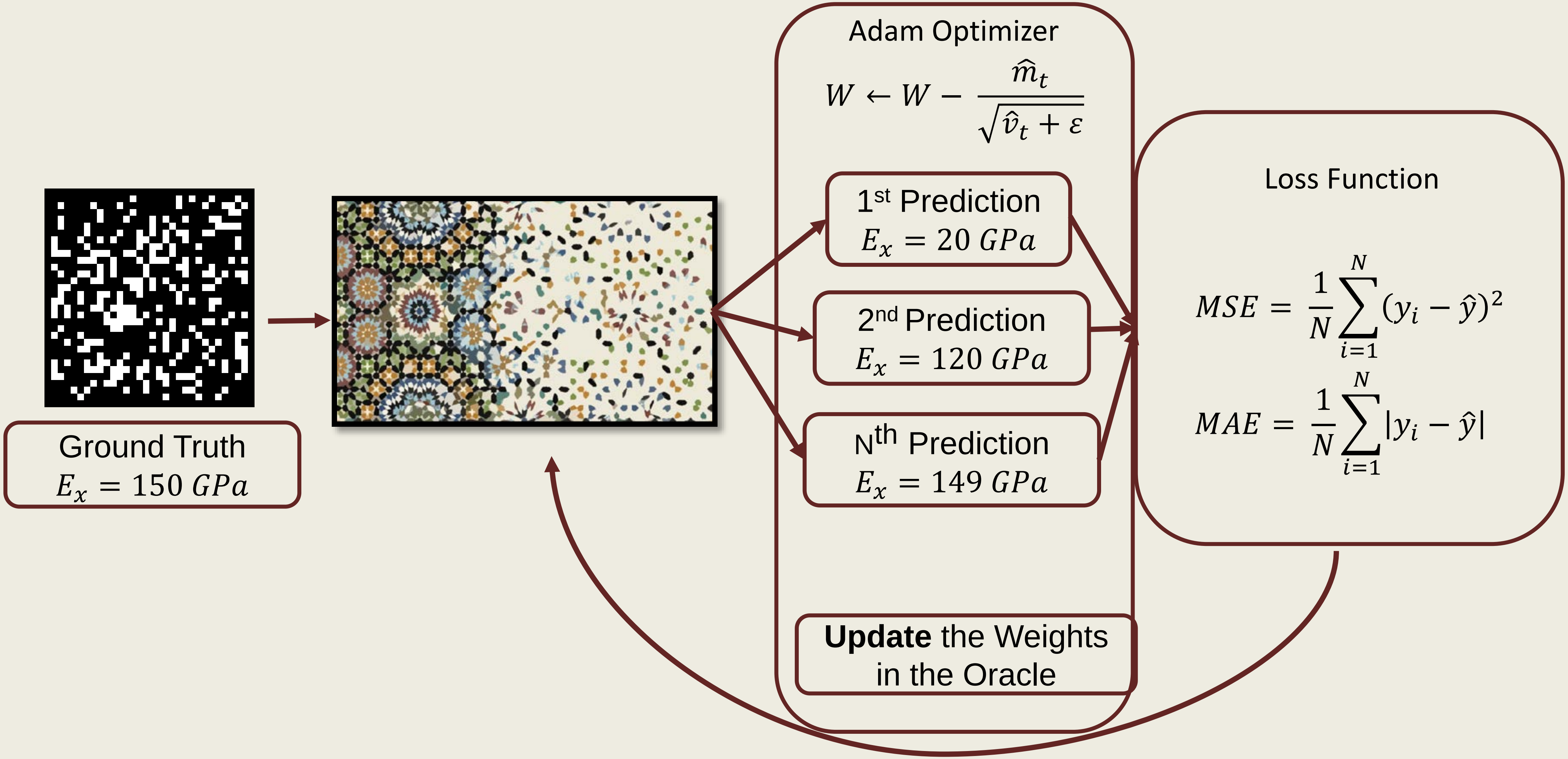
90% classification accuracy.



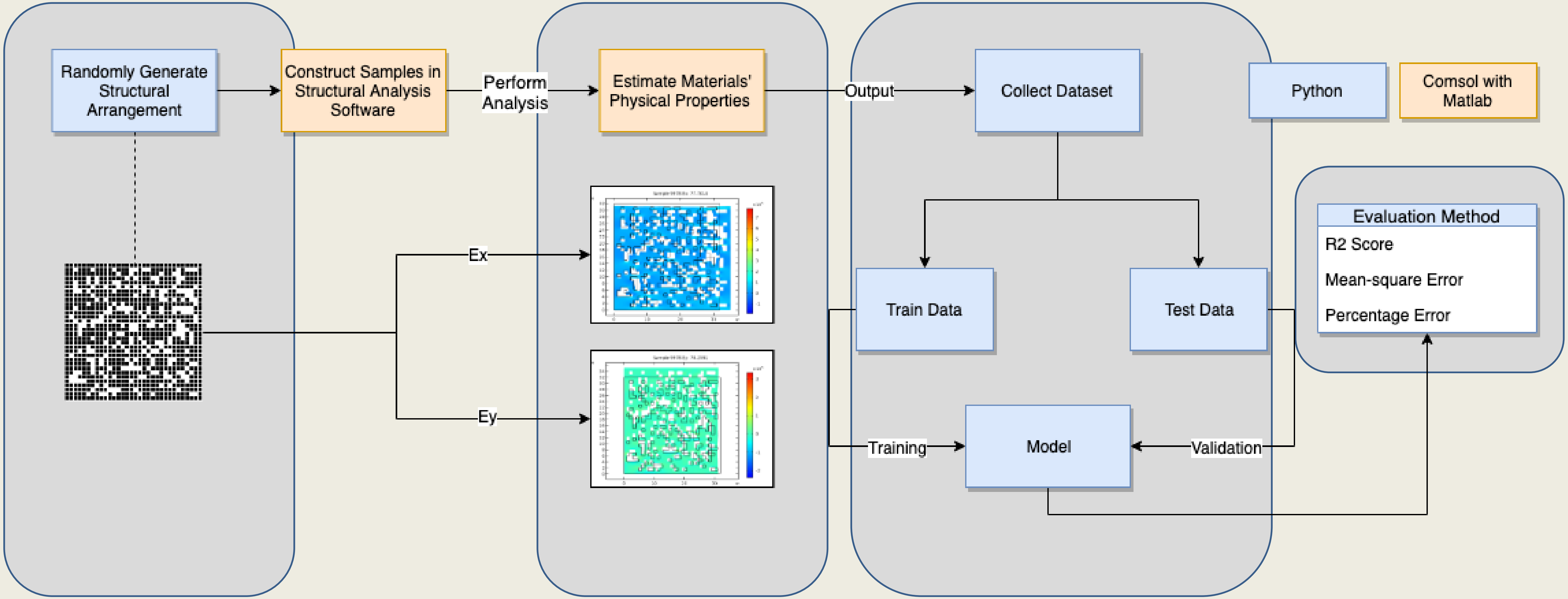
ImageNet Large Scale Visual Recognition Competition
over 10 million image data and 1000 classes



Loss and Optimizer



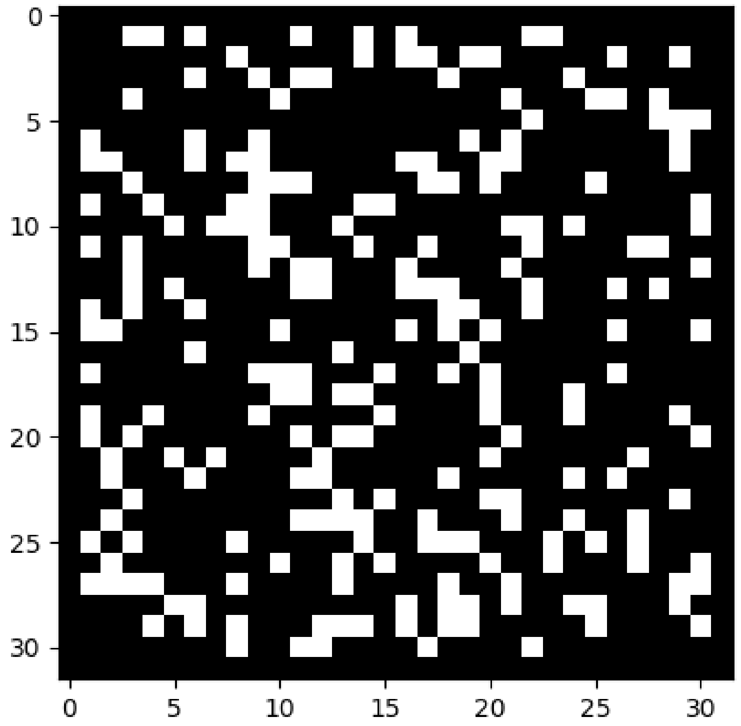
Flow Chart



Randomly Generate Structural Arrangement
Construct Samples in Structural Analysis Software
Perform Analysis
Estimate Materials' Physical Properties
Output
Collect Dataset
Python
Comsol with Matlab
Ex
Ey
Train Data
Test Data
Evaluation Method
R2 Score
Mean-square Error
Percentage Error
Training
Model
Validation

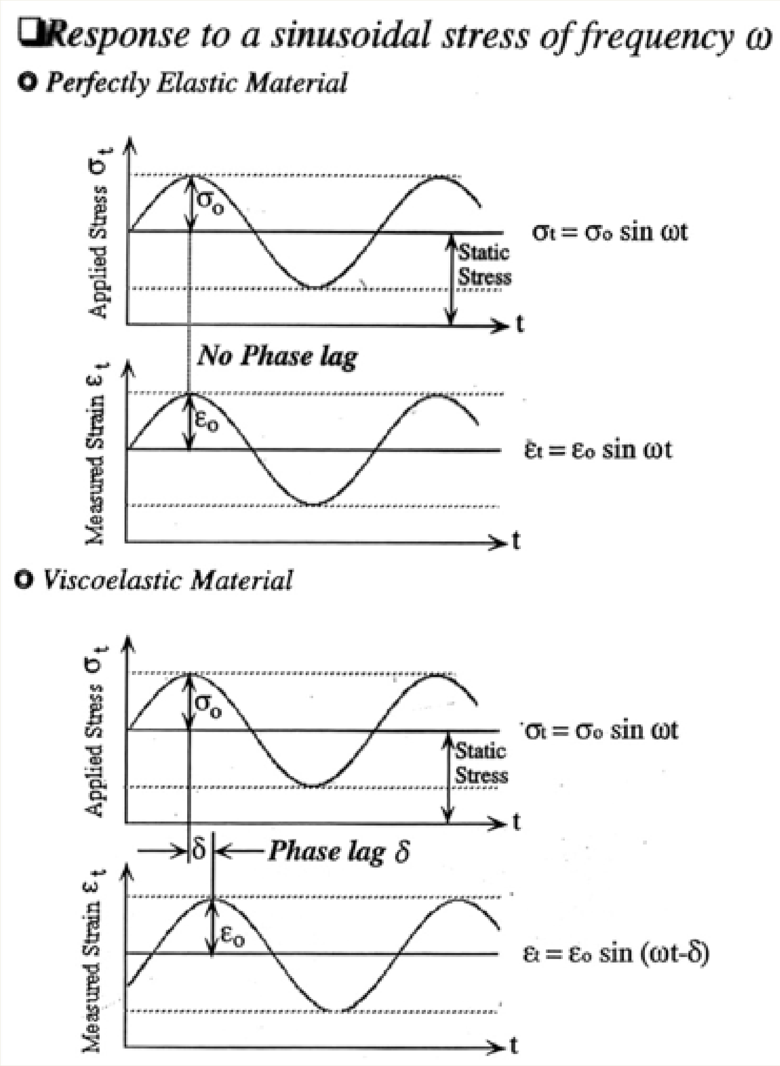
Samples

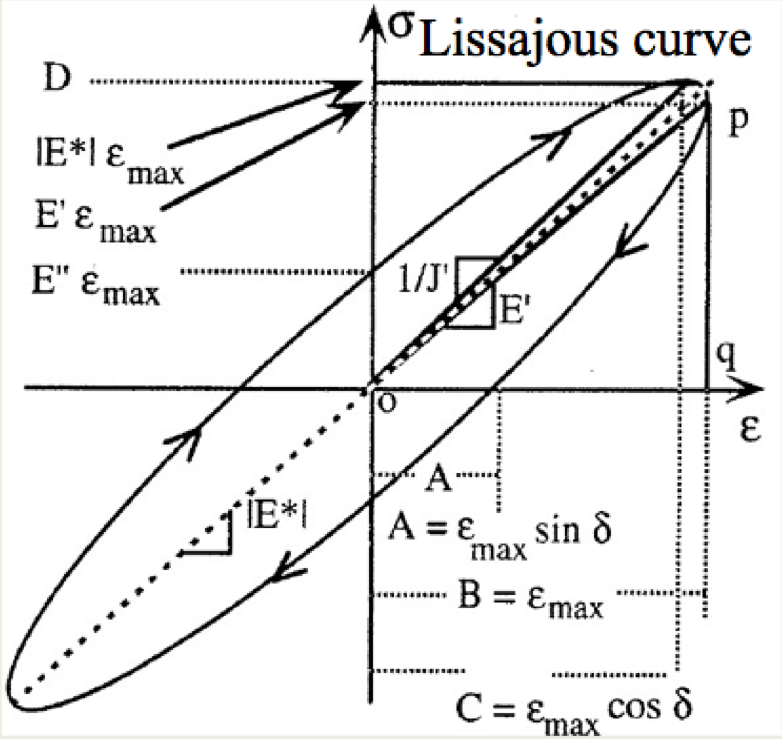
Solid Boundary



Smooth Angle

Linear viscoelasticity: dynamic response





Complex modulus

$$E^* = E' + iE''$$

Complex compliance

$$J^* = J' - iJ''$$

Loss tangent $\tan\delta = E''/E' = A/C$

Figure of merit $E'\tan\delta = E''$

Linear Elastic Material
The Navier Equation

For isotropic elasticity, the Navier equation is to be solved for displacement fields **u**.

$$\mu\nabla^2\mathbf{u}+(\lambda+\mu)\nabla(\nabla\cdot\mathbf{u})=\rho\ddot{\mathbf{u}} \quad \text{or} \quad \nabla\bullet\boldsymbol{\sigma}=\rho\ddot{\mathbf{u}}$$

In index notation

$$\mu u_{i,kk}+(\lambda+\mu)u_{k,k,i}=\rho u_{i,tt} \quad \text{or} \quad C_{ijkl}u_{k,jl}=\rho u_{i,tt}$$

With the engineering strain, Stress tensor can be found.

$$\varepsilon_{ij}=\frac{1}{2}(u_{i,j}+u_{j,i}) \quad \sigma_{ij}=C_{ijkl}\varepsilon_{kl}=C_{ijkl}u_{k,l} \quad \bar{\sigma}_{ij}=\bar{C}_{ijkl}\bar{\varepsilon}_{kl}$$

With the coefficients

$$\bar{C}_{ijkl}=\bar{\lambda}\delta_{ij}\delta_{kl}+\bar{\mu}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$$

The volume-averaged stress and strain are defined by

$$\bar{\sigma}_{ij}=\frac{1}{V}\int_{\Omega}\sigma_{ij}\,dV=\frac{1}{V}\int_{\partial\Omega}t_i x_j\,dA \quad \bar{\varepsilon}_{ij}=\frac{1}{V}\int_{\Omega}\varepsilon_{ij}\,dV=\frac{1}{2V}\int_{\partial\Omega}\left(u_i n_j+u_j n_i\right)dA$$

When **viscoelastic properties** are considered, the Boltzmann superposition leads to the following constitutive relation in time domain.

$$\sigma_{ij}\left(t,x_1,x_2,x_3\right)=\int_0^t E_{ijkl}\left(t-\tau,x_1,x_2,x_3\right)\frac{\partial\varepsilon_{kl}\left(\tau,x_1,x_2,x_3\right)}{\partial\tau}d\tau$$

$$\tilde{\sigma}_{ij}\left(\omega,x_1,x_2,x_3\right)=E^*_{ijkl}\left(\omega,x_1,x_2,x_3\right)\tilde{\varepsilon}_{kl}\left(\omega,x_1,x_2,x_3\right)$$

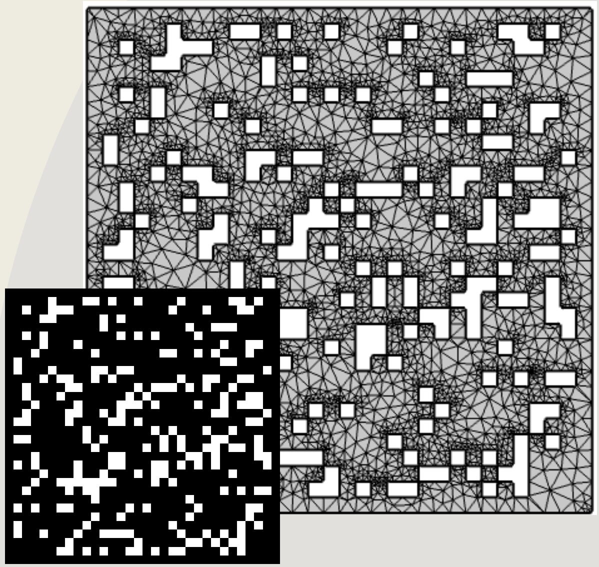
$$E^*\left(\omega\right)=E'\left(\omega\right)+iE''\left(\omega\right)$$

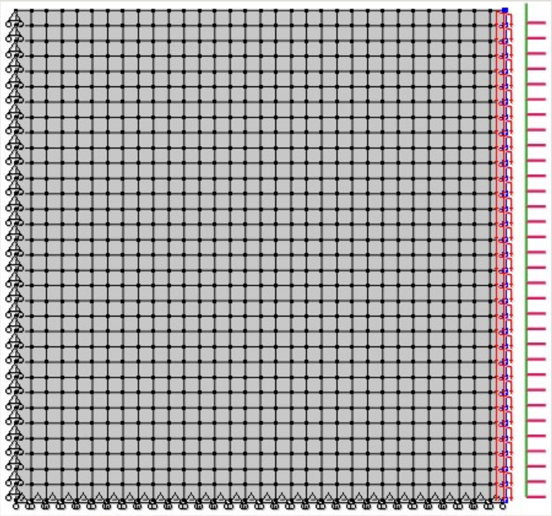
$$\tan\delta\left(\omega\right)=\frac{E''\left(\omega\right)}{E'\left(\omega\right)}$$

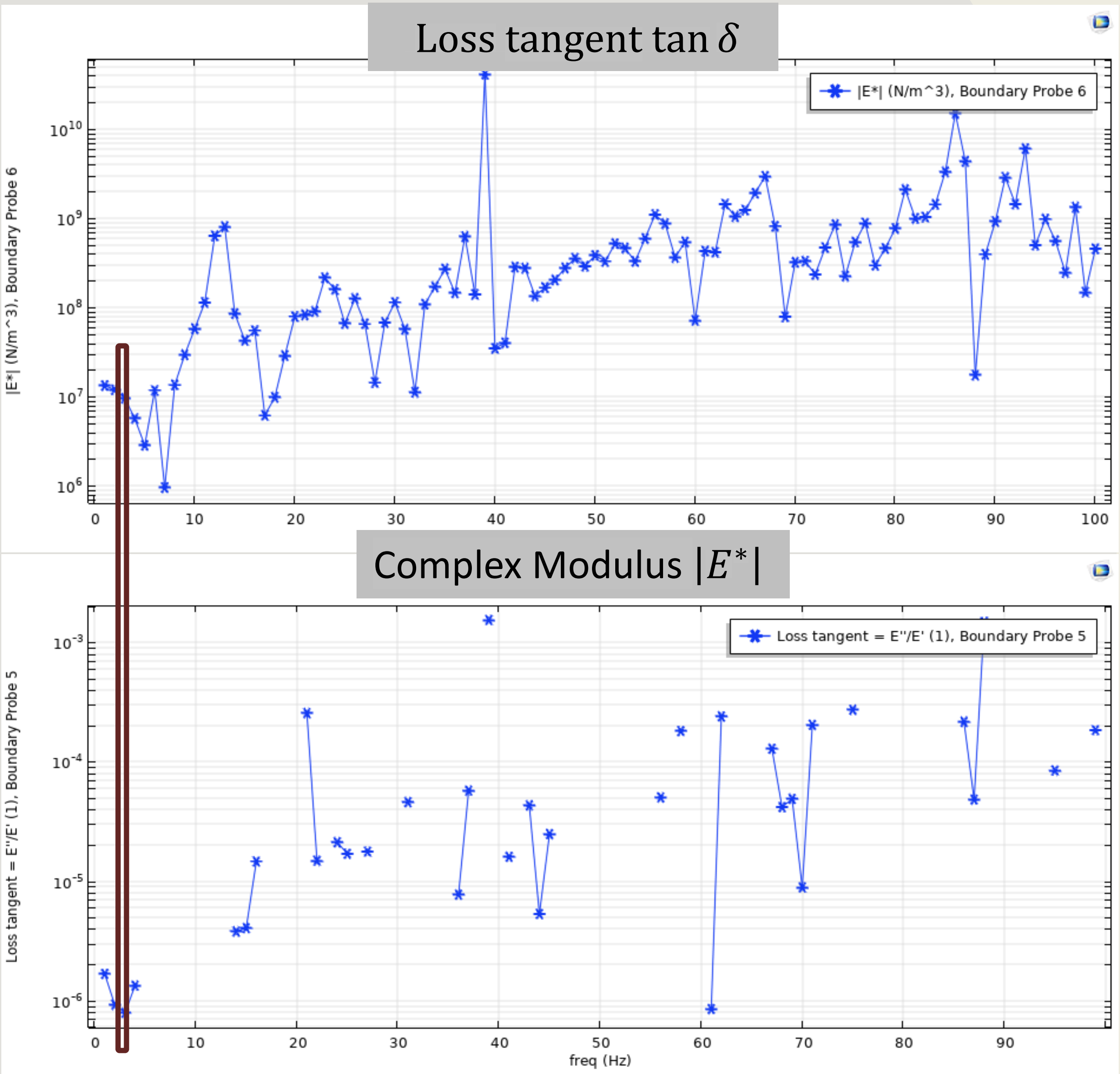
$$\left[M_{jk}-\rho c^2\delta_{jk}\right]f''_k=0 \quad u_k=f_k\left(\mathbf{n}\bullet\mathbf{x}-ct\right)$$

$$M_{jk}=n_i C_{ijkl} n_l \quad \det\left[M_{jk}-\rho c^2\delta_{jk}\right]=0$$

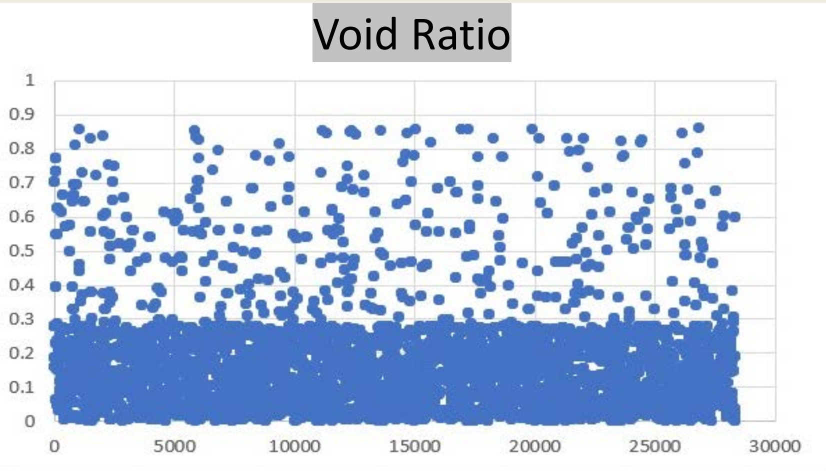
FEM Calculations for Elastic or Viscoelastic Properties

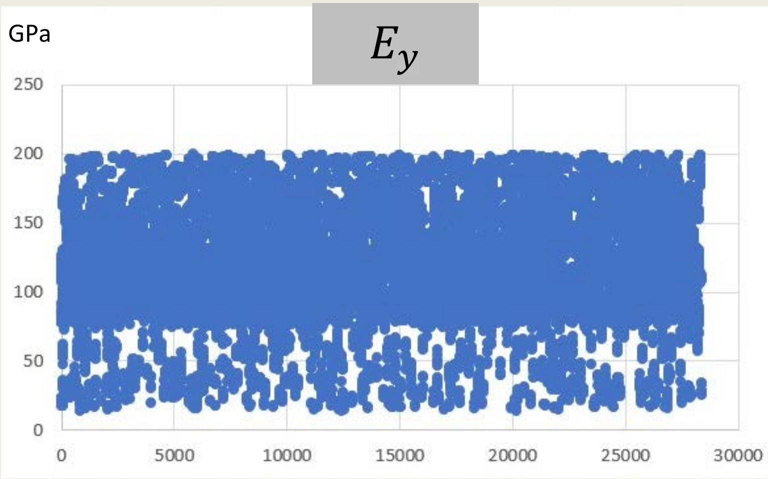


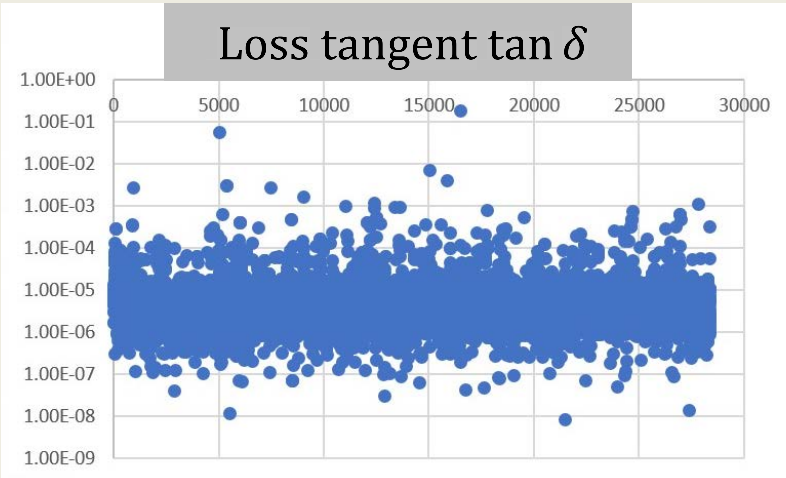


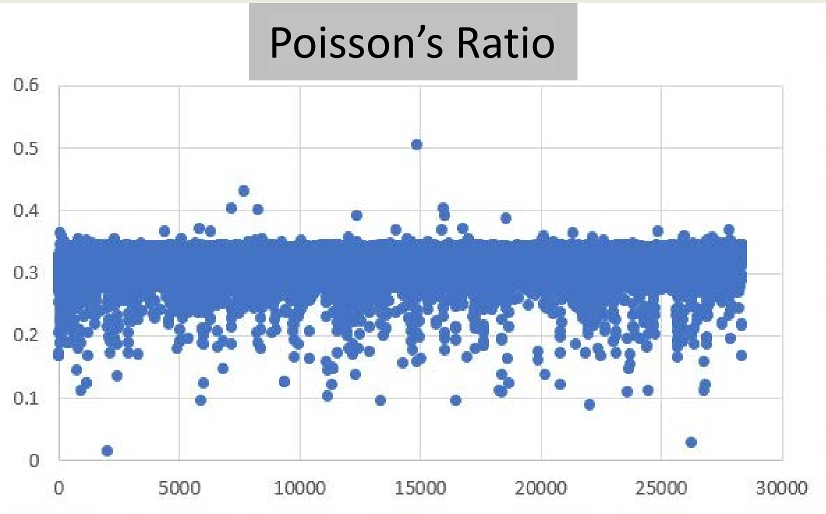


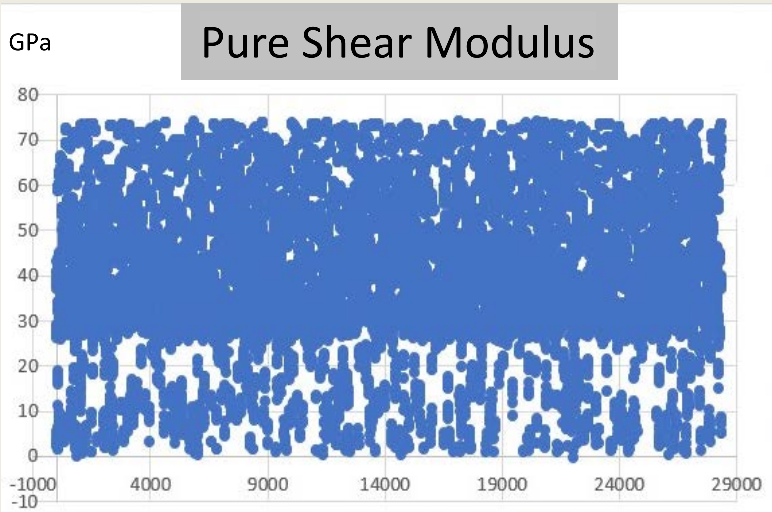
Data Distribution

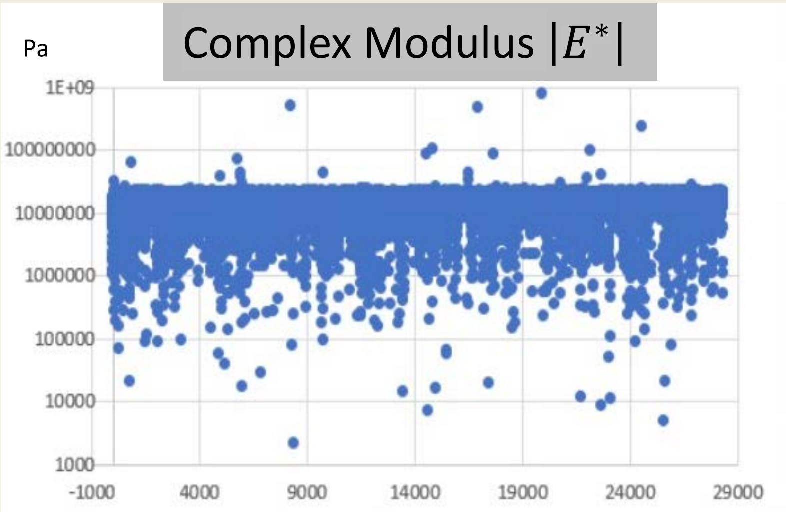




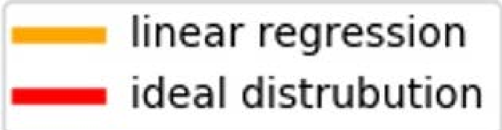








Results



*Error Percentage

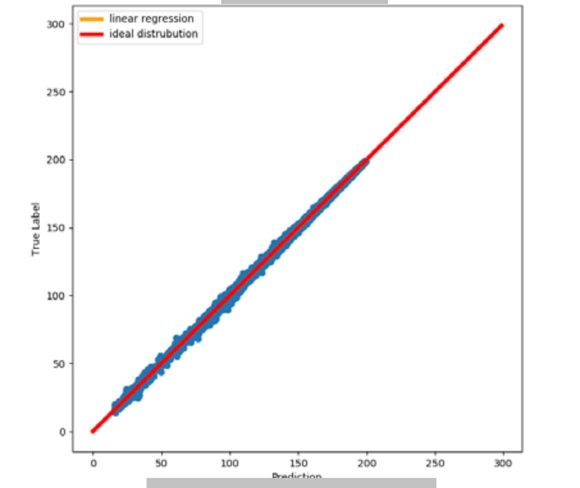
E_x

Ground Truth

Prediction

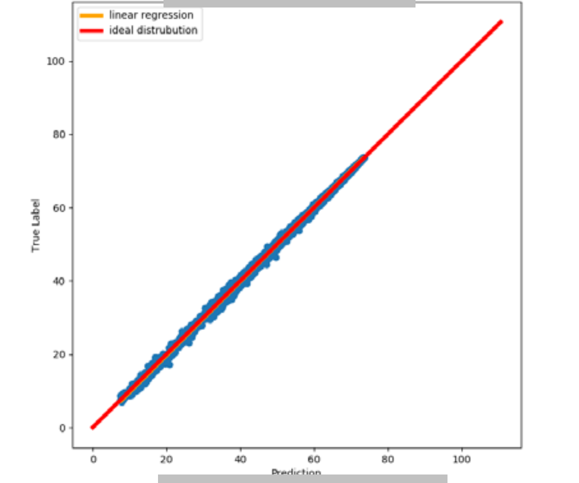
1.18200427 %*

E_y



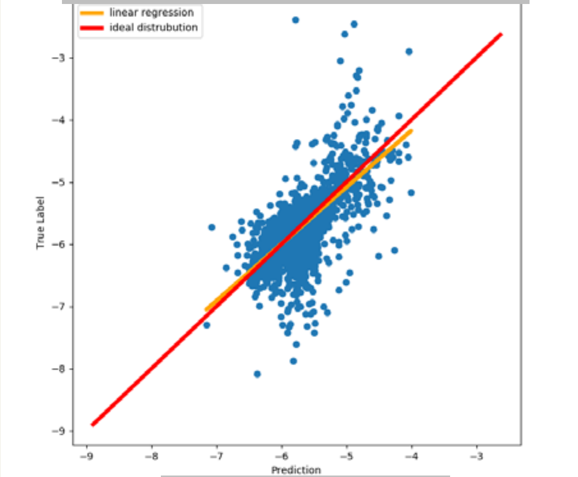
0.75872028%*

Bulk Shear



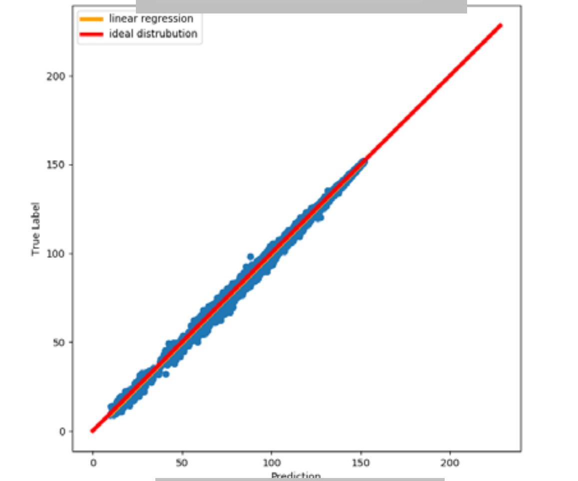
0.75519656%*

Loss tangent $\tan\delta$



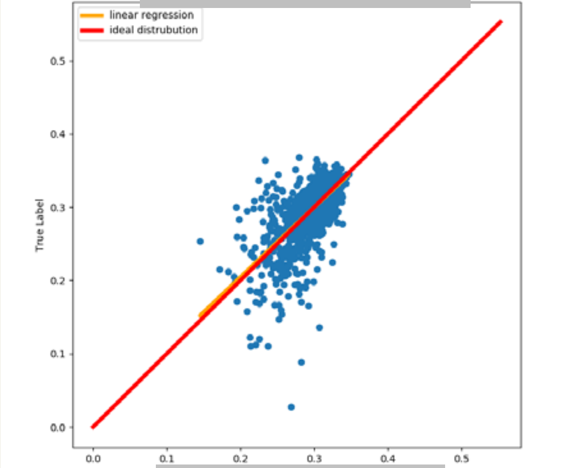
2.06561051%*

Bulk Modulus



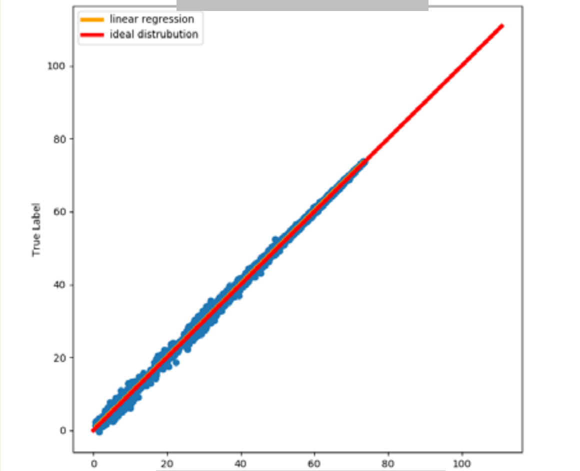
1.36850339%*

Poisson's Ratio



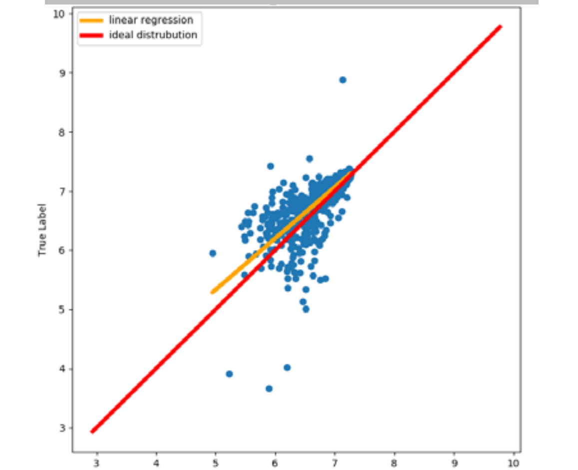
1.94843323%*

Pure Shear



1.04467757%*

Complex Modulus $|E^*|$



0.91550227%*

Application

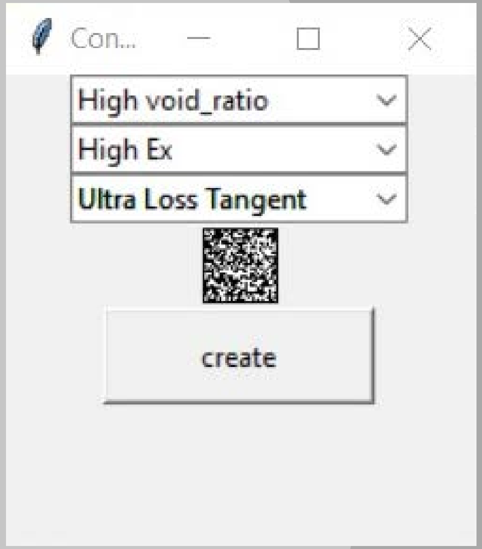
Classical

```
Generating sample
Caculating No.19779
Time cost: 9.906250 sec
Start running analysis
Storage elastic modulus E_p at 3 = 20079083.285715 N/m^3
Loss elastic modulus E_pp at 3 =     7.264534 N/m^3
Tensile loss tangent at 3 = 0.000000361796
Complex elastic modulus |E*| at 3 = 20079083.285716 N/m^3


time cost: 0.593750 sec

total time cost: 10.500000 sec
Generating sample
Caculating No.19780
```

Machine Learning

Raspbian Pi Deployment

Quick DEMO



Lower computation cost when scale up.
Fast and easy to deploy with high accuracy.
Implies a convenient path to the topology optimization process.

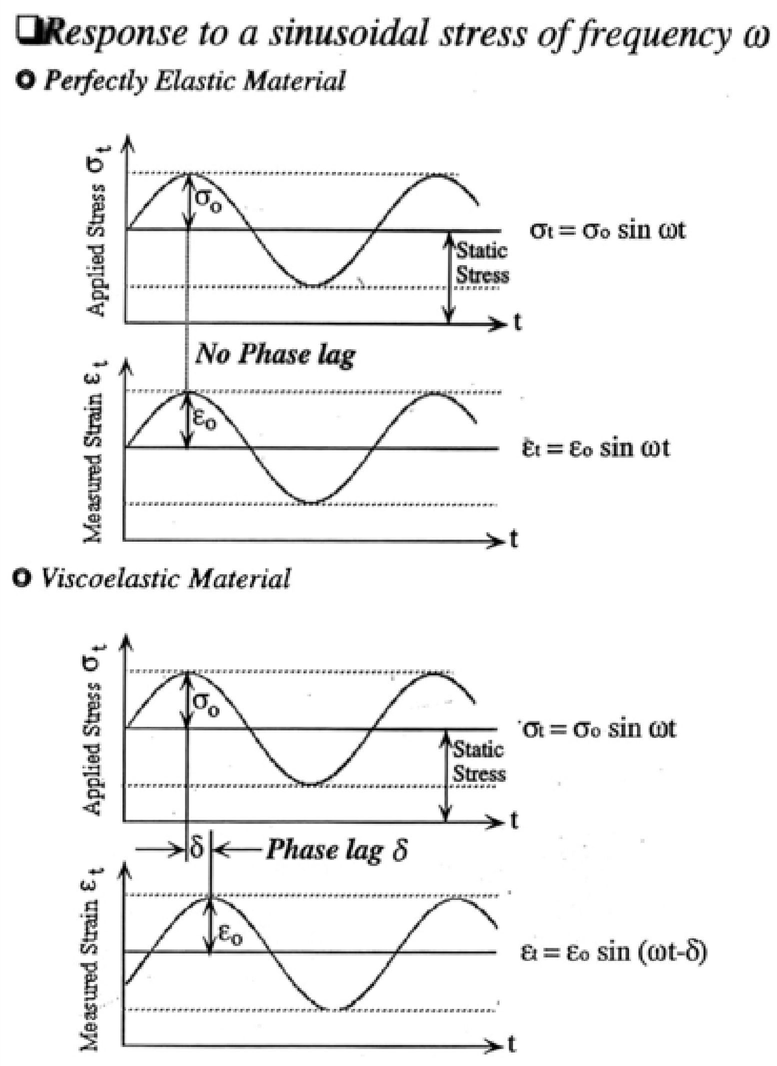
Summary

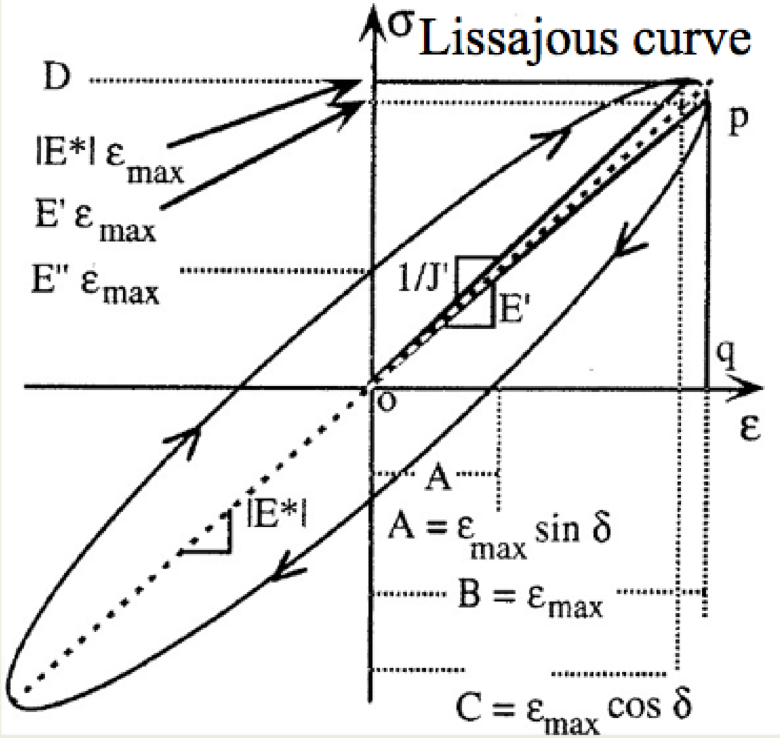
- VGG network architecture was introduced to design materials for desired elastic or viscoelastic properties.
- Well-trained DNN may provide lower computational cost, without loosing prediction accuracy, as oppose to full FEM calculations.

Questions or Comments

Appendix

Linear viscoelasticity: dynamic response





Complex modulus

$$E^* = E' + iE''$$

Complex compliance

$$J^* = J' - iJ''$$

Loss tangent

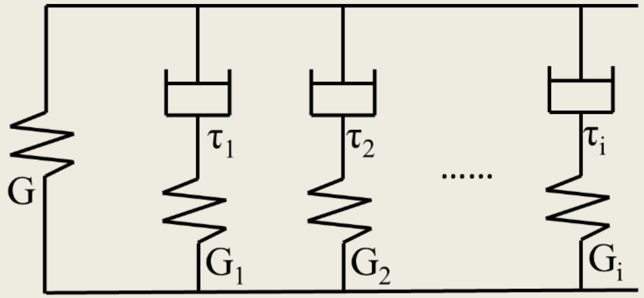
$$\tan\delta = E''/E' = A/C$$

Figure of merit

$$E'\tan\delta = E''$$

Viscoelastic Material Model for high damping rubber

- Bulk modulus (K=400 MPa) is assumed to be purely elastic
- Generalized Maxwell model for shear modulus with the elastic branch G=58.6 kPa



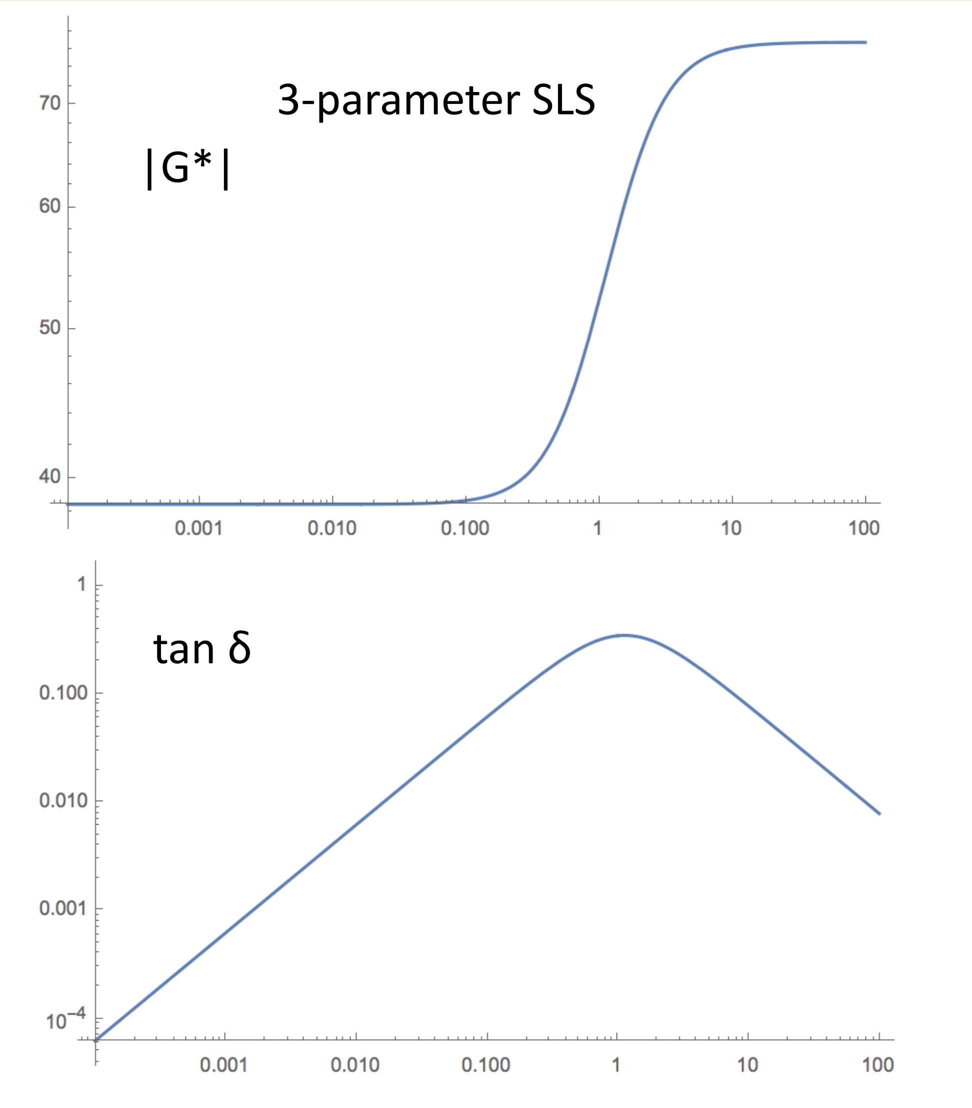
$$G'(\omega) = G + \sum_{m=1}^{N} G_m \frac{(\omega\tau_m)^2}{1+(\omega\tau_m)^2}$$

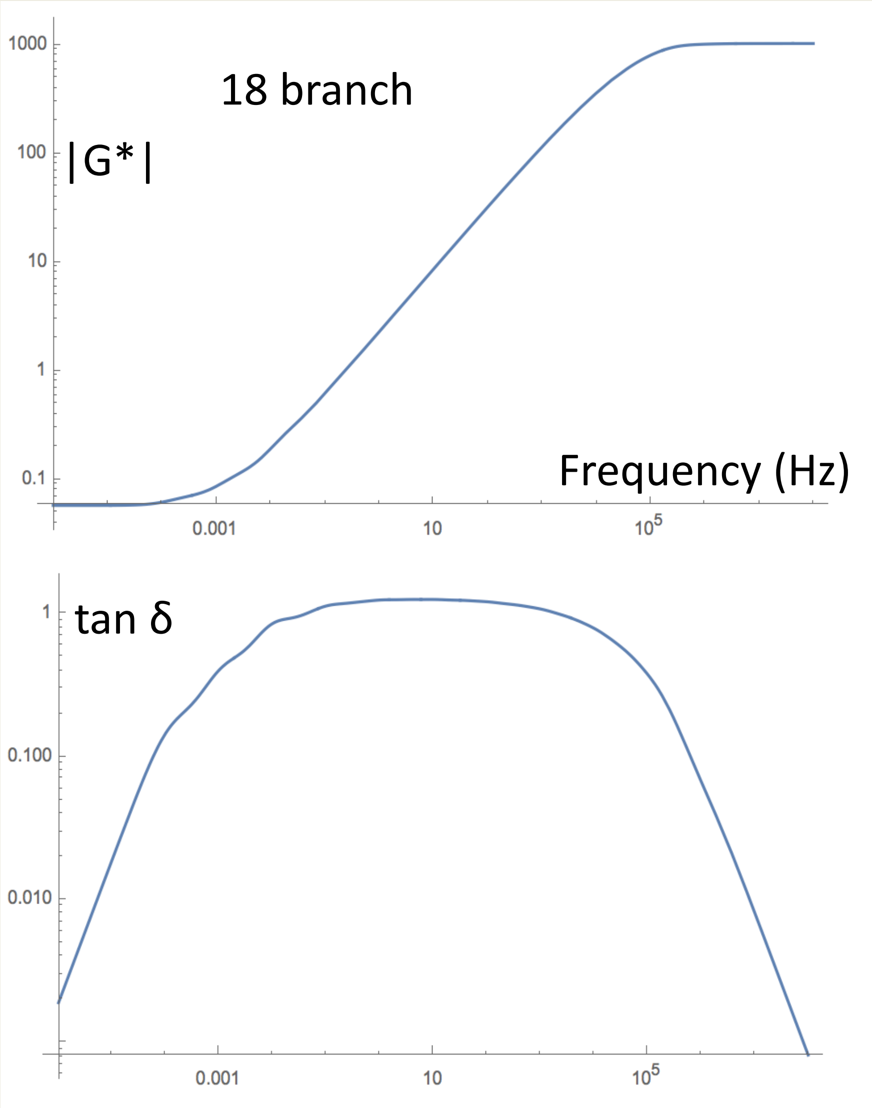
$$G''(\omega) = \sum_{m=1}^{N} G_m \frac{\omega\tau_m}{1+(\omega\tau_m)^2}$$

Parameters for the 18-branch shear modulus to realistically describe a high damping viscoelastic material

1) 13.3[MPa] 1e-7[sec]
2) 286[MPa] 1e-6[sec]
3) 291[MPa] 3.16e-6[sec]
4) 212[MPa] 1e-5[sec]
5) 112[MPa] 3.16e-5[sec]
6) 61.6[MPa] 1e-4[sec]
7) 29.8[MPa] 3.16e-4[sec]
8) 16.1[MPa] 1e-3[sec]
9) 7.83[MPa] 3.16e-3[sec]
10) 4.15[MPa] 1e-2[sec]
11) 2.03[MPa] 3.16e-2[sec]
12) 1.11[MPa] 1e-1[sec]
13) 0.491[MPa] 3.16e-1[sec]
14) 0.326[MPa] 1[sec]
15) 0.0825[MPa] 3.16[sec]
16) 0.126[MPa] 10[sec]
17) 0.0373[MPa] 100[sec]
18) 0.0118[MPa] 1000[sec]

Viscoelastic Spectra of the Models





K=83.33 MPa, G=38.46 MPa

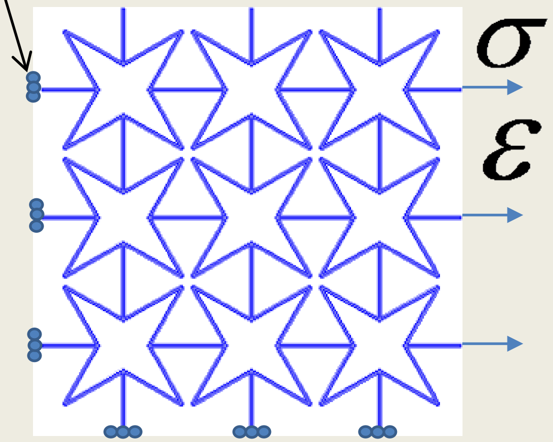
G_1=G, τ=0.1 s

Frequency (Hz)

Boundary, Loading Conditions and Elastic Constants

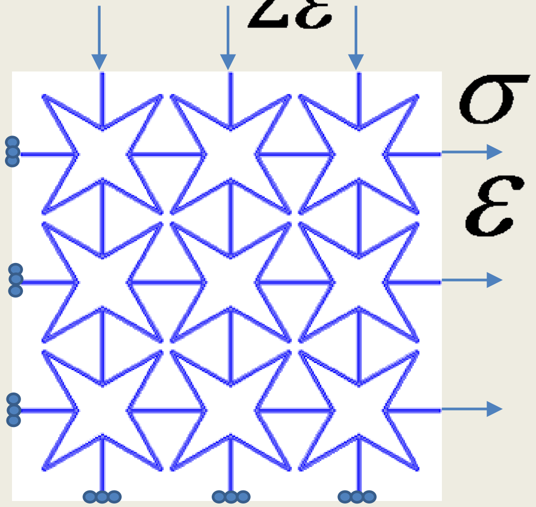
Roller

$$E = \frac{\sigma}{\varepsilon}$$



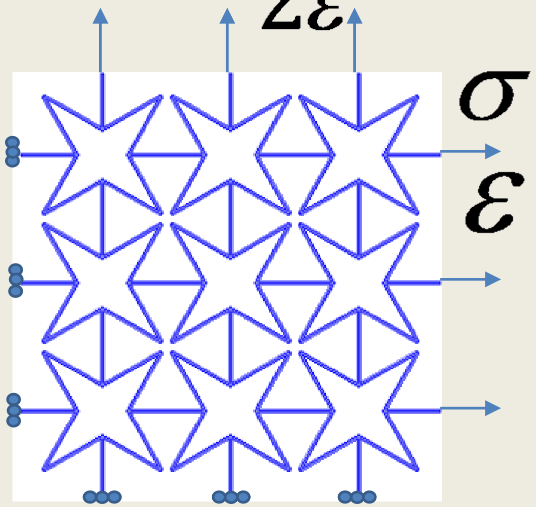
Uniaxial mode

$$G = \frac{\sigma}{2\varepsilon}$$



Bi-axial shear mode

$$K_{2D} = \frac{\sigma}{2\varepsilon}$$



Bi-axial bulk mode

Poisson's ratio $$\nu = -\frac{\varepsilon_{yy}}{\varepsilon_{xx}}$$