Topology optimization of lattice materials with nonlinear elasticity law

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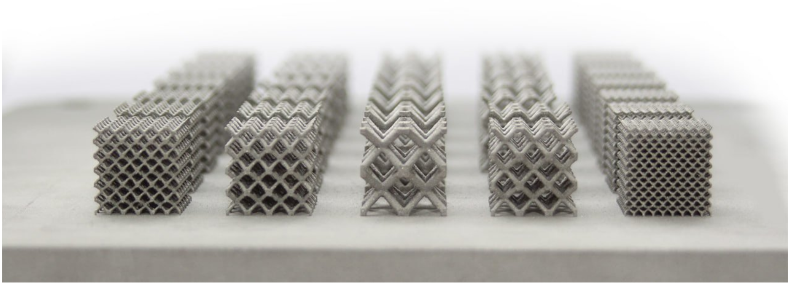
Lattice structures and metamaterials



Design lattices with linear elastic law

Weak form of the modified linear elasticity equation:
find $\boldsymbol{u} \in U = \left\{ \boldsymbol{v} \in \left(H^1(\Omega)\right)^2 : \boldsymbol{u} = 0 \text{ on } \Gamma_D \right\}$
s.t.

$$a(\boldsymbol{u}, \boldsymbol{v}) = C(\boldsymbol{v}) \ \ \forall \boldsymbol{v} \in U$$

with

$$a(\boldsymbol{u}, \boldsymbol{v}) = \int_\Omega \sigma_{\boldsymbol{p}}(\boldsymbol{u}) : \varepsilon(\boldsymbol{v}) \ \ d\boldsymbol{x}$$

$$C(\boldsymbol{v}) = \int_{\Gamma_N} \boldsymbol{f} \cdot \boldsymbol{v} \ \ d\gamma$$

$$\sigma_{\boldsymbol{p}}(\boldsymbol{u}) = \rho^{\boldsymbol{p}} \sigma(\boldsymbol{u})$$

Topology Optimization

Algorithm 1: SIMP on a fixed grid

Result: ρ

Input: TOL, kmax, ρ_{min}, α;

Set: $\rho_h^0 \leftarrow 1$, $k \leftarrow 0$, err $\leftarrow 1 + TOL$

while $err > TOL$ & $k < kmax$ **do**

1. $\rho_h^{k+1} \leftarrow \text{IPOPT}(\rho_h^k,\ \rho_{\text{min}}, Mit = 10, \alpha,\ \ldots);$
2. $\rho_h^{k+1} \leftarrow \text{HELMHOLTZ}\left(\rho_h^{k+1}, \tau\right);$
3. $\text{err} \leftarrow \|\rho_h^{k+1} - \rho_h^k\|_\infty;$
4. $k \leftarrow k + 1;$

end

Algorithm 2: SIMPATY: SIMP with AdaptiviTY

Result: ρ

Input: CTOL, MTOL, kmax, $\rho_{\min}$, $\mathcal{T}_h^0$, α;

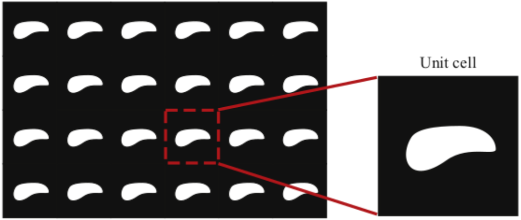
Set: $\rho_h^0 \leftarrow 1$, $k \leftarrow 0$, errC $\leftarrow 1 + TOL$

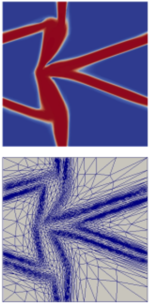
while $errC > TOL$ & $k < kmax$ **do**

1. $\rho_h^{k+1} \leftarrow \mathrm{IPOPT}\big(\rho_h^k, \rho_{\min}, Mit = nk, \alpha, ...\big)$;
2. $\mathcal{T}_h^{k+1} \leftarrow adaptmesh\left(\mathcal{T}_h^k, \rho_h^{k+1}, MTOL, method\right)$;
3. errC $\leftarrow |\#\mathcal{T}_h^{k+1} - \#\mathcal{T}_h^k| / \#\mathcal{T}_h^k$;
4. $k \leftarrow k + 1$;

end

Homogenization applied to linear elasticity law





$$\int_Y E_{ijpq}\varepsilon_{pq}^{*,kl}\varepsilon_{ij}(v)\ dY = \int_Y E_{ijpq}\varepsilon_{pq}^{0,kl}\varepsilon_{ij}(v)\ dY \ \forall v \in V \qquad (1)$$

$$E_{ijkl}^{H} = \frac{1}{|Y|}\int_Y E_{pqrs}\left(\varepsilon_{pq}^{0,kl} - \varepsilon_{pq}^{*,kl}\right)\left(\varepsilon_{rs}^{0,ij} - \varepsilon_{rs}^{*,ij}\right)\ dY \qquad (2)$$

$$J = \sum_{ijkl}\left(E_{ijkl}^{H}(\rho) - E_{ijkl}^{W}\right)^2 \qquad (3)$$

Design lattices with nonlinear elastic law

TO problem

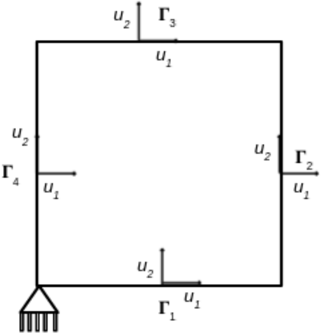
Find ρ such that $\min_{\rho \in L^\infty(Y)} J(\rho)$ is achieved under constraints

1. State equation for nonlinear material is satisfied by $\boldsymbol{u}(\rho)$
2. $+$ Periodicity conditions
3. $\int_Y \rho \, dY \leqslant \alpha |Y|$
4. $\rho_{\min} \leqslant \rho \leqslant 1$

$$J(\boldsymbol{u}) = \frac{1}{2}\left(c(\boldsymbol{u}) - c^*\right)^2 = \frac{1}{2}\left(\nu(\boldsymbol{u}) - \nu^*\right)^2$$

Design lattices with nonlinear elastic law

- Boundary conditions and Poisson's ratio ν
- Nonlinear model
- Lagrange method for `IPOPT`
- Tests to validate the model
- Final algorithm and parameters tuning



$$\begin{cases} \boldsymbol{u}\cdot\boldsymbol{n} = u_1 & = 0 & \text{on } \Gamma_1 \\ \boldsymbol{u}\cdot\boldsymbol{n} = u_2 & = 0 & \text{on } \Gamma_4 \\ \quad u_1 & = d_1 & \text{on } \Gamma_2 \\ \frac{\partial\Psi(\boldsymbol{u})}{\partial\boldsymbol{u}}\cdot\boldsymbol{n} & = 0 & \text{on } \Gamma_3 \end{cases}$$

Poisson's ratio is computed with

$$\nu_{12} = -\frac{\int_{\Gamma_3} u_2 - \int_{\Gamma_1} u_2}{d_1}$$

where d_1 is the traction imposed at the right boundary and $u_2 = 0$ *on* Γ_1 because of symmetry conditions

Linear model

$$\Psi\left(\rho,\boldsymbol{u}\right)=\sigma_{\rho}\left(\boldsymbol{u}\right):\varepsilon\left(\boldsymbol{u}\right)=\frac{1}{2}\lambda_{L}\left(E_{kk}\right)^{2}+\mu E_{ij}E_{ij}$$

In our study we have used

$$\Psi\left(\rho,\boldsymbol{u}\right)=\frac{\lambda_{L}}{2}\left(J-1\right)^{2}+\mu E_{ij}E_{ij}$$

to circumvent the drawbacks of the Kirchhoff-St.Venant model under excessive compression (formula (6d) from ref. [2])

Lagrange functional:

$$\mathscr{L}\left(\rho, \boldsymbol{u}, \boldsymbol{\lambda}\right) = J\left(\boldsymbol{u}\right) + \int_Y \rho^p \frac{\partial \Psi\left(\boldsymbol{u}\right)}{\partial \boldsymbol{u}} \; \boldsymbol{\lambda} \; dY$$

By requiring that the Gateaux derivatives of $\mathscr{L}$ with respect to the variables $\rho, \boldsymbol{u}, \boldsymbol{\lambda}$ evaluated at the solution $\left(\hat{\rho}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}\right)$ vanish for any test function properly chosen, we obtain the state equation , the adjoint equation and the gradient of the cost function.

Design lattices with nonlinear elastic law

State equation

To retrieve the state equation, we imposed
$\frac{\partial \mathscr{L}}{\partial \boldsymbol{\lambda}} \left(\hat{\rho}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}} \right) \varphi = 0 \ \forall \varphi \in V$
Find $\hat{\boldsymbol{u}} \in V$ such that

$$\int_Y \hat{\rho}^p \frac{\partial \Psi \left(\hat{\boldsymbol{u}} \right)}{\partial \boldsymbol{u}} \varphi dY = \ 0 \ \forall \varphi \in V$$

Newton tangent problem

Given $\boldsymbol{u}^0 \ \forall \ k = 0, 1, \ldots$ up to convergence, solve:

$$\begin{cases} \frac{\partial}{\partial \boldsymbol{u}} \left[\int_Y \hat{\rho}^p \frac{\partial \Psi \left(\boldsymbol{u}^k \right)}{\partial \boldsymbol{u}} \boldsymbol{\delta u} \ dY \right] \varphi = - \int_Y \hat{\rho}^p \frac{\partial \Psi \left(\boldsymbol{u}^k \right)}{\partial \boldsymbol{u}} \boldsymbol{u}^k \varphi dY \quad \forall \ \varphi \ \in V \\ \boldsymbol{u}^{k+1} = \boldsymbol{u}^k + \boldsymbol{\delta u} \end{cases} \tag{4}$$

The adjoint equation in the optimization procedure has been derived imposing $\frac{\partial \mathscr{L}}{\partial \boldsymbol{u}}\left(\hat{\rho}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}\right) \boldsymbol{\psi} = 0 \ \forall \boldsymbol{\psi} \in V$

Dual problem

Find $\hat{\boldsymbol{\lambda}} \in V$ such that

$$\frac{\partial}{\partial \boldsymbol{u}}\left(\int_Y \rho^p \frac{\partial \boldsymbol{\psi}\left(\hat{\boldsymbol{u}}\right)}{\partial \boldsymbol{u}} \hat{\boldsymbol{\lambda}} \; dY\right) \boldsymbol{\psi} + \frac{\partial J\left(\boldsymbol{u}\right)}{\partial \boldsymbol{u}} \boldsymbol{\psi} = 0 \quad \forall \boldsymbol{\psi} \in V \tag{5}$$

$$\frac{\partial J\left(\boldsymbol{u}\right)}{\partial \boldsymbol{u}} \boldsymbol{\psi} = \frac{-\left(\nu_{12} - \nu^*\right)}{d_1} \int_{\Gamma_3} \psi_2$$

Derivative of the Lagrange functional with respect to the control variable:

$$\frac{\partial \mathscr{L}\left(\hat{\rho}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}\right)}{\partial \rho}\left(\hat{\rho}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{\lambda}}\right) v = \int_Y p \hat{\rho}^{p-1} v \frac{\partial \Psi\left(\hat{\boldsymbol{u}}\right)}{\partial \boldsymbol{u}} \hat{\boldsymbol{\lambda}} dY \qquad (6)$$

Example of possible filter inside `IPOPT`

$$\bar{\rho} = \frac{\tanh\left(\beta\eta\right) + \tanh\left(\beta\left(\rho - \eta\right)\right)}{\tanh\left(\beta\eta\right) + \tanh\left(\beta\left(1 - \eta\right)\right)} \qquad p\bar{\rho}^{p-1} \frac{\partial \bar{\rho}}{\partial \rho} v = p\bar{\rho}^{p-1} \frac{1}{\tanh\left(\beta\eta\right) + \tanh\left(\beta\left(1 - \eta\right)\right)} \frac{\beta}{\cosh\left(\beta\left(\hat{\rho} - \eta\right)\right)^2} v$$

Validation of the model

Poisson's coefficient computation

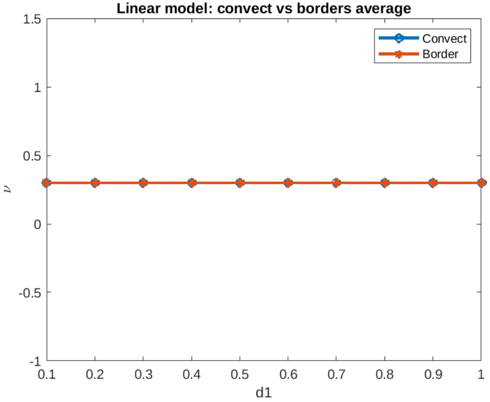
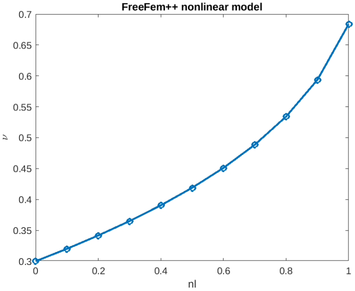
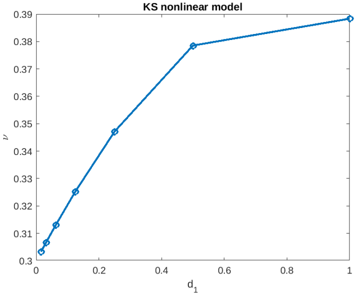


Figure: Check on the linear model for the computation of Poisson's ratio



(a) FreeFem++ nonlinear model



(b) KS nonlinear model

Figure: Check on the nonlinear model

Validation of the model

GradJ and Newton's method

$$\left\| \frac{\left[F\left(\boldsymbol{u}+\varepsilon\ \boldsymbol{du}\right)-F\left(\boldsymbol{u}-\varepsilon\ \boldsymbol{du}\right)\right]}{2\varepsilon}-Jac\left(\boldsymbol{u}\right)\right\|_{L^{\infty}}=9.09059e-08$$

$$\left\| \frac{J\left(\rho+\varepsilon\ d\rho\right)-J\left(\rho-\varepsilon\ d\rho\right)}{2\varepsilon}-gradJ\left(\rho\right)\right\|_{L^{\infty}}=7.18473e-12$$

Final algorithm and parameters tuning

Algorithm 3: Final Algorithm

Result: ρ
Input: CTOL, MTOL, maxit, $\rho_{\min}$, $\mathcal{T}_h^0$, α;
Set: ρ_h^0, $k \leftarrow 0$, errC $\leftarrow 1 + TOL$
while $errC > TOL \ \&\ k < maxit$ **do**

1. $p^{k+1} \leftarrow p_{\max} - 2e^{-k/2}$
2. $\rho_h^{k+1} \leftarrow \mathrm{IPOPT}(\rho_h^k, \rho_{\min}, Mit = IPOPTmaxiter, tol = IPOPTtol, \ldots)$;
3. $\rho_h^{k+1} \leftarrow \mathrm{HELMHOLTZ}\left(\rho_h^{k+1}, \tau\right)$;
4. $\mathcal{T}_h^{k+1} \leftarrow adaptmesh\left(\mathcal{T}_h^k, \rho_h^{k+1}, MTOL, method\right)$;
5. $\rho_h^{k+1} \leftarrow \mathrm{HEAVISIDE}\left(\rho_h^{k+1}, \beta_H\right)$;
6. $\rho_h^{k+1} \leftarrow \mathrm{SIGMUND}\left(\rho_h^{k+1}, \beta = \beta^k, \eta = \eta^k\right)$;
7. errC $\leftarrow |\#\mathcal{T}_h^{k+1} - \#\mathcal{T}_h^k| / \#\mathcal{T}_h^k$;
8. $k \leftarrow k + 1$;

end

Optimized materials obtained

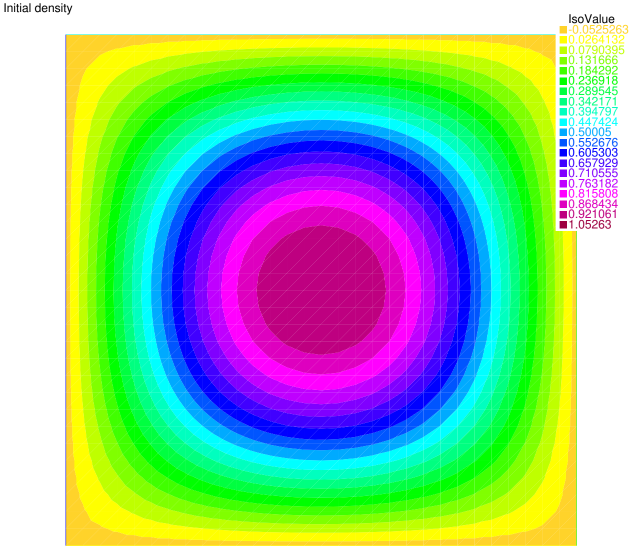


Figure: Initial density

Optimized materials obtained

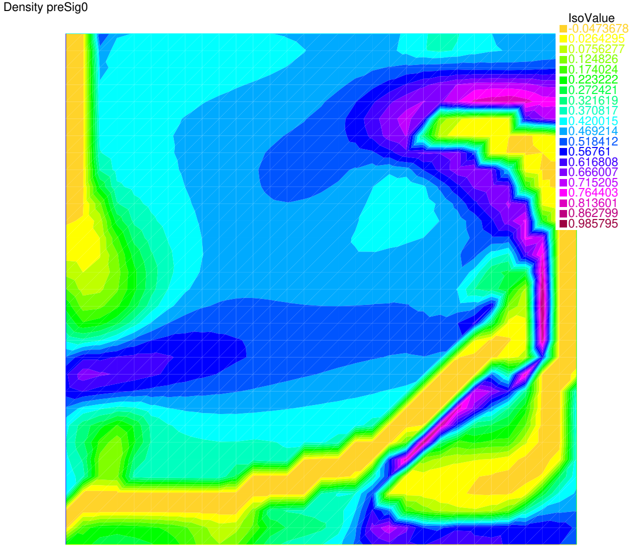
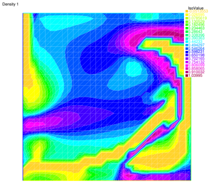


Figure: Density after the first IPOPT cycle

Optimized materials obtained



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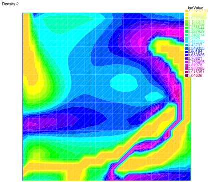
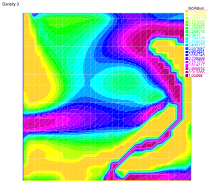
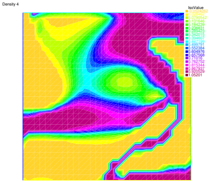


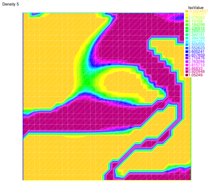
(b) ii = 2



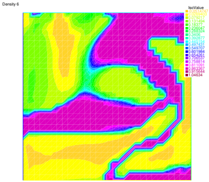
(c) ii = 3



(d) ii = 4



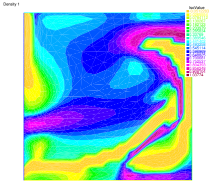
(e) ii = 5



(f) ii = 6

Figure: Structure with increasing Sigmund filters parameters

Optimized materials obtained



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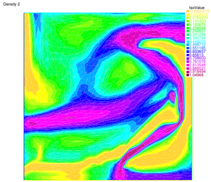

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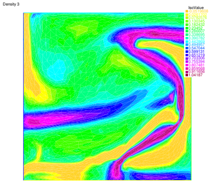

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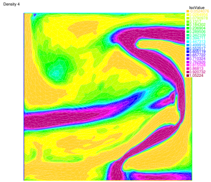

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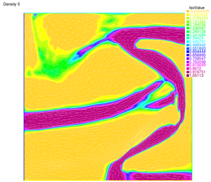

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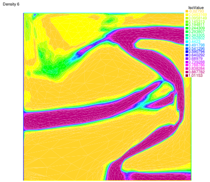
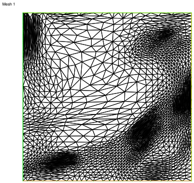


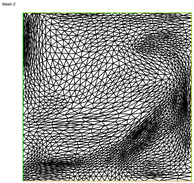
(f) ii = 6

Figure: Structure with increasing Sigmund filters parameters and grid adaptation

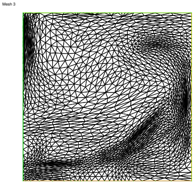
Optimized materials obtained



(a) ii $= 1$



(b) ii $= 2$



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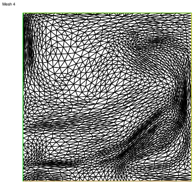
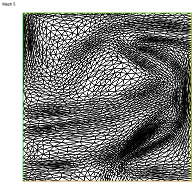
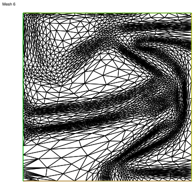


(d) ii $= 4$



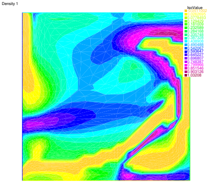
(e) ii $= 5$



(f) ii $= 6$

Figure: Mesh of structures with increasing Sigmund filters parameters and grid adaptation

Optimized materials obtained



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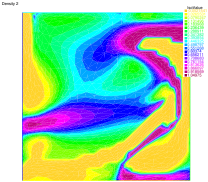

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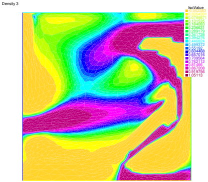
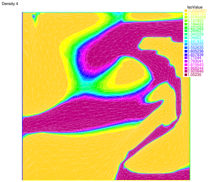


(c) ii = 3



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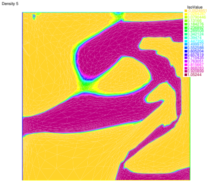

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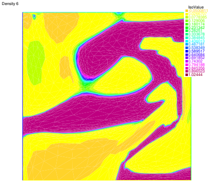
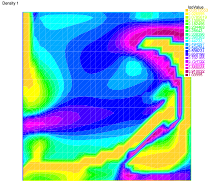


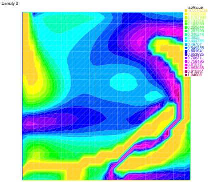
(f) ii = 6

Figure: Structure with fixed $\eta = 0.5$ and grid adaptation

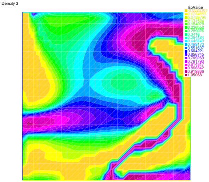
Optimized materials obtained



(a) ii = 1



(b) ii = 2



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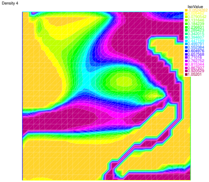

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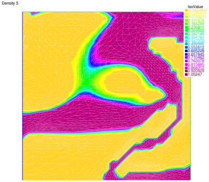
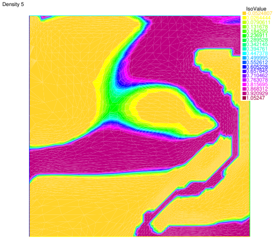


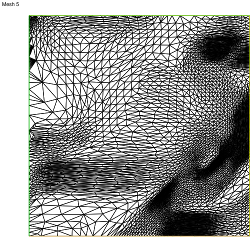
(e) ii = 5

Figure: Final structure optimization

Conclusions



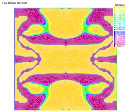
(a) Final structure



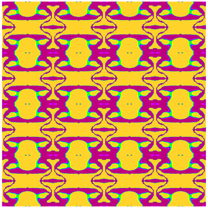
(b) Final mesh

Figure: Final structure and mesh

Conclusions



(a) Structure



(b) Lattice material

Figure: Reflected (2×2) final structure and lattice material

- Poisson's ratio computed on 2×2 cells: $\nu = -1.35916$
- Model reliability validated
- Big issue of parameters tuning: problem specific
- Future studies: extend to other TO problems and to 3D setting

Essential bibliography

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