A Mixed-Integer Programming Approach to Design of Periodic Structures with Negative Thermal Expansion

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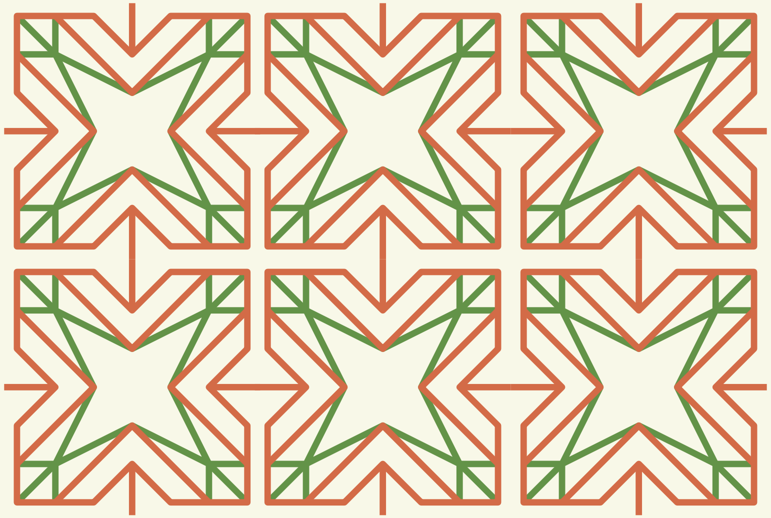
structures with negative thermal expansion

- ...contract when heated.



- high (positive) TE
- low (positive) TE

mixed-integer programming

- m-i linear prog.:

$$\begin{array}{ll} \min & \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{r}^{\mathrm{T}}\boldsymbol{y} \\ \mathrm{s.\,t.} & \boldsymbol{a}_i^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{g}_i^{\mathrm{T}}\boldsymbol{y} \geq b_i \quad (i = 1, \dots, m), \\ & \boldsymbol{x} \in \{0, 1\}^n, \quad \boldsymbol{y} \in \mathbb{R}^l \end{array}$$

- "mixed":
  - x_j : integer (discrete) variable
  - y_l : real (continuous) variable
- replace $\boldsymbol{x} \in \{0, 1\}^n$ with $\mathbf{0} \leq \boldsymbol{x} \leq \mathbf{1}$
  $\rightarrow$ linear prog. relaxation
- can be solved with, e.g., a branch-and-bound method

negative thermal expansion

- materials with NTE
  - zirconium tungstate family [Martinek & Hummel '68]
  - zeolite [Lightfoot, Woodcock, Maple, Villaescusa, & Wright '01]

negative thermal expansion

- materials with NTE
  - zirconium tungstate family [Martinek & Hummel ’68]
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- (possible) applications
  - to reduce thermal stress in a structure
  - thermal fastener [Sigmond & Torquato ’96]
    - inserted into a hole at high temperature
    - fitted tightly into the hole when it cools down
  - sensitive temperature sensors [Sleight ’98]
    - combination of two thin films with large PTE and large NTE

optimization to achieve NTE

- existing methods:
  - continuum & homogenization method

    [Sigmund & Torquato '97], [Chen, Silva, & Kikuchi '01]

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- fabrication of opt. sol.
  - direct metal deposition:
    powdered metals are melted
    by laser [Chen, Silva, & Kikuchi '01]
  - oxide co-extrusion:
    powder based thermoplastic
    processing [Qi & Halloran, 04]

optimization to achieve NTE

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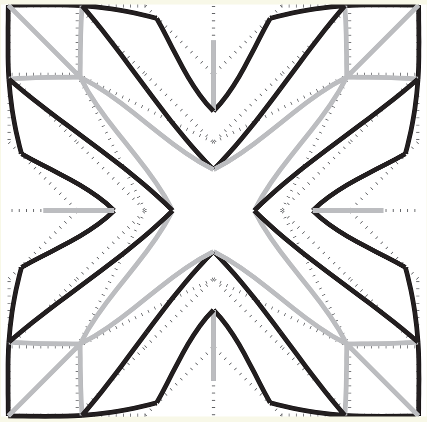
- our method:
  - periodic frame structure
  - stress constraints & pre-determined beam sections

    $\rightarrow$ no hinge, no thin member



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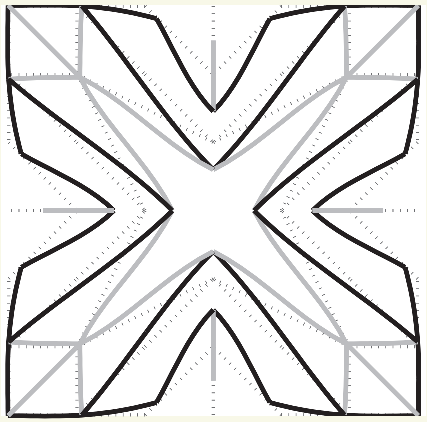


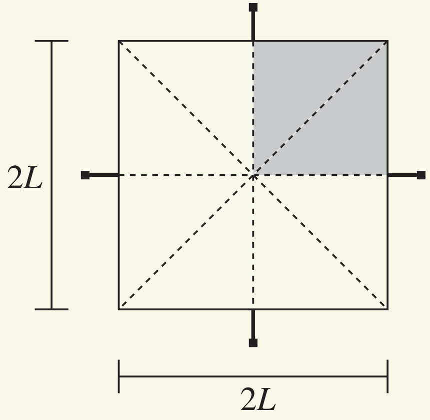
[our method]

- $\rightarrow$ manufacturability (no post-processing)
- $\rightarrow$ global optim.
  - an idea — MILP for truss

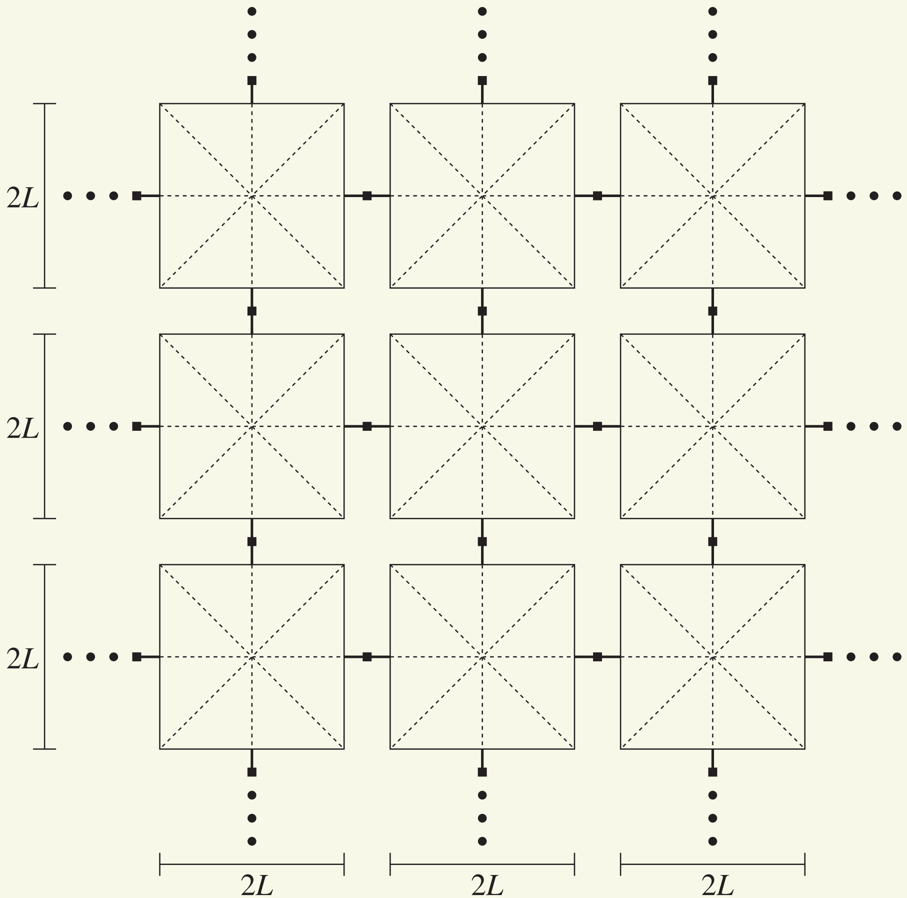
    [Rasmussen & Stolpe '08] [K. & Guo '10]

problem setting

- assume periodicity & symmetry
- unit cell: planar frame structure
- design variables: sections of members



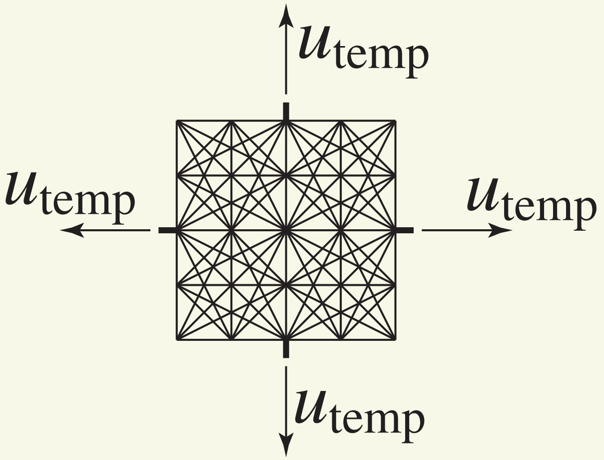
unit cell



periodicity

problem setting

- design of base cell
  - prepare candidate members, e.g.,



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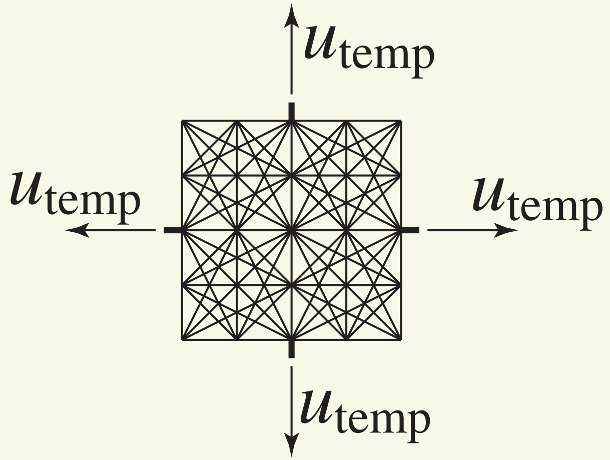

- two materials (w/ different positive TECs)
  - Determine

$$\text{member } e = \begin{cases} \text{material 1} \\ \text{material 2} \\ \text{void} \end{cases}$$

so as to minimize u_{temp} due to temperature elevation.

optimization problem

$$\begin{array}{ll} \max & u_{\rm temp} \\ {\rm s.\,t.} & \text{equil. eq. at elevated temperature} \\ & \text{stress constraints} \\ & \text{avoiding member intersection, etc.} \end{array}$$

- integer variables
  - for member i,

$$\begin{array}{lcl} (x_e, y_e) = (1, 0) & \Leftrightarrow & e \in M_1 \text{ (material 1)} \\ (x_e, y_e) = (0, 1) & \Leftrightarrow & e \in M_2 \text{ (material 2)} \\ (x_e, y_e) = (0, 0) & \Leftrightarrow & e \in N \text{ (void)} \end{array}$$

- $\rightarrow$ can be reduced to MIP.

reduction to MIP (1)

- stiffness matrix:

$$K = \sum_{e=1}^{m} \sum_{j=1}^{3} k_{et} \boldsymbol{b}_{et} \boldsymbol{b}_{et}^{\mathrm{T}} \qquad (\boldsymbol{b}_{et} : \text{const. vec.})$$

- member stiffnesses:

$$k_{et} = \bar{k}_{et1} x_e + \bar{k}_{et2} y_e \qquad (\bar{k}_{etp} : \text{const.})$$

- member TECs:

$$\alpha_e = \bar{\alpha}_{e1} x_e + \bar{\alpha}_{e2} y_e \qquad (\bar{\alpha}_{ep} : \text{const.})$$

- integer variables for member e:

$$x_e = \begin{cases} 1 & \text{if } M_1 \text{ is used} \\ 0 & \text{otherwise} \end{cases} \qquad y_e = \begin{cases} 1 & \text{if } M_2 \text{ is used} \\ 0 & \text{otherwise} \end{cases}$$

reduction to MIP (2)

- thermoelastic equil. eq. $K\boldsymbol{u} = \boldsymbol{f}(\Delta t) \;\Leftrightarrow$

$$\sum_{e=1}^{m} \sum_{j=1}^{3} s_{et} \boldsymbol{b}_{et} = \boldsymbol{0} \qquad \text{(force-balance)}$$

$$s_{et} = \begin{cases} \bar{k}_{et1}(\boldsymbol{b}_{et}^{\mathrm{T}} \boldsymbol{u} - \bar{\alpha}_{e1} \Delta T) & \text{if } x_e = 1 \quad (\diamondsuit 1) \\ \bar{k}_{et2}(\boldsymbol{b}_{et}^{\mathrm{T}} \boldsymbol{u} - \bar{\alpha}_{e2} \Delta T) & \text{if } y_e = 1 \quad (\diamondsuit 2) \\ 0 & \text{otherwise} \quad (\clubsuit) \end{cases} \qquad \text{(compatibility)}$$

- stress constraints:

$$|q_e(\boldsymbol{u})| / q_e^{\mathrm{y}} + |m_e(\boldsymbol{u})| / m_e^{\mathrm{y}} \le 1 \qquad (\spadesuit)$$

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- $(\clubsuit)$ & $(\spadesuit)$ $\Leftrightarrow$ $|s_{e1}|/s_{e1}^{\max} + \cdots + |s_{e3}|/s_{e3}^{\max} \le x_e + y_e$

- $(\diamondsuit 1)$ $\Leftrightarrow$ $|s_{et} - \bar{k}_{et1}(\boldsymbol{b}_{et}^{\mathrm{T}}\boldsymbol{u} - \bar{\alpha}_{e1}\Delta T)| \le M(1 - x_e)$

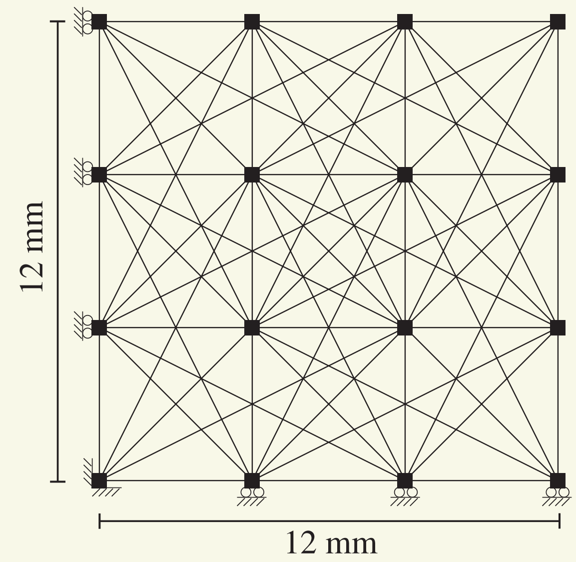
  ($M \gg 0$: const.)

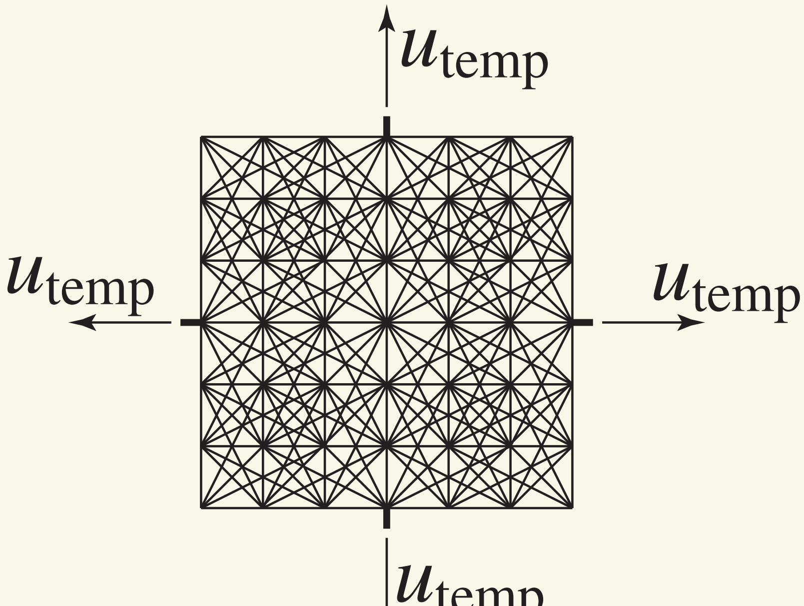
goal: MIP formulation

$$
\begin{aligned}
\max \quad & u_{\mathrm{temp}} \\
\mathrm{s.\,t.} \quad & \sum_{e=1}^{m} \sum_{j=1}^{3} s_{et} \boldsymbol{b}_{et} = \boldsymbol{f}, \\
& |s_{et} - \bar{k}_{et1}(\boldsymbol{b}_{et}^{\mathrm{T}} \boldsymbol{u} - \bar{\alpha}_{e1} \Delta T)| \le M(1 - x_e), & \forall t, \ \forall e, \\
& |s_{et} - \bar{k}_{et2}(\boldsymbol{b}_{et}^{\mathrm{T}} \boldsymbol{u} - \bar{\alpha}_{e2} \Delta T)| \le M(1 - y_e), & \forall t, \ \forall e, \\
& \sum_{t=1}^{3} \frac{|s_{et}|}{s_{et}^{\max}} \le x_e + y_e, & \forall i, \\
& x_e, y_e \in \{0, 1\}, & \forall i.
\end{aligned}
$$

ex.) global optimization

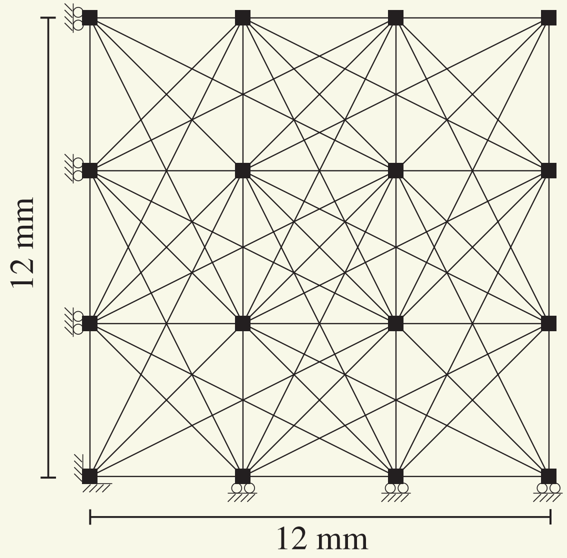
- 66 candidate members
- Timoshenko beam element
- solver: CPLEX ver. 12.2
- $u_{\mathrm{temp}} \to \min$
- beam cross-section
  - (width) $\times$ (thickness) $= 1 \times 1\,\mathrm{mm}$

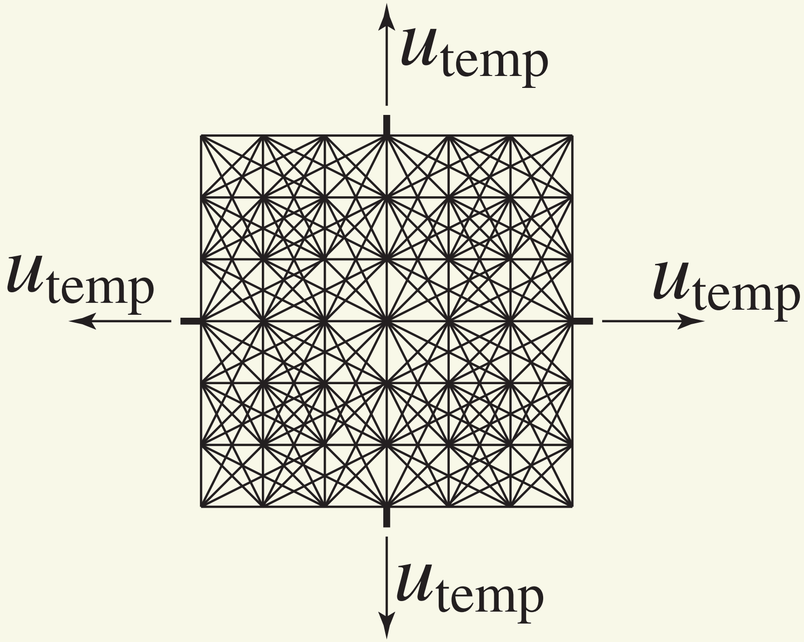


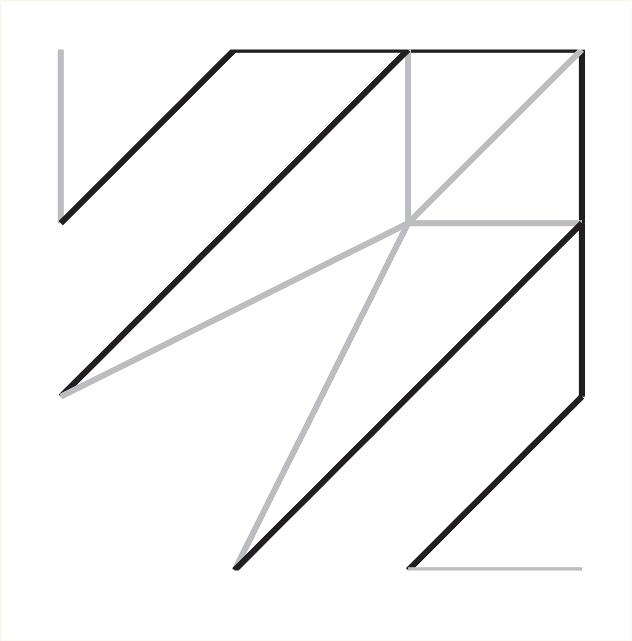


ex.) global optimization

- 66 candidate members
- $\alpha = -4.19275 \times 10^{-5}\,\mathrm{K}^{-1}$
- Time: $237{,}713\,\mathrm{s}$







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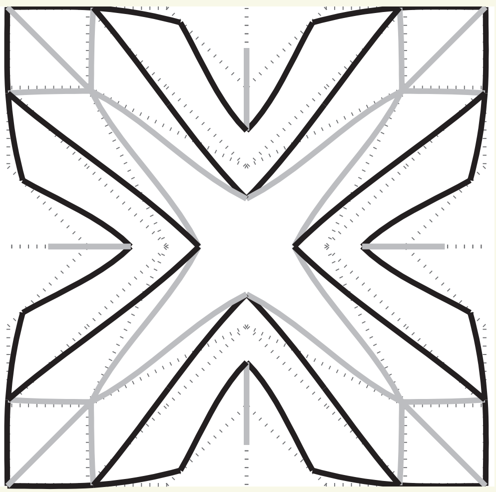

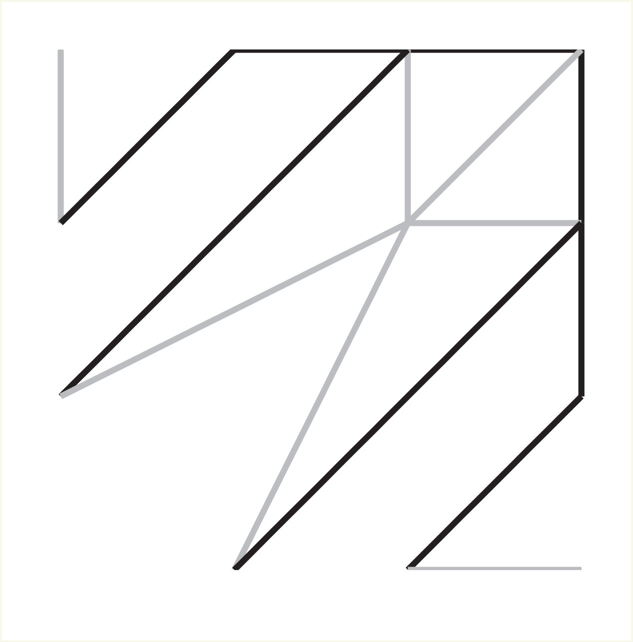

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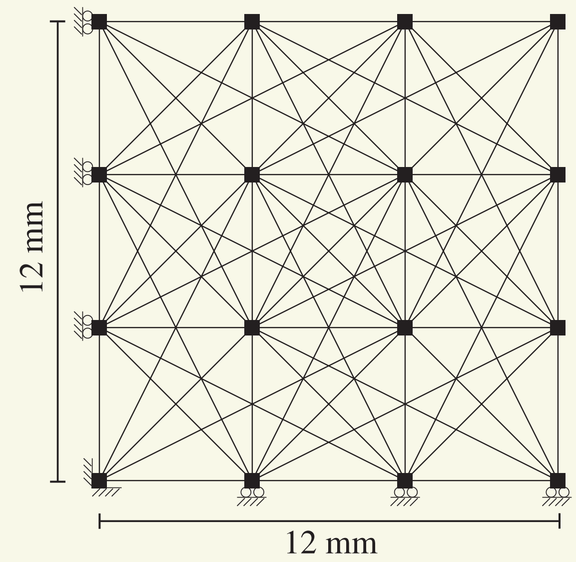

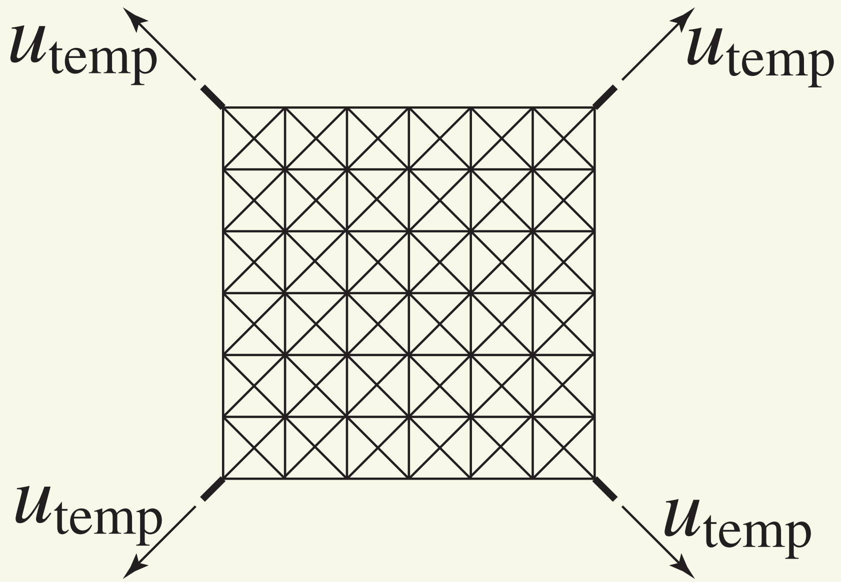

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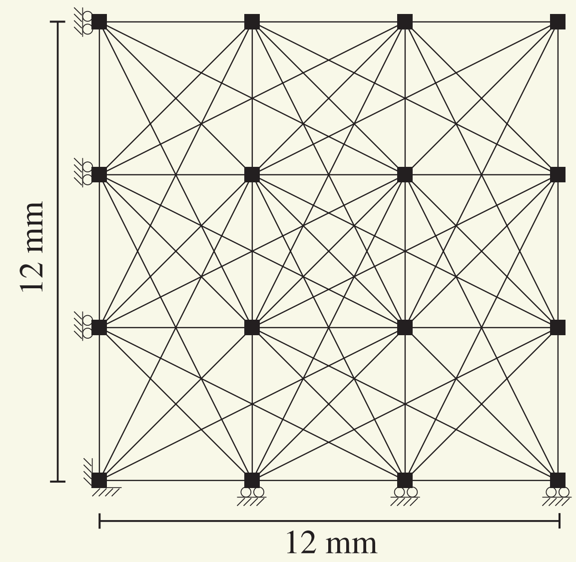

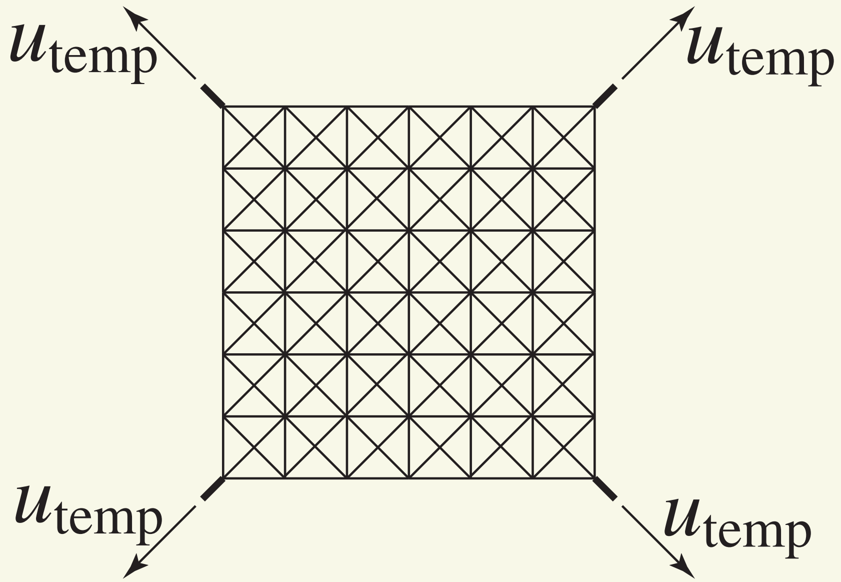

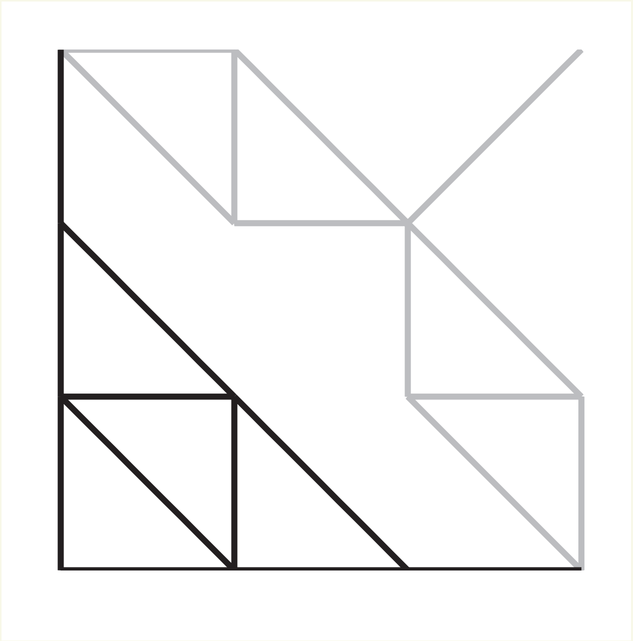

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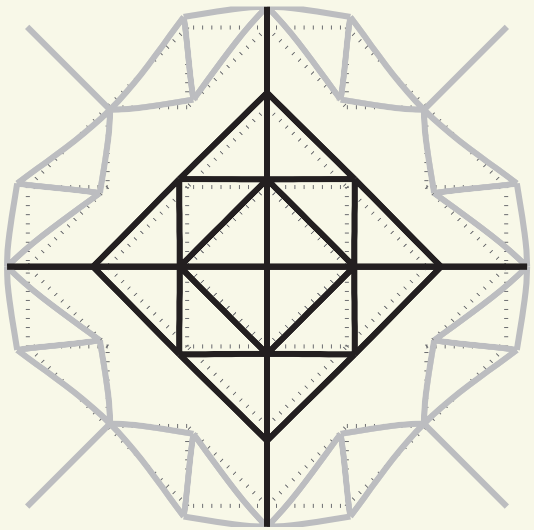
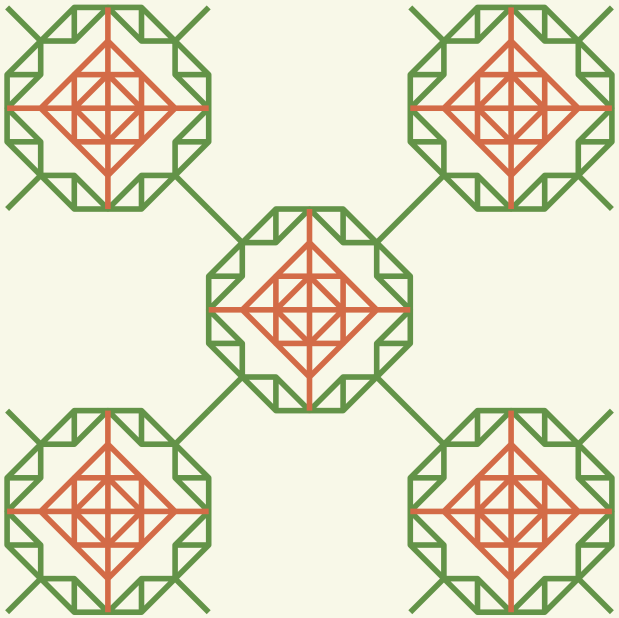
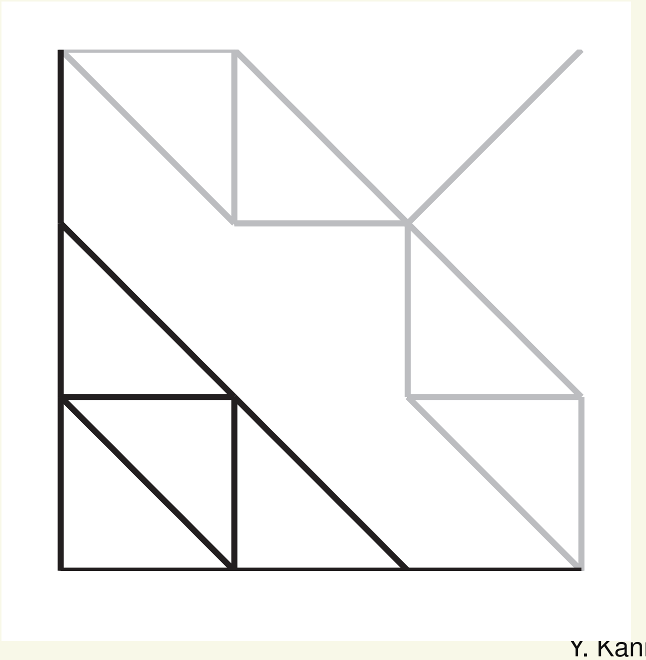




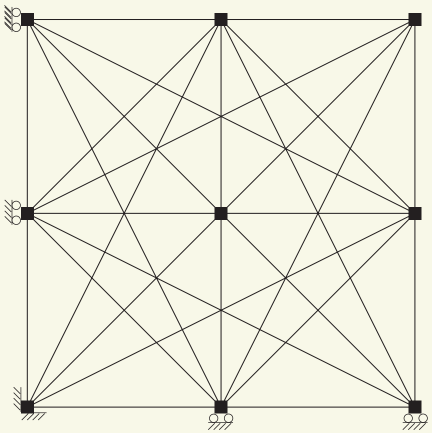


towards large-scale examples

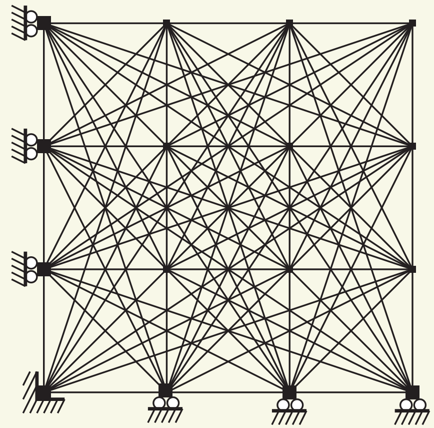
- use heuristics implemented in the MILP solver
- lose guarantee of global optimality
- CPLEX option
  - `emphasis mip` $= 4$
    (emphasize to find hidden feasible solutions)
  - `timelimit` $= 1{,}000\,\mathrm{s}$
    (limit run time, report the best feasible solution)

  $\rightarrow$ Global opt. sols. were found for all the examples above.
  - After that, e.g., $66\,\mathrm{h}$ were spent to prove global optimality.
- try larger examples with this heuristic...

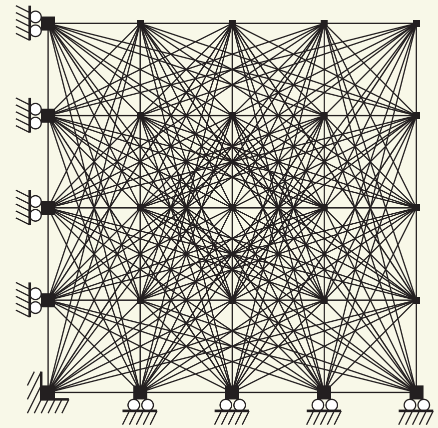
more examples



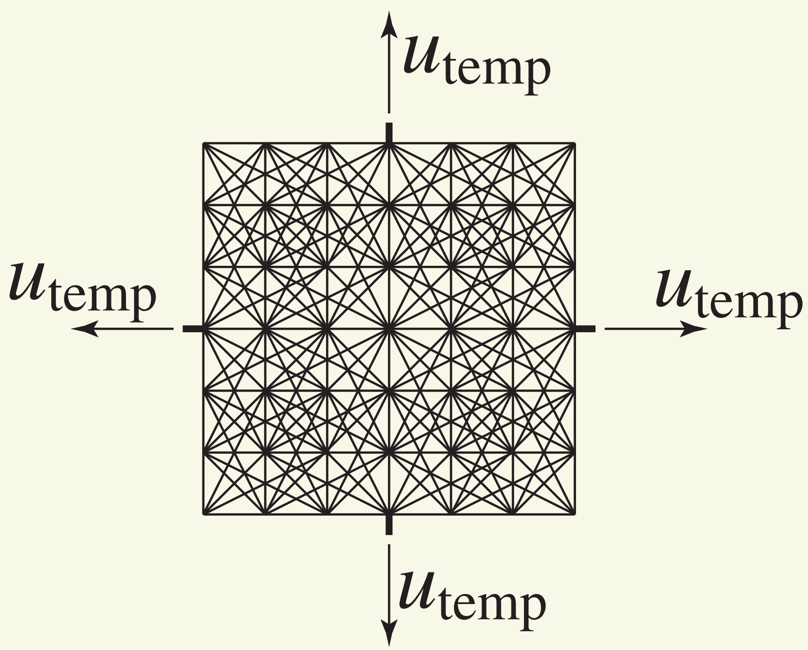
28 members



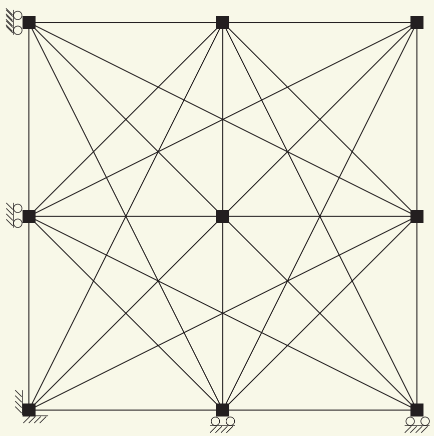
86 members

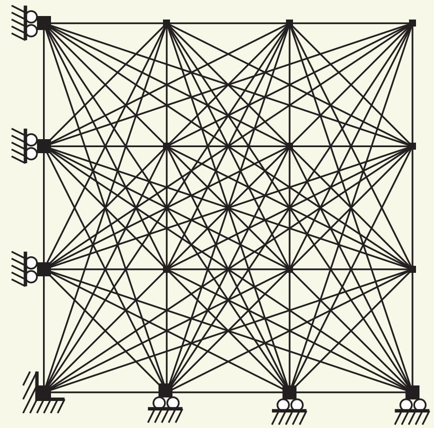


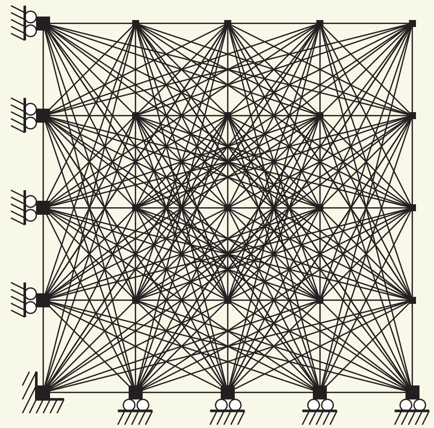
200 members

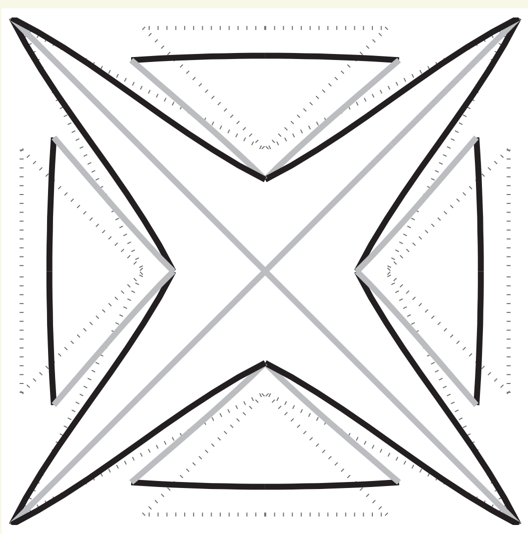


more examples

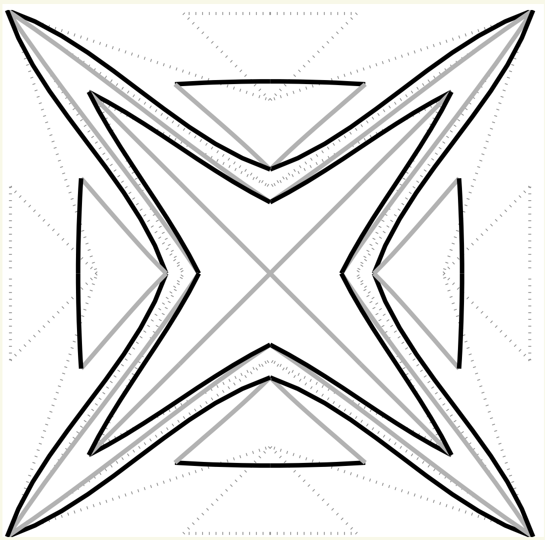




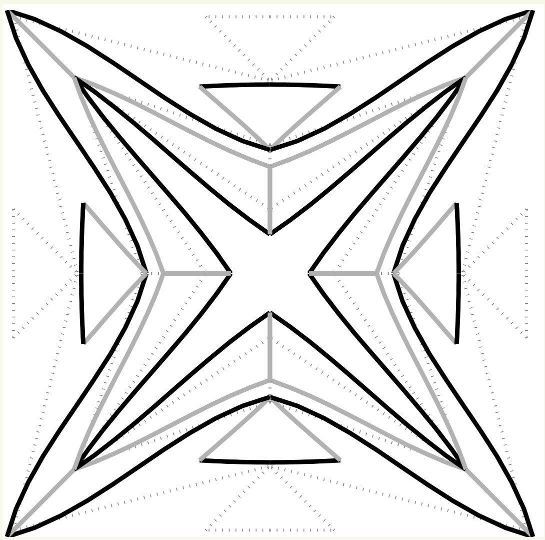




$-2.86604 \times 10^{-5}\,\mathrm{K}^{-1}$
(global opt.)



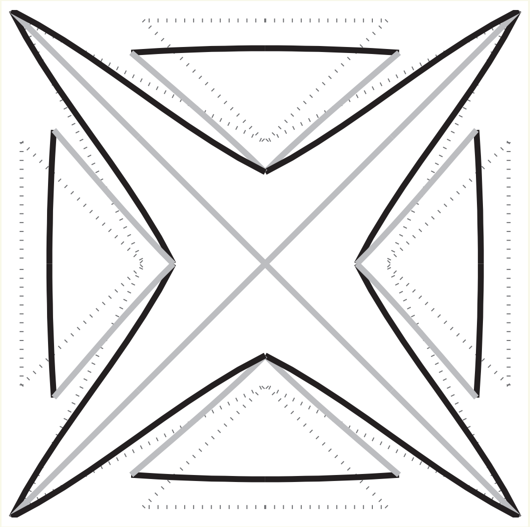
$-6.52129 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)



$-6.60450 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)

more examples

- Small TECs are achieved.
- Two materials are placed alternately.
  $\rightarrow$ Explore "simpler" solutions.



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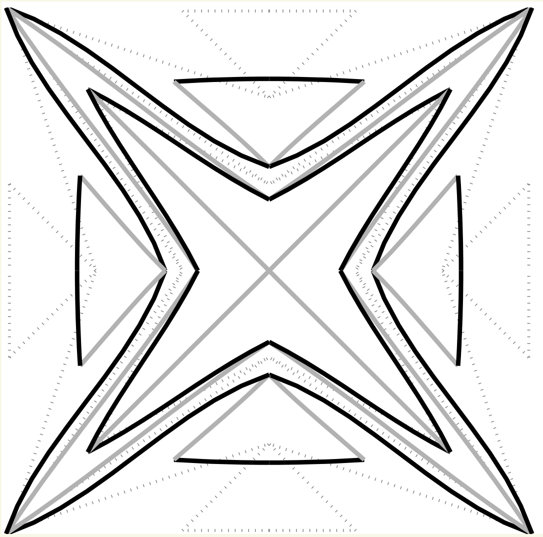

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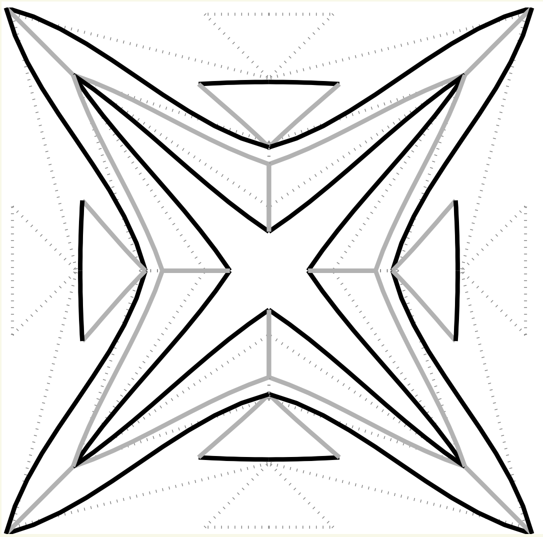

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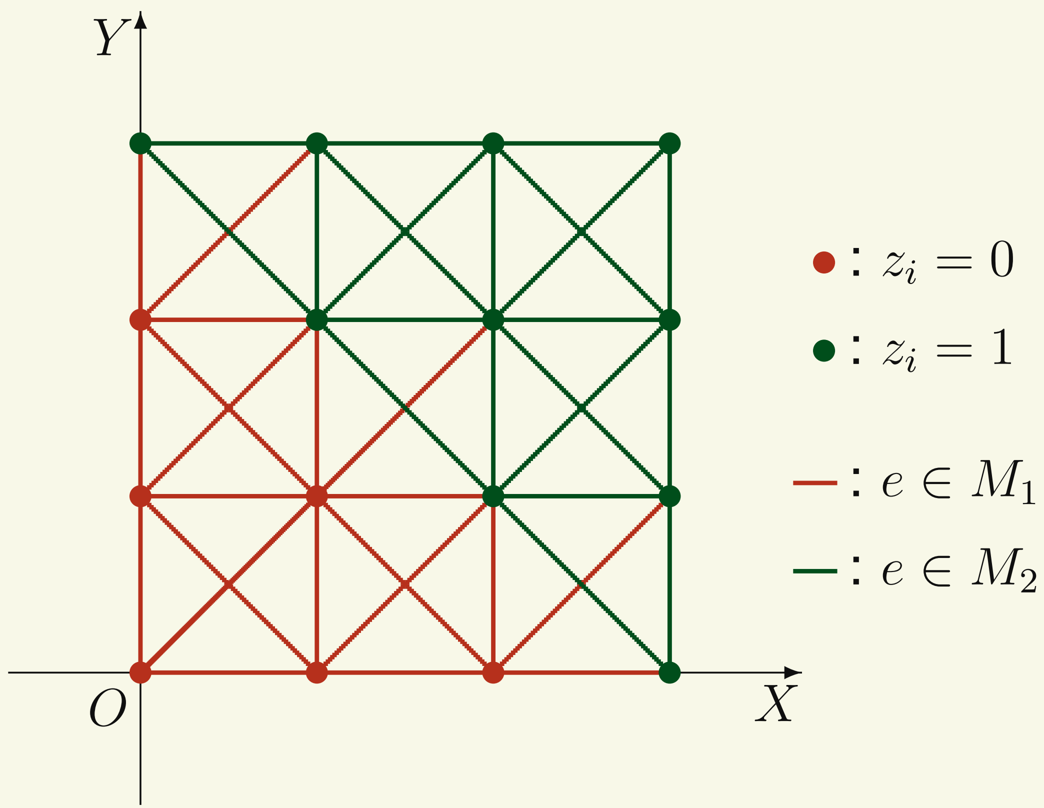
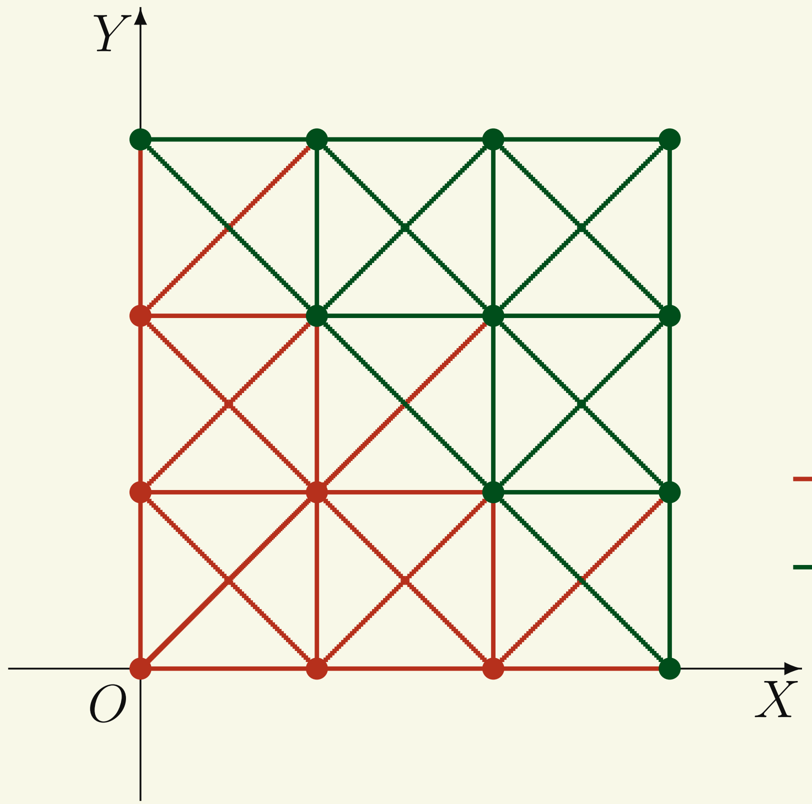
separation of material distributions: motivation



- separation constraint
  - interior:
    M_1 (high TEC)
  - exterior:
    M_2 (low TEC)
- for avoiding small pieces

- compressions act on interfaces between M_1 and M_2
  - $\rightarrow$ Bonding will be strengthened when temperature elevates.

separation of material distributions: formulation

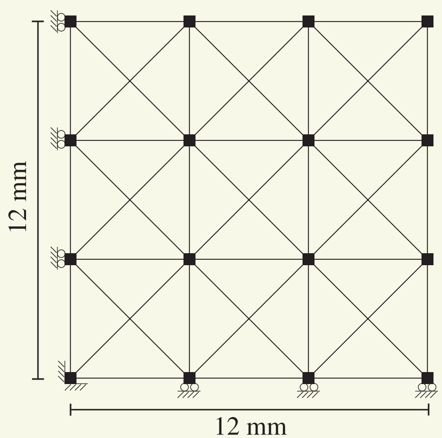


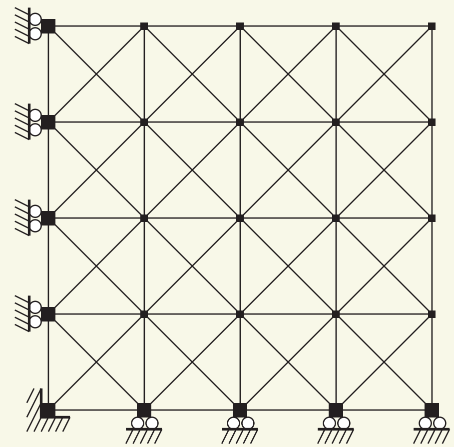
- : $z_i = 0$
- : $z_i = 1$
- : $e \in M_1$
- : $e \in M_2$

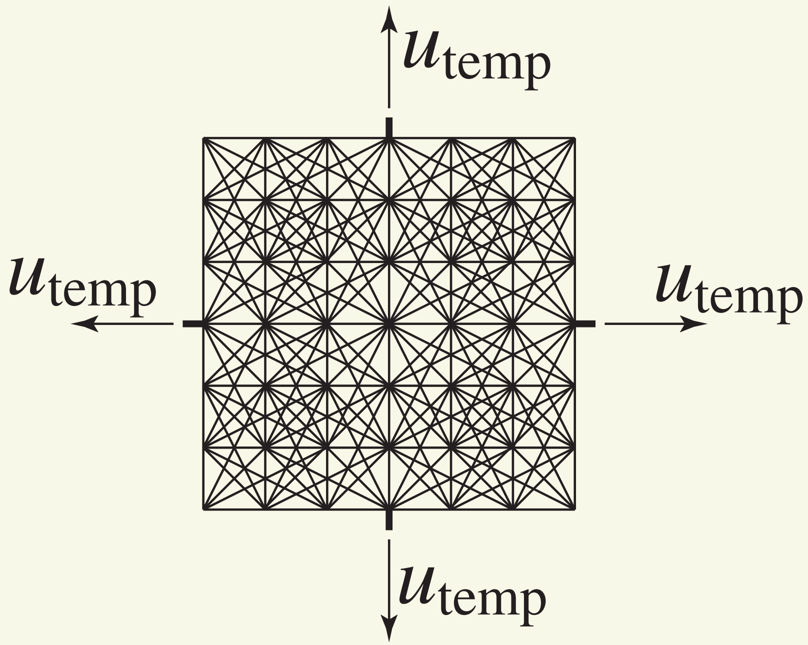
- 0-1 variables
  - x_e : indicates existence of member e
  - z_i : classifies node i
    - if node i : interior & node j : exterior $\Rightarrow z_i \leq z_j$
- notation: $e = (i, j)$
- material selection rule:

$$
\begin{aligned}
x_e = 1,\ z_i + z_j \leq 1 \quad &\Leftrightarrow \quad e \in \mathcal{M}_1, \\
x_e = 1,\ z_i + z_j = 2 \quad &\Leftrightarrow \quad e \in \mathcal{M}_2, \\
x_e = 0,\ z_i + z_j \leq 2 \quad &\Leftrightarrow \quad e \in \mathcal{N}.
\end{aligned}
$$

ex.) w/ separation constraints







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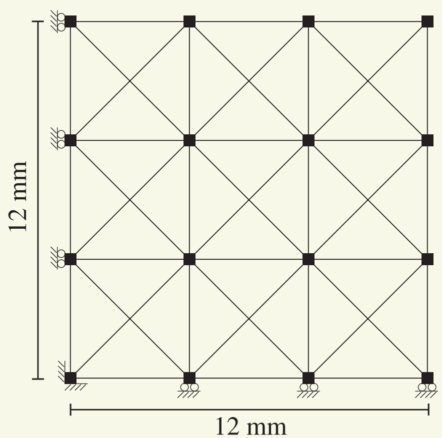
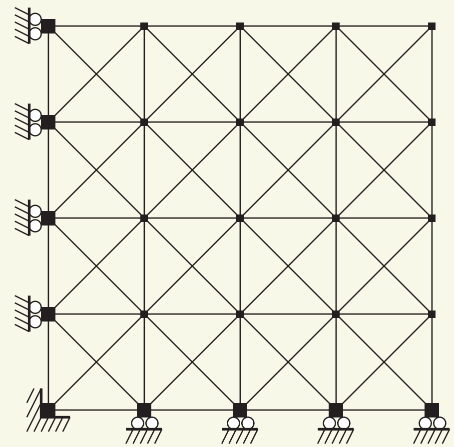
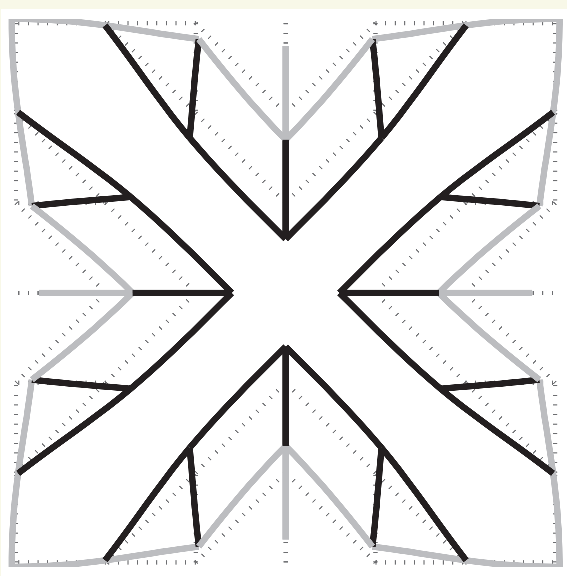
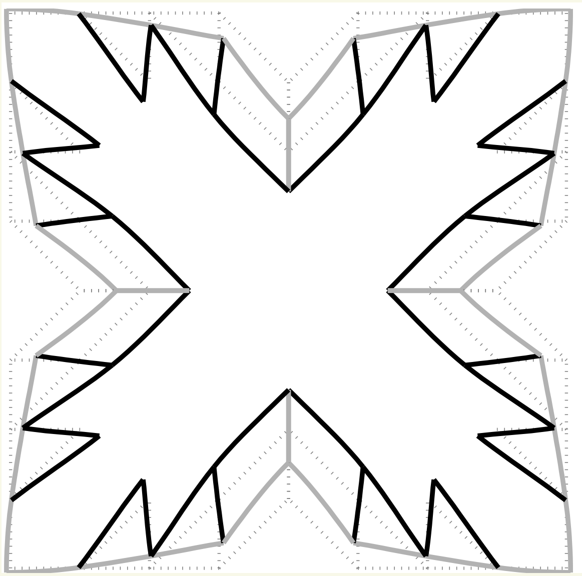




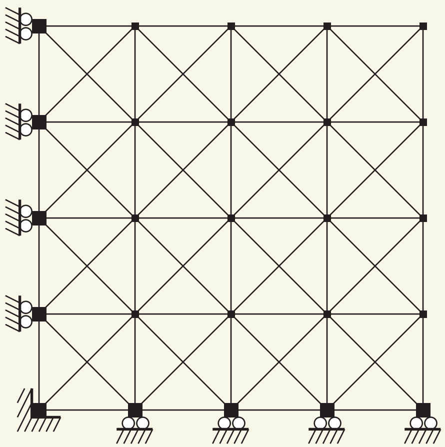


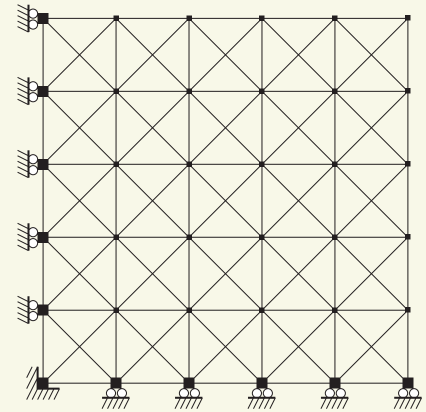
$-2.12746 \times 10^{-5}\,\mathrm{K}^{-1}$
(global, $9{,}500\,\mathrm{s}$)

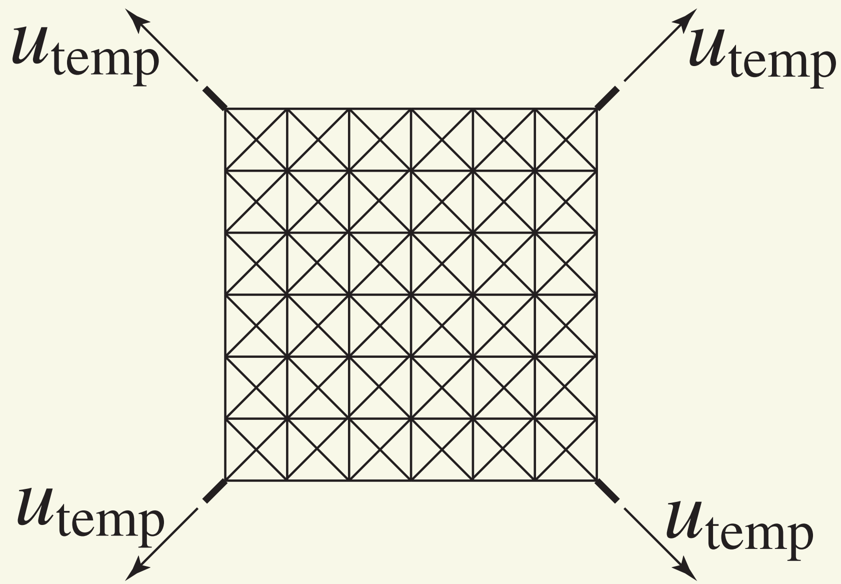


$-3.01329 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)

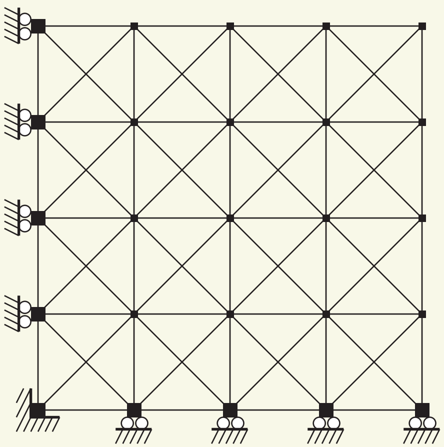
ex.) w/ separation constraints

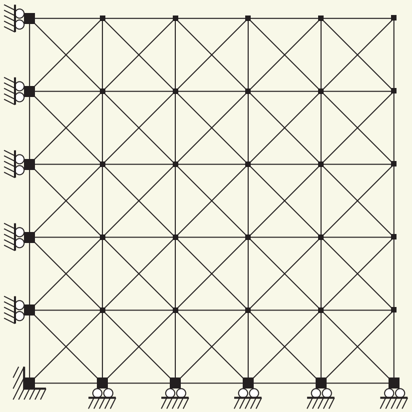


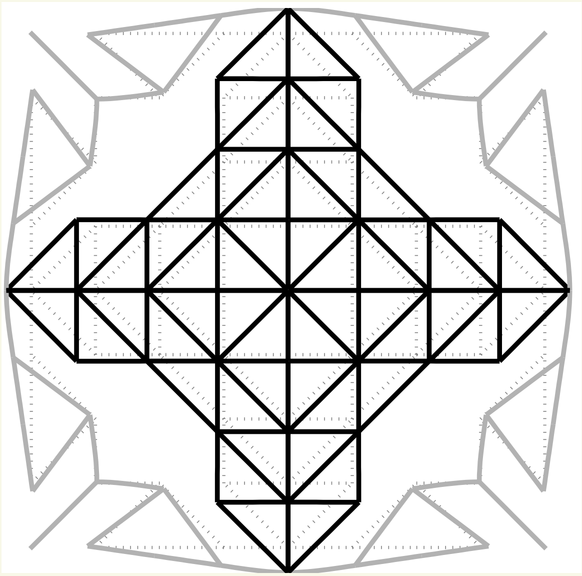




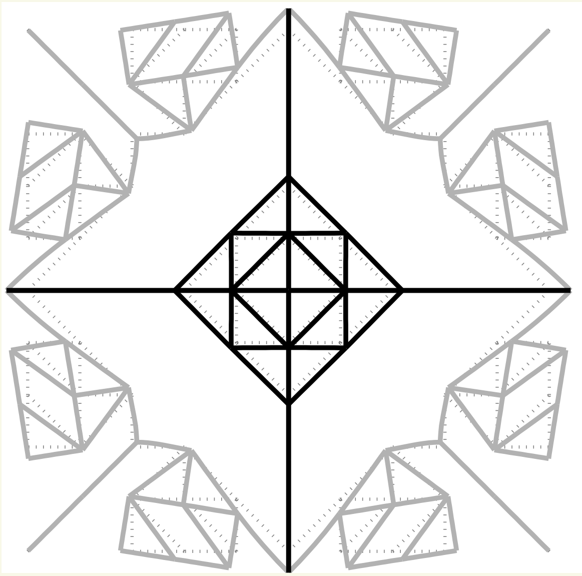
ex.) w/ separation constraints







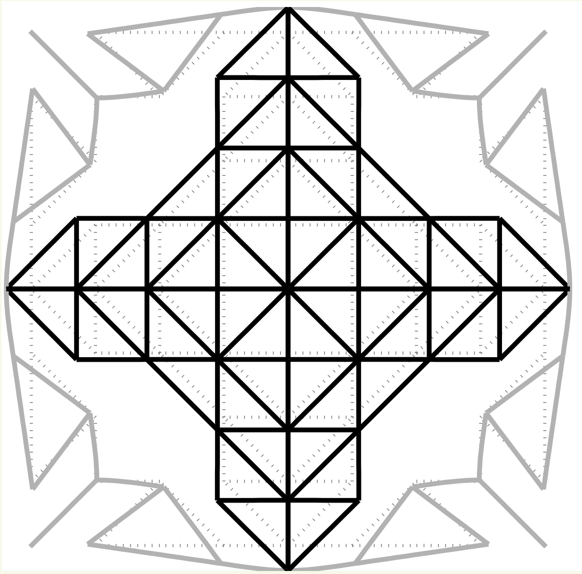
$0.08285 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)



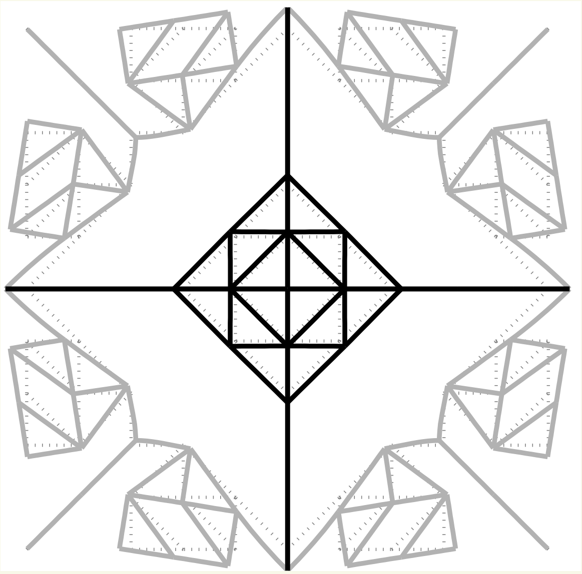
$-0.04296 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)

ex.) w/ separation constraints

- fabrication
  - lattice consisting of M_2 (exterior)
  - pieces consisting of M_1 (interior)
  - heating M_2 and inserting M_1
    $\rightarrow$ Bonding will be strengthened automatically.



$0.08285 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)



$-0.04296 \times 10^{-5}\,\mathrm{K}^{-1}$
(12 h)

summary

- design of counterintuitive structures
  - $\rightarrow$ Optimization might be a helpful tool.
- structures with negative thermal expansion
  - topology optimization of frame structures
    - min. the displacement at elevated temperature
    - mixed-integer programming
  - selection of material of member e $\leftarrow$ integer variables
    - two materials (w/ positive TECs) and void
  - stress constraints
  - no hinge, no thin member, no post-processing