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A plugin framework for large-scale multi-formulation topology optimization

Mateus B. Neiva[1], Andrea Nale[2], Ivan F. Menezes[1], Andrea Chiozzi[3]

1: Department of Mechanical Engineering, Pontifical Catholic University of Rio de Janeiro, Rua Marquês de SãoVicente, 225, Rio de Janeiro 22453, Brazil
2: Department of Architecture University of Ferrara, Via della Ghiara 36 - 44121 Ferrara, Italy
3: Department of Environmental and Prevention Sciences, University of Ferrara, C.so Ercole I d'Este, 32 - 44121 Ferrara, Italy

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SUMMARY

1. MOTIVATIONS & OBJECTIVES

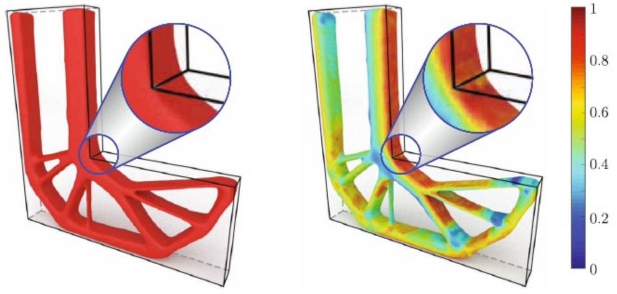
2. TOPOLOGY OPTIMIZATION

3. TOPSIM FRAMEWORK

4. RESULTS

5. CONCLUSIONS & FUTURE WORK

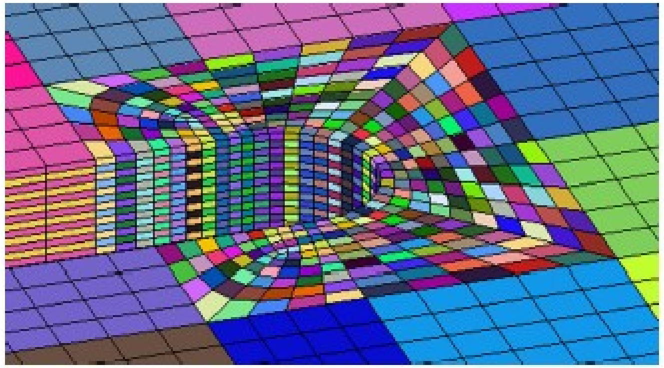
Bridge Domain - Zegard (2016)



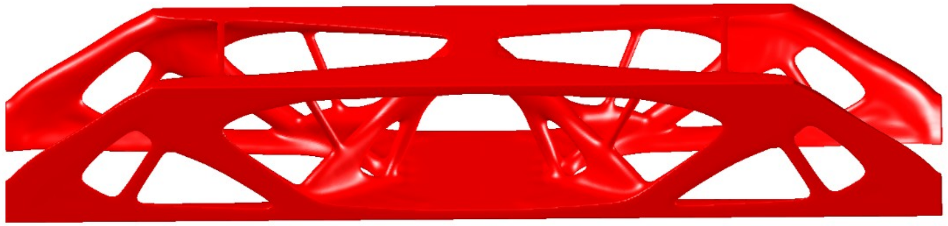
L-Bracket Domain - Senhora (2020)

MOTIVATIONS & OBJECTIVES

- Development of an efficient plugin framework for topology optimization
- Propose a plugin structure for single and multimaterial formulations
- Simulation of multi-scale problems
- Improve filter computation complexity
- Congruent elements algorithm



Elements Congruency - Yadav (2014)



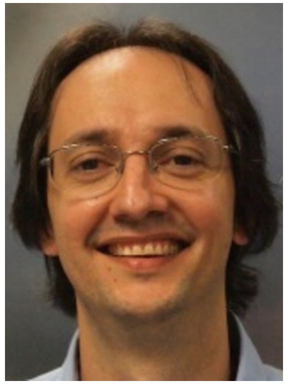
MBB Domain PolyTop++ Leonardo (2015)

RESEARCH COLLABORATION

PUC RIO

Università degli Studi di Ferrara

Mateus B. Neiva
PhD Student



Ivan F. Menezes
Associate Professor

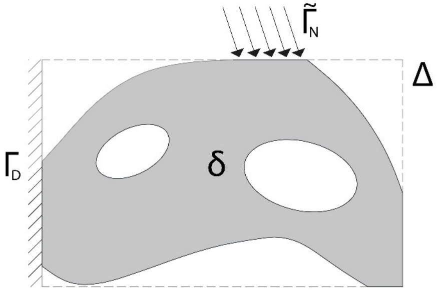
Andrea Nale
PhD Student

Andrea Chiozzi
Assistant Professor

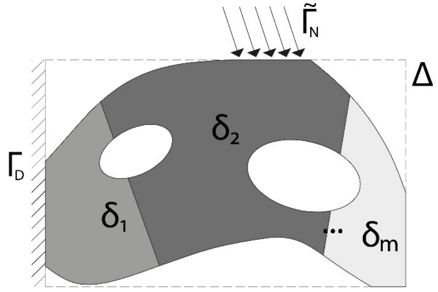
TOPOLOGY OPTIMIZATION

The approach adopted is a multi-material topology optimization[1]:

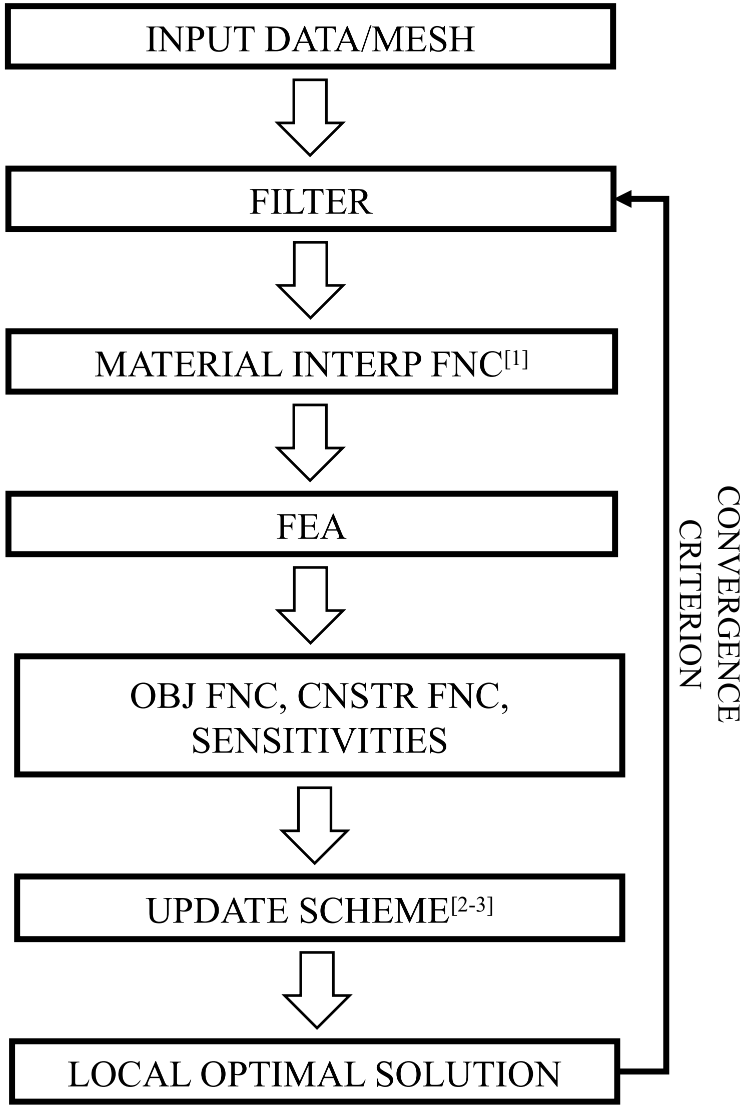
$$
\begin{aligned}
\min_{\mathbf{z}} \quad & C = \mathbf{F}^T\,\mathbf{U}(\mathbf{z}) \\
\text{s.t.} \quad & g_j = \frac{\sum_{m\in\mathcal{G}_j}\sum_{\ell\in\mathcal{E}_j} V_\ell m_v(y_{\ell m})}{\sum_{\ell\in\mathcal{E}_j} V_\ell} - \overline{v}_j \le 0,\ j = 1, \dots N^c \\
\text{with} \quad & \mathbf{K}(\mathbf{z})\,\mathbf{U}(\mathbf{z}) = \mathbf{F} \\
& \mathbf{y}(\mathbf{z}) = \mathcal{H}(\mathbf{z}) \\
& 0 \le \mathbf{z} \le 1
\end{aligned}
$$



TopOpt
Single Material



TopOpt
Multimaterial



[1] Stegmann, J., & Lund, E. (2005). Discrete material optimization of general composite shell structures. International Journal for Numerical Methods in Engineering, 62(14), 2009-2027.
[2] Bendsoe, M. P., & Sigmund, O. (2013). Topology optimization: theory, methods, and applications. Springer Science & Business Media.
[3] Zhang, X. S., Paulino, G. H., & Ramos, A. S. (2018). Multi-material topology optimization with multiple volume constraints: a general approach applied to ground structures with material nonlinearity. Structural and Multidisciplinary Optimization, 57, 161-182.

MULTISCALE APPROACH

The topology optimization approach adopted for multimaterial is a **homogenization-based structural optimization**[1]:

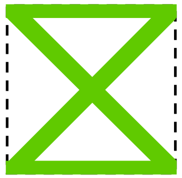
PREDEFINED RVEs

↓

COMPUTATIONAL HOMOGENIZATION[2]

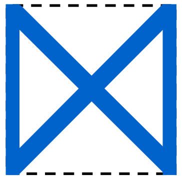
↓

TOPOLOGY OPTIMIZATION



$E_1 = 0.75\,\mathrm{MPa}$

$\nu_1 = 0.3$



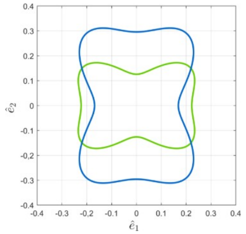
$E_1 = 1\,\mathrm{MPa}$

$\nu_1 = 0.3$

Periodic Microstructures

$$D_1^H = \begin{bmatrix} 0.284 & 0.099 & 0 \\ 0.099 & 0.161 & 0 \\ 0 & 0 & 0.0104 \end{bmatrix} \qquad D_2^H = \begin{bmatrix} 0.215 & 0.132 & 0 \\ 0.132 & 0.377 & 0 \\ 0 & 0 & 0.0139 \end{bmatrix}$$

Homogenized Elasticity Matrix



Directional Tensile Modulus

[1] Wu, J., Sigmund, O., & Groen, J. P. (2021). Topology optimization of multi-scale structures: a review. Structural and Multidisciplinary Optimization, 63, 1455-1480.
[2] Hassani, B., & Hinton, E. (2012). Homogenization and structural topology optimization: theory, practice and software. Springer Science & Business Media.

MULTI-MATERIAL INTERPOLATION

The material interpolation is used to define the constitutive properties of each element and to penalize mixing:

$$m_E = m_M \circ m_W$$

The material interpolation is accomplished in two main steps:

1) a **material penalty function** to push the element densities toward zero and one. Using modified SIMP method (void are considered as Ersatz Material) the penalized element densities are computed as:

$$w_{li} = m_W = y_{li}^p$$

2) a **multi-material interpolation function** to determine the stiffness properties in each element and penalize mixing. The element stiffness elasticity matrix is interpolated as follows:

$$K_\ell = m_M = \sum_{m=1}^{N^m} w_{\ell i} \prod_{\substack{j=1 \\ j \neq m}}^{N^m} (1 - \gamma w_{\ell j}) K_\ell^H$$

OPTIMALITY CRITERIA

The structural optimization problem is solved using the approximated problem at the current design point:

$$\begin{array}{ll} \min\limits_{\mathbf{z}} & f_{\text{app}}(\mathbf{z}) \\ \text{subject to} & g_{\text{app}}(\mathbf{z}) \leq 0 \\ \text{with} & \mathbf{z} \in [0,1]^{N^e} \end{array}$$

The OC[1] design variable update scheme is obtained by the linearization of the objective function in exponential intermediate variables

$$\frac{\partial f_{\text{app}}}{\partial z_\ell} + \lambda \frac{\partial g_{\text{app}}}{\partial z_\ell} = 0$$

$$f_{\text{app}}(\mathbf{z}) = f(\mathbf{z}^0) + \frac{\partial f}{\partial z_\ell}\bigg|_{\mathbf{z}=\mathbf{z}^0} \frac{1}{a} z_\ell^0 \left[\left(\frac{z_\ell}{z_\ell^0}\right)^a - 1 \right]$$

$$g_{\text{app}}(\mathbf{z}) = g(\mathbf{z}^0) + \frac{\partial g}{\partial g}\bigg|_{\mathbf{z}=\mathbf{z}^0} \left(z_\ell - z_\ell^0 \right)$$

$$\left(\frac{z_\ell - 1}{z_\ell^0 - 0}\right)^{(1-a)} = -\frac{\frac{\partial f}{\partial \ell}|_{z=z^0}}{\lambda_j \frac{\partial g_j}{\partial \ell}|_{z=z^0}} := B_\ell$$

The sensitivities are defined as:

$$\frac{\partial f}{\partial z_\ell} = \boxed{\frac{\partial y_\ell}{\partial z_\ell}} \boxed{\frac{\partial E_\ell}{\partial y_\ell}} \boxed{\frac{\partial f}{\partial E_\ell}} \qquad \frac{\partial g}{\partial z_\ell} = \boxed{\frac{\partial y_\ell}{\partial z_\ell}} \boxed{\frac{\partial g}{\partial y_\ell}}$$

$$\boxed{\frac{\partial y_\ell}{\partial z_\ell} = P^T} \qquad \boxed{\frac{\partial E_k}{\partial y_\ell} = \begin{cases} p y_\ell^{p-1}, & \text{if } \ell = k \\ 0, & \text{otherwise} \end{cases}}$$

$$\boxed{\frac{\partial f}{\partial w_{\ell m}} = -U^T \frac{\partial K}{\partial w_{\ell m}} U} \qquad \frac{\partial K_\ell}{\partial w_\ell} = \frac{\partial K_\ell^0}{\partial w_\ell} \qquad \boxed{\frac{\partial g_j}{\partial v_\ell} = \frac{A_\ell}{\sum_{\ell \in \mathcal{E}_j} A_\ell}}$$

The design variables are updated as:

$$z_\ell^k = \begin{cases} z_\ell^+, & \text{if } z_\ell^* \geq z_\ell^+ \\ z_\ell^-, & \text{if } z_\ell^* \geq z_\ell^+ \\ z_\ell^*, & \text{otherwise} \end{cases} \qquad \begin{aligned} z^0 &= z_\ell^0, \ldots, z_{N^e}^0 \\ z_\ell^- &= \max\{0, z_\ell^0 - \text{move}\} \\ z_\ell^+ &= \min\{1, z_\ell^0 + \text{move}\} \end{aligned}$$

$$z_\ell^* = B_\ell^{\frac{1}{1+\alpha}} z_\ell^0 \qquad B_\ell = -\frac{\frac{\partial f}{\partial \ell}|_{z=z^0}}{\lambda_j \frac{\partial g_j}{\partial \ell}|_{z=z^0}}$$

The convergence criteria is set as:

$$||z_\ell^k - z_\ell^{k-1}||_2 \leq \text{tol}$$

[1] Bendsoe, M. P., & Sigmund, O. (2013). Topology optimization: theory, methods, and applications. Springer Science & Business Media.

ZPR UPDATE SCHEME

The sensitivities of:

- objective function f: $\dfrac{\partial f}{\partial z_{\ell m}} = \boxed{\dfrac{\partial y_{\ell m}}{\partial z_{\ell m}}}\boxed{\dfrac{\partial w_{\ell m}}{\partial y_{\ell m}}}\boxed{\dfrac{\partial f}{\partial w_{\ell m}}}$

- constraint function g: $\dfrac{\partial g}{\partial z_{\ell m}} = \boxed{\dfrac{\partial y_{\ell m}}{\partial z_{\ell m}}}\boxed{\dfrac{\partial v_{\ell m}}{\partial y_{\ell m}}}\boxed{\dfrac{\partial g}{\partial v_{\ell m}}}$

$$\boxed{\frac{\partial y_{\ell m}}{\partial z_{\ell m}} = P^T} \qquad \boxed{\frac{\partial w_{kj}}{\partial y_{\ell m}} = \begin{cases} p y_{\ell m}^{p-1}, & \text{if } \ell = k \text{ and } j = m \\ 0, & \text{otherwise} \end{cases}}$$

$$\boxed{\frac{\partial f}{\partial w_{\ell m}} = -U^T \frac{\partial K}{\partial w_{\ell m}} U}$$

$$\frac{\partial K_\ell}{\partial w_{\ell m}} = \prod_{\substack{j=1 \\ j\neq m}}^{N^m} (1-\gamma w_{\ell j}) K_\ell^H - \sum_{\substack{p=1 \\ p\neq m}}^{N^m} w_{\ell p} \prod_{\substack{r=1 \\ r\neq p \\ r\neq m}}^{N^m} (1-\gamma w_{\ell r}) K_{\ell p}^H$$

$$\boxed{\frac{\partial v_{li}}{\partial y_{jk}} = \begin{cases} \rho_\ell, & \text{if } \ell = k \text{ and } j = m \\ 0, & \text{otherwise} \end{cases}} \qquad \boxed{\frac{\partial g_j}{\partial v_{\ell i}} = \frac{A_\ell}{\sum_{\ell \in \varepsilon_j} A_\ell}}$$

The ZPR[1] (Zhang-Paulino-Ramos) design variable update scheme uses the Lagrangian duality to solve a series of convex approximate subproblems around the current design to move toward an optimal point:

$$z_{\ell m}^k = \begin{cases} z_{\ell m}^+, & \text{if } z_{\ell m}^* \geq z_{\ell m}^+ \\ z_{\ell m}^-, & \text{if } z_{\ell m}^* \geq z_{\ell m}^+ \\ z_{\ell m}^*, & \text{otherwise} \end{cases} \qquad \begin{aligned} z^0 &= z_{\ell m}^0, \ldots, z_{\ell N^m}^0 \\ z_{\ell m}^- &= \max\{0, z_{\ell m}^0 - \text{move}\} \\ z_{\ell m}^+ &= \min\{1, z_{\ell m}^0 + \text{move}\} \end{aligned}$$

$$z_{\ell m}^* = B_{\ell m}^{\frac{1}{1+\alpha}} \sum_{k=1}^{N^e} P_{\ell k} z_{ki}^0 \qquad B_{\ell m} = -\frac{\frac{\partial f}{\partial \ell m}|_{z=z^0}}{\lambda_j \frac{\partial g_j}{\partial \ell m}|_{z=z^0}}$$

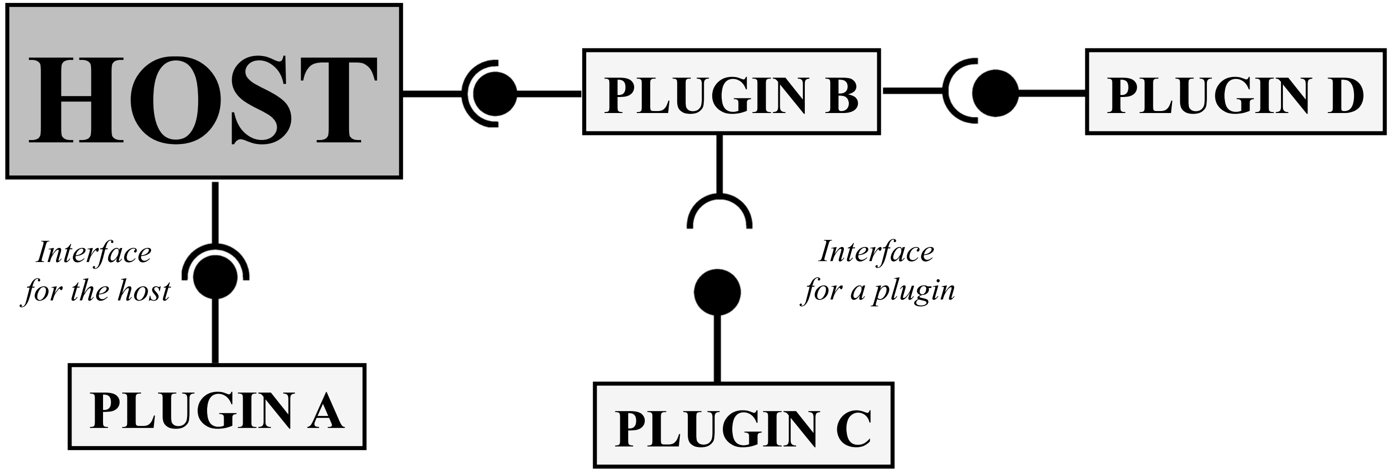
The optimization problem is considered to have converged when a prescribed maximum number of iterations is reached or when:

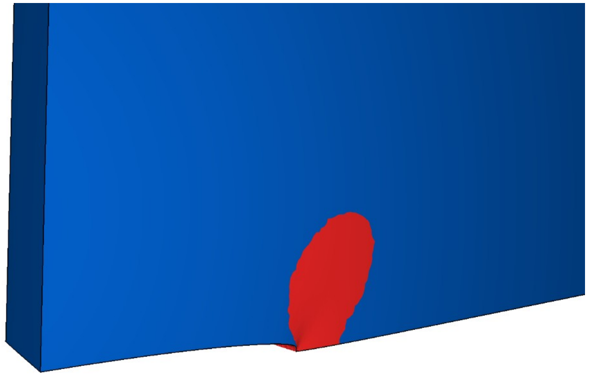
$$||z_{\ell m}^k - z_{\ell m}^{k-1}||_2 \leq \text{tol}$$

[3] Zhang, X. S., Paulino, G. H., & Ramos, A. S. (2018). Multi-material topology optimization with multiple volume constraints: a general approach applied to ground structures with material nonlinearity. Structural and Multidisciplinary Optimization, 57, 161-182.

TOPSIM FRAMEWORK

Architecture:
- plugins can define or request an interface;
- plugins define a specific algorithm for high performance;





- Computational tool focusing in developing numerical models for different applications;

- Environment based in plugin, which allows flexibility and extensibility:
  - Plugins are loaded in executing time under a specific application

- Supports different programming languages in the plugins:
  - C++, C, FORTRAN, [Lua…]

- Supports large scale simulation (millions of elements)
  - Serial and parallel code for either machines or *cluster;*
  - Focus on efficient use of memory and performance

- Plugin framework allows implementation of complex models but also their proper reduction for simpler cases.
  Ex. FEM with large strain, plasticity and thermal expansion can simply not being load;

- Uses Tops[1], an efficient computational data structure for topological domain.

[1] Celes, W., Paulino, G. H., & Espinha, R. (2005). A compact adjacency-based topological data structure for finite element mesh representation. International journal for numerical methods in engineering, 64(11), 1529-1556.

COMPUTATIONAL POINT OF VIEW

PLUGINS:
Commonly, new applications are statically defined in the code (in compilation time) with the use of conditions (if…else, switch).
Example: Updated Schemes: Optimality Criterion, ZPR, Steepest Descent, MMA, GCMMA, Interior Point, SLP, etc.

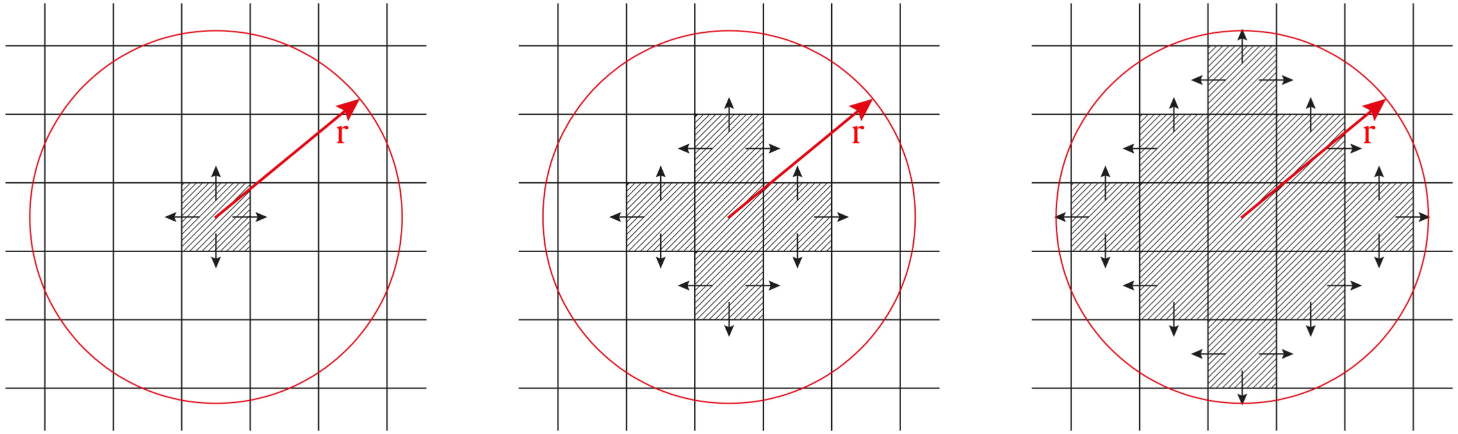
As a consequence:
- Code should handle several previous established models arrange
- Complex Input file, that recurrently needs to be changed for every new application
- Difficult to share reduced code versions

TOPOPT EDUCATIONAL CODES:
- same type of element (99 lines [1])
- assumes all elements to be equal (PolyStress 3D[2])
- pre-compute stiffness matrix (PolyMat[3]), which leads to not using the classic element assemble loop

[1] Sigmund, O. (2001). A 99 line topology optimization code written in Matlab. Structural and multidisciplinary optimization, 21, 120-127.
[2] Giraldo-Londoño, O., & Paulino, G. H. (2020). A unified approach for topology optimization with local stress constraints considering various failure criteria: von Mises, Drucker–Prager, Tresca, Mohr–Coulomb, Bresler–Pister and Willam–Warnke. Proceedings of the Royal Society A, 476(2238), 20190861.
[3] Sanders, E. D., Pereira, A., Aguiló, M. A., & Paulino, G. H. (2018). PolyMat: an efficient Matlab code for multi-material topology optimization. Structural and Multidisciplinary Optimization, 58, 2727-2759.

FILTER: RECURSIVE FUNCTION

$$P_{ij} = \frac{w_{ij} v_j}{\sum_{k=1}^{N^e} w_{ij} v_j}, \text{with, } w_{ij} = \max \left[0, 1 - \frac{||x_i - x_j||_2}{r} \right]^q$$



FILTER ALGORITHM ORDER

Conventional:

for every element (reference) a loop over elements computes the distance between them

$$O(n)$$

once a vector distance is obtained a sort is performed

$$O(n\log(n))$$

total:

$$O(n^2\log(n))$$

TopSim:

using Tops (sort is built-in)

$$O(n\log(n))$$

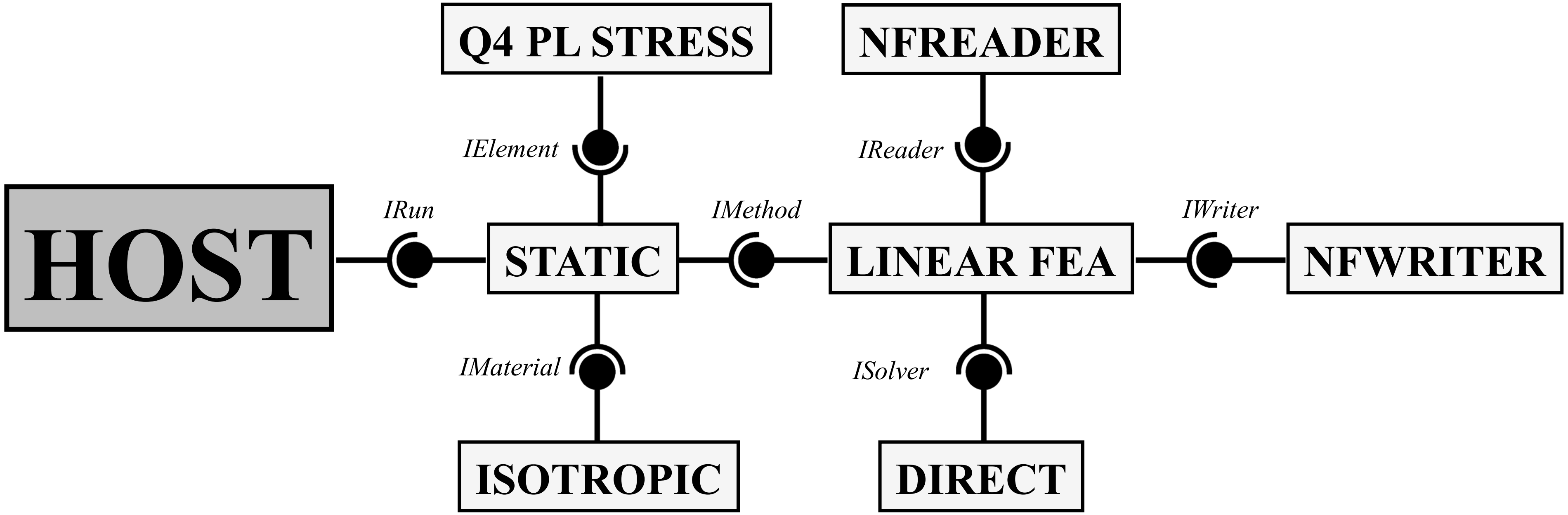
recursion

$$O(n)$$

total:

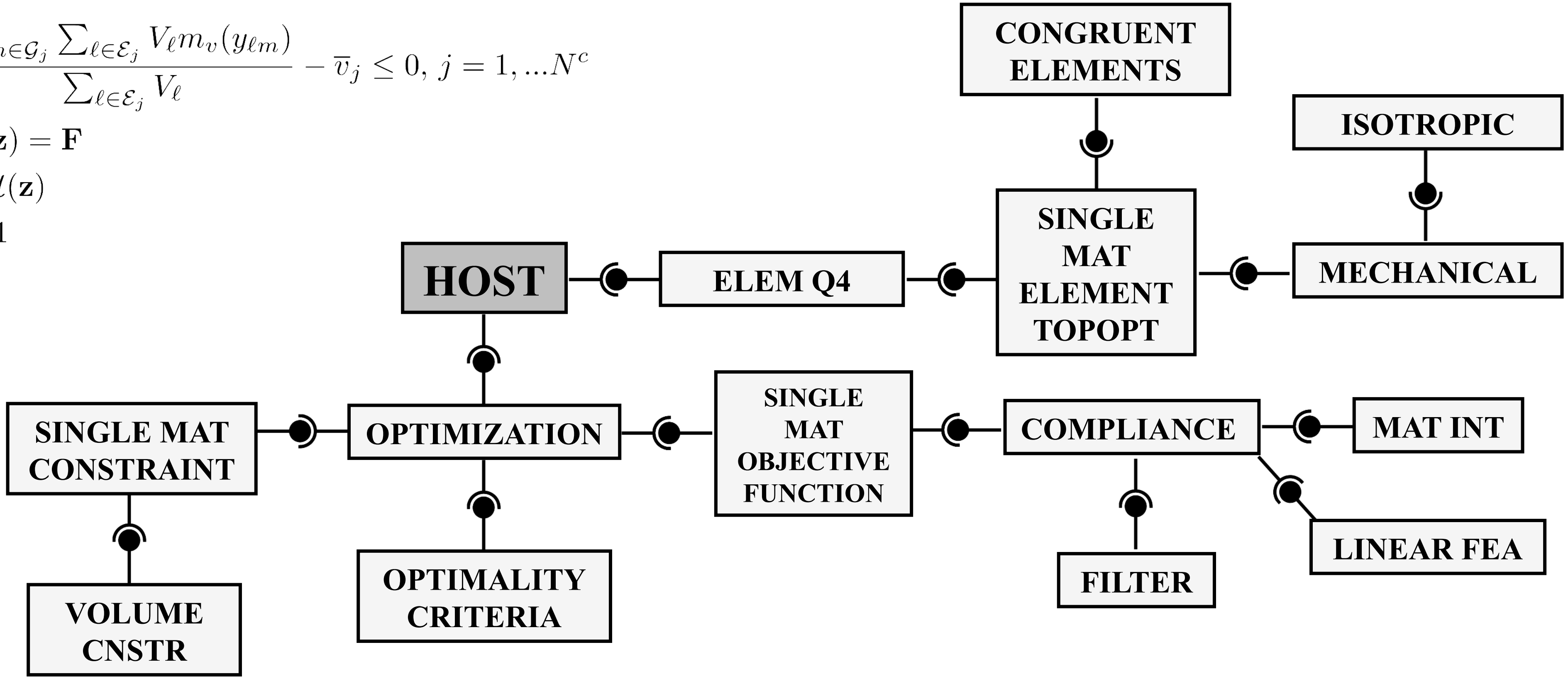
$$O(n)$$

PLUGIN-BASED FRAMEWORK: LINEAR ELASTOSTATIC FEA



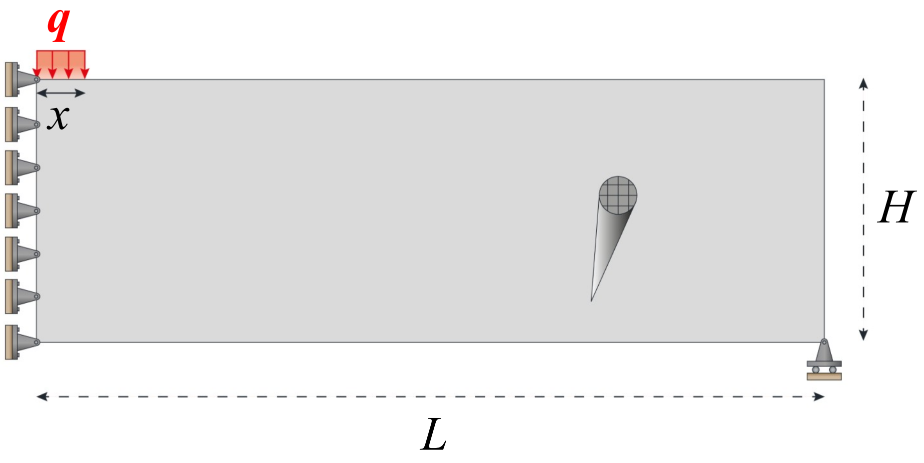
TOP-OPT COMPLIANCE-BASED VOLUME-CONSTRAINED

$$
\begin{aligned}
\min_{\mathbf{z}} \quad & C = \mathbf{F}^T\,\mathbf{U}(\mathbf{z}) \\
\text{s.t.} \quad & g_j = \frac{\sum_{m\in\mathcal{G}_j}\sum_{\ell\in\mathcal{E}_j} V_\ell m_v(y_{\ell m})}{\sum_{\ell\in\mathcal{E}_j} V_\ell} - \overline{v}_j \le 0,\; j = 1, \ldots N^c \\
\text{with} \quad & \mathbf{K}(\mathbf{z})\,\mathbf{U}(\mathbf{z}) = \mathbf{F} \\
& \mathbf{y}(\mathbf{z}) = \mathcal{H}(\mathbf{z}) \\
& 0 \le \mathbf{z} \le 1
\end{aligned}
$$



Plugin-based Q4Opt Framework

MBB DOMAIN



GEOMETRY
$L = 3$
$H = 1$
$x = L/16$

ELEMENTS
quad4

DISCRETIZATION
3000x1000

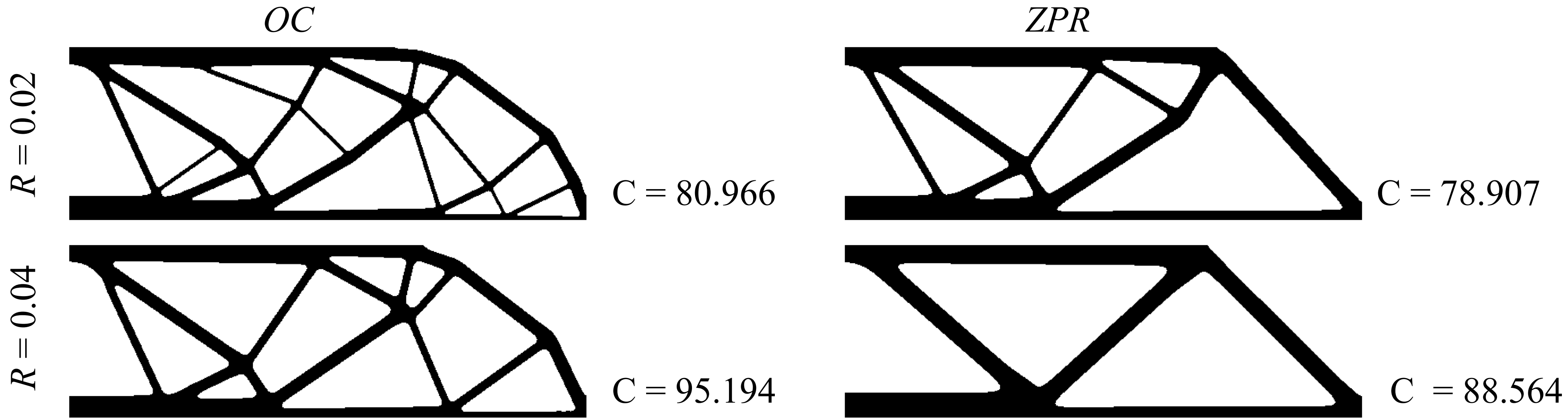
MATERIAL
isotropic
E = 1
ν = 0.3

OC & ZPR
move = 0.2
eta = 1/2

TOPOPT
$p = 1{:}0.5{:}4$
VolFrac = 0.3

FILTER
R = variable
q = linear order

LOAD
P = 0.5/(L/16)



TOPOPT
p = [1:0.5:4]
VolFrac = 0.3

ZPR
move = 0.2
eta = 1/2

FILTER
R = 0.04
q = linear order

ELEMENTS
quad4

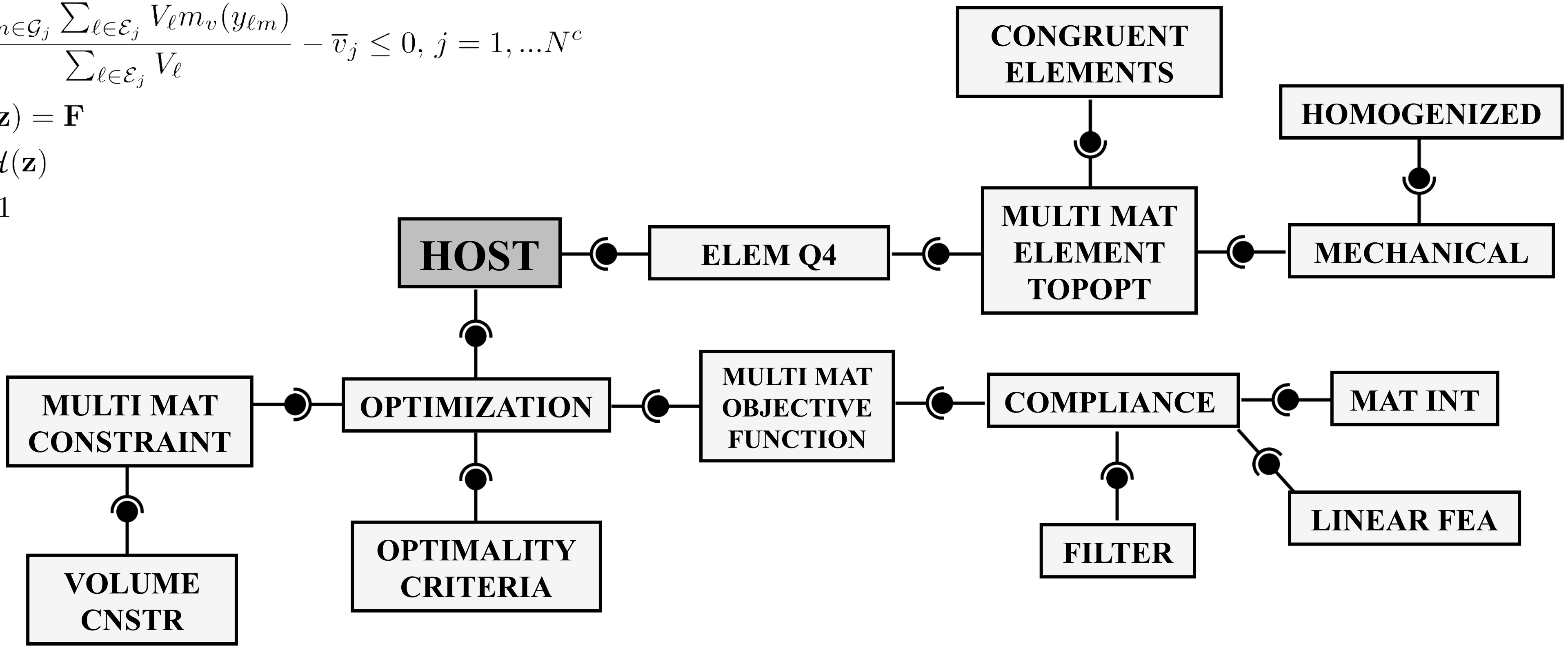
DISCRETIZATION
1200x300

C = 130.69633

NUMBER OF DOFS
723002

TOP-OPT MULTIMATERIAL COMPLIANCE-BASED VOLUME-CONSTRAINED

$$
\begin{aligned}
\min_{\mathbf{z}} \quad & C = \mathbf{F}^T\,\mathbf{U}(\mathbf{z}) \\
\text{s.t.} \quad & g_j = \frac{\sum_{m\in\mathcal{G}_j}\sum_{\ell\in\mathcal{E}_j} V_\ell m_v(y_{\ell m})}{\sum_{\ell\in\mathcal{E}_j} V_\ell} - \overline{v}_j \le 0,\ j = 1,\ldots N^c \\
\text{with} \quad & \mathbf{K}(\mathbf{z})\,\mathbf{U}(\mathbf{z}) = \mathbf{F} \\
& \mathbf{y}(\mathbf{z}) = \mathcal{H}(\mathbf{z}) \\
& 0 \le \mathbf{z} \le 1
\end{aligned}
$$

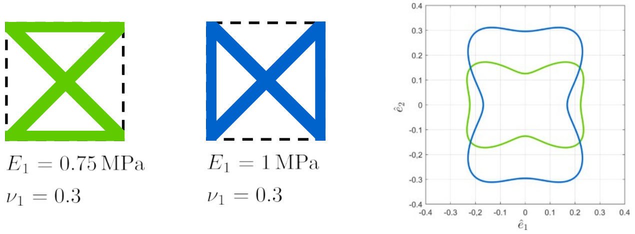


Plugin-based Q4Opt Framework

TOPOPT
p = [1 1.5 2 3 4]
γ = [0 0.2 0.5 0.8 1]
VolFrac = 0.3

ZPR
move = 0.2
eta = 1/2

FILTER
R = variable
q = linear order



R = 0.02

C = 201.459

R = 0.04

C = 221.367

R = 0.06

C = 240.008

R = 0.08

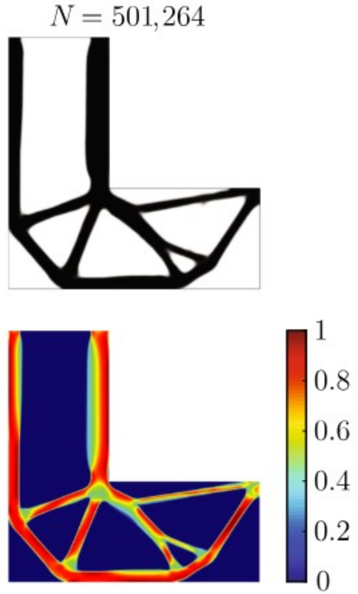
C = 268.923

R = 0.10

C = 286.017

CONCLUSION

- Versatile code for multi formulation in topology optimization;
- Implementation of an efficient filter with less computational resources (order);
- Reproduce large-scale simulation problems (without cluster)



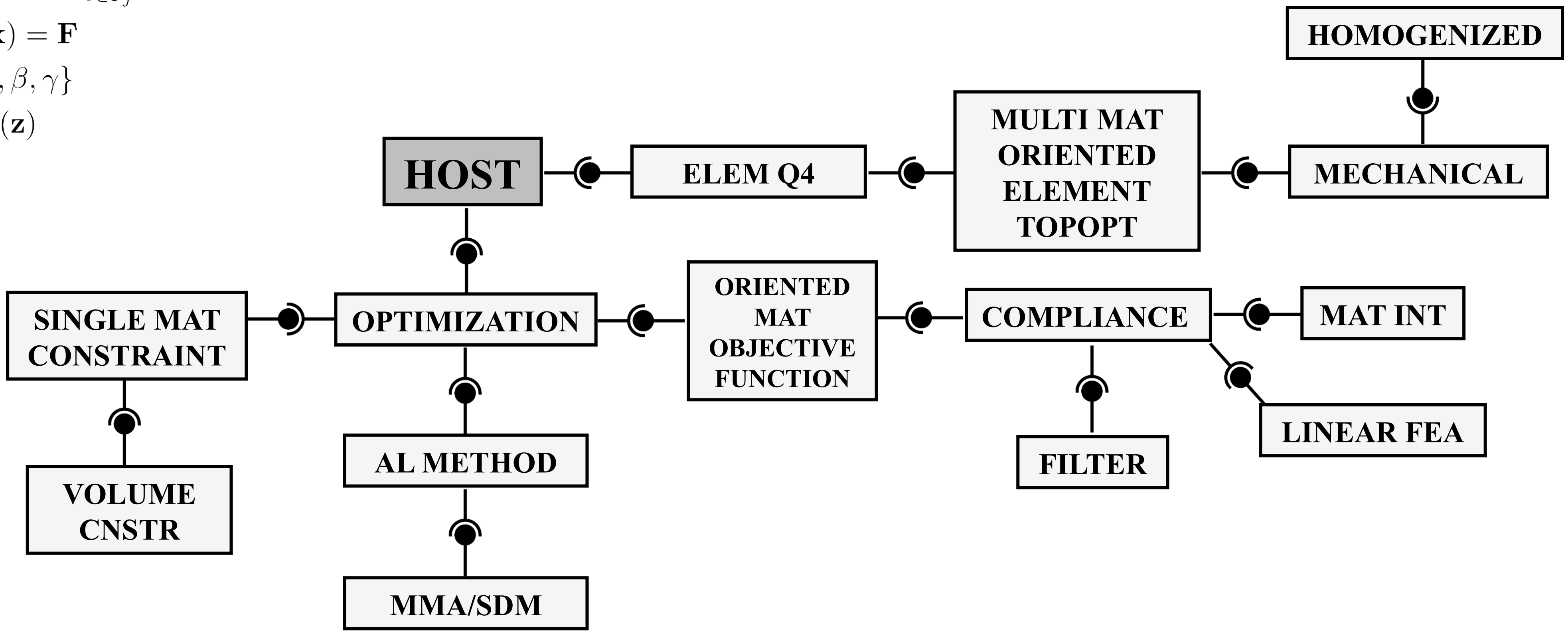
PolyStress

FUTURE WORK

- Study of efficiency with TopSim
- Material orientation
- Stress constraint

TOP-OPT COMPLIANCE-BASED VOLUME-CONSTRAINED MATERIAL-ORIENTED

$$
\begin{aligned}
\min_{\mathbf{x}} \quad & C = \mathbf{F}^T\,\mathbf{U}(\mathbf{x}) \\
\text{s.t.} \quad & g_j = \frac{\sum_{m\in\mathcal{G}_j}\sum_{\ell\in\mathcal{E}_j} V_\ell m_v(y_{\ell m})}{\sum_{\ell\in\mathcal{E}_j} V_\ell} - \overline{v}_j \leq 0,\ j = 1, \ldots N^c \\
\text{with} \quad & \mathbf{K}(\mathbf{x})\,\mathbf{U}(\mathbf{x}) = \mathbf{F} \\
& \mathbf{x} = \{\mathbf{z}, \alpha, \beta, \gamma\} \\
& \mathbf{y}(\mathbf{z}) = \mathcal{H}(\mathbf{z}) \\
& 0 \leq \mathbf{z} \leq 1
\end{aligned}
$$



Plugin-based Q4Opt Framework

TOP-OPT VOLUME MINIMIZATION STRESS-CONSTRAINED

$$\min_{\mathbf{z}} \quad V(\mathbf{z}) = \frac{1}{|\Omega|}\sum_{e=1}^{N^e} \tilde{y}_e ve$$

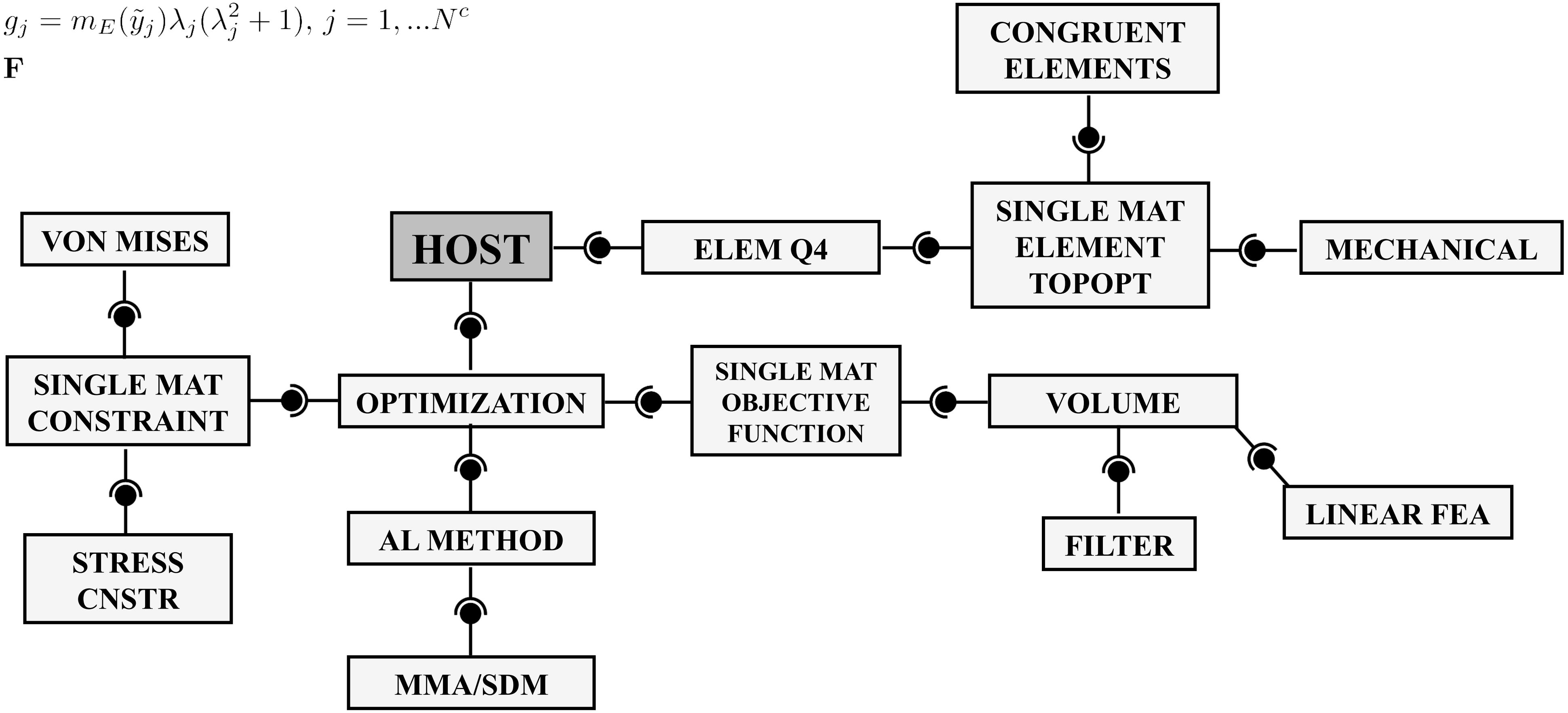
$$\text{s.t.} \quad g_j(\mathbf{z},\mathbf{u}) \leq 0,\ \ g_j = m_E(\tilde{y}_j)\lambda_j(\lambda_j^2+1),\ j = 1,\ldots N^c$$

$$\text{with} \quad \mathbf{K}(\mathbf{z})\,\mathbf{U}(\mathbf{z}) = \mathbf{F}$$

$$\lambda_j = \sigma_j^{eq} - 1$$

$$\tilde{\mathbf{y}}(\mathbf{z}) = \mathcal{H}(\mathbf{z})$$

$$0 \leq \mathbf{z} \leq 1$$



Plugin-based Q4Opt Framework

Thank you for your attention!

ALIS GRAVE NIL

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