Simple, accurate surrogate models of the elastic response of three-dimensional open truss micro-architectures with applications to multiscale topology design

TOP Webinar 7

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This presentation is based on three journal papers

- S. Watts *et al.* Simple, accurate surrogate models of the elastic response of three-dimensional open truss micro-architectures with applications to multiscale topology design. *SAMO* **60,** 1887–1920 (2019) DOI 10.1007/s00158-019-02297-5
- S. Watts *et al.* Correction to: Simple, accurate surrogate models of the elastic response of three-dimensional open truss micro-architectures with applications to multiscale topology design. *SAMO* **61**, 1759–1762 (2020) DOI 10.1007/s00158-019-02425-1
- S. Watts. Elastic response of hollow truss lattice micro-architectures. *IJSS* **206**, 472–564 (2020) DOI 10.1016/j.ijsolstr.2020.08.018

We focus on the first paper; the other two correct and extend these results.

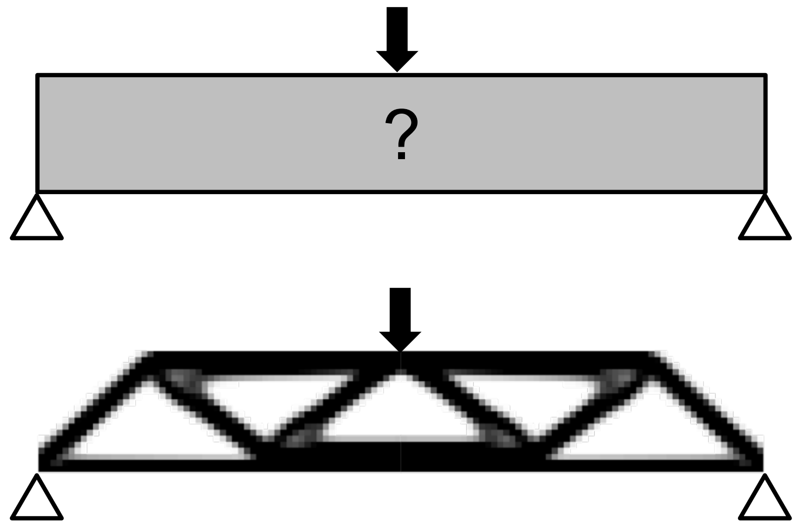
Topology optimization can be thought of as material design

- We are choosing constitutive response throughout the domain
- Traditional density and level set parameterizations obtain 0/1 designs that we can interpret as something we can fabricate

$$\min_{\underline{\rho}} \int_\Omega \left\langle \nabla \underline{u}, \mathbb{C}\left(\underline{\rho}\right) \nabla \underline{u} \right\rangle dv$$

$$\frac{1}{|\Omega|} \int_\Omega \underline{\rho}\, dv \leq \vartheta$$

$$\begin{aligned} \operatorname{div}\left(\mathbb{C}\left(\underline{\rho}\right)\left[\nabla \underline{u}\right]\right) &= -\underline{b} \quad \text{on } \Omega \\ \underline{u} &= \underline{0} \quad \text{on } \partial\Omega_e \\ \left(\mathbb{C}\left(\underline{\rho}\right)\left[\nabla \underline{u}\right]\right) \cdot \underline{n} &= \underline{t} \quad \text{on } \partial\Omega_n \end{aligned}$$



O. Sigmund. *SAMO* ***21*** (2001)

Additive manufacturing has greatly expanded the feasibility of fabricating optimized designs.

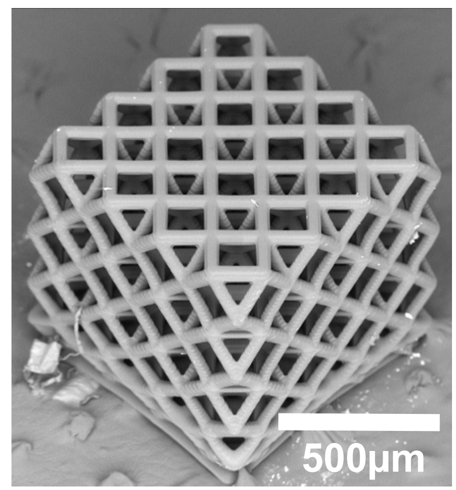
Advances in additive manufacturing enable micro-architected materials with variable density

- We'd like to be able to design an optimal microstructure
- Macroscale design can use homogenized response of microscale
- Intermediate macro-densities are no longer problematic
- FE^2 approaches have general design space but extremely high cost

$$\operatorname{div}\left(\mathbb{C}^h\left(\underline{\rho}\right)\left[\nabla \underline{u}\right]\right) = -\underline{b}^h \quad \text{on } \Omega_c$$

$$\mathbb{C}^h = \sum_{ij} \frac{1}{\left|\Omega_f\right|} \int_{\Omega_f} \mathbb{C}\left(\mathbb{I} + \nabla\chi^{ij} \otimes E_{ij}\right) dv$$

$$\operatorname{div} \mathbb{C}\left[\chi^{ij}\right] = -\operatorname{div} \mathbb{C}\left[E_{ij}\right] \text{ on } \Omega_f, \chi^{ij} \text{ periodic}$$

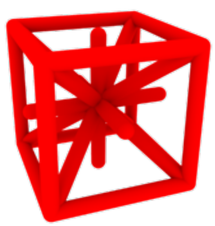


W. Chen et al.
Sci Adv ***5*** (2019)

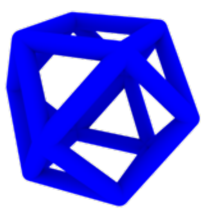
Surrogate model replaces *assumed* interpolated material properties with *realizable* ones.

Restricting the micro-architecture to a low-dimensional design space has several benefits

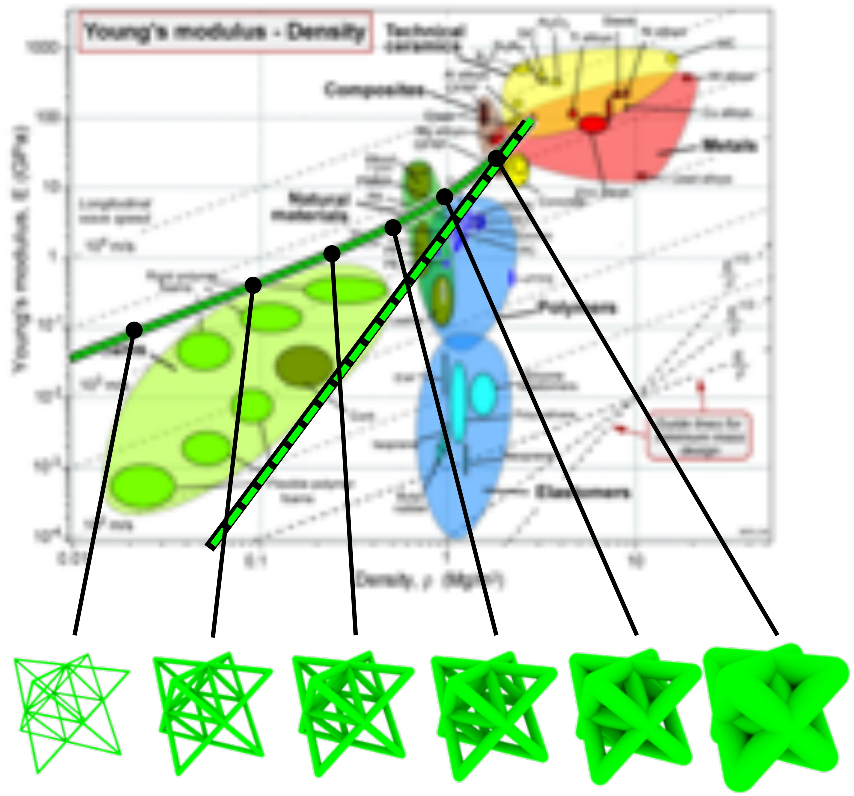
- Enables *pre-computation* of response and surrogate *modeling*
- Well-matched to using “known printable” micro-architectures
- Ensures long-range continuity of the lattice *a priori*



Isotruss



ORC truss



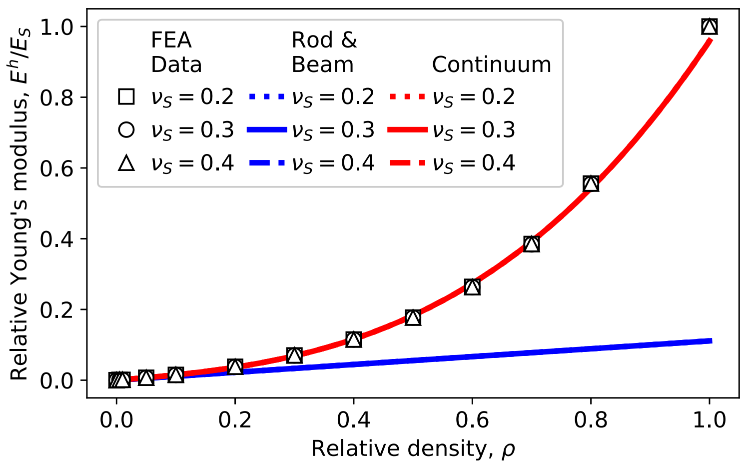
Octet truss

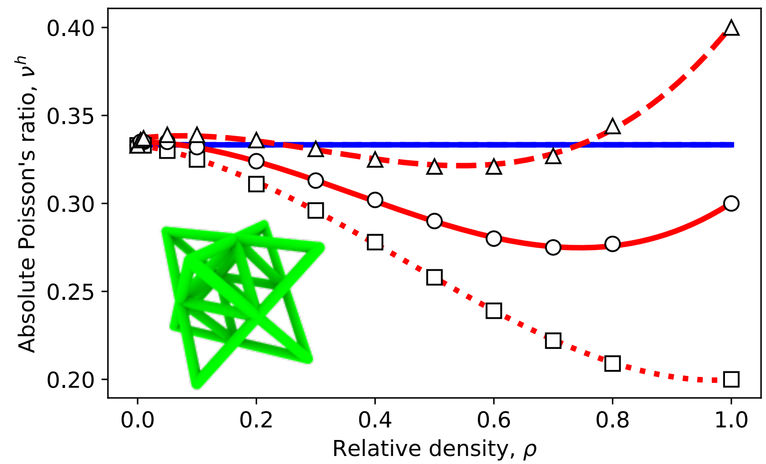
Surrogate model design approaches trade *generality* of design for *speed* of solution.

Existing surrogate models can be inaccurate for large regions of the design space

- Models using rod and beam theory have simple analytical forms that are easy to implement
- These models are accurate at low densities, but become less so as the density increases

$$C_{11}^h = \frac{\rho}{6} \qquad C_{12}^h = \frac{\rho}{12} \qquad C_{44}^h = \frac{\rho}{12}$$

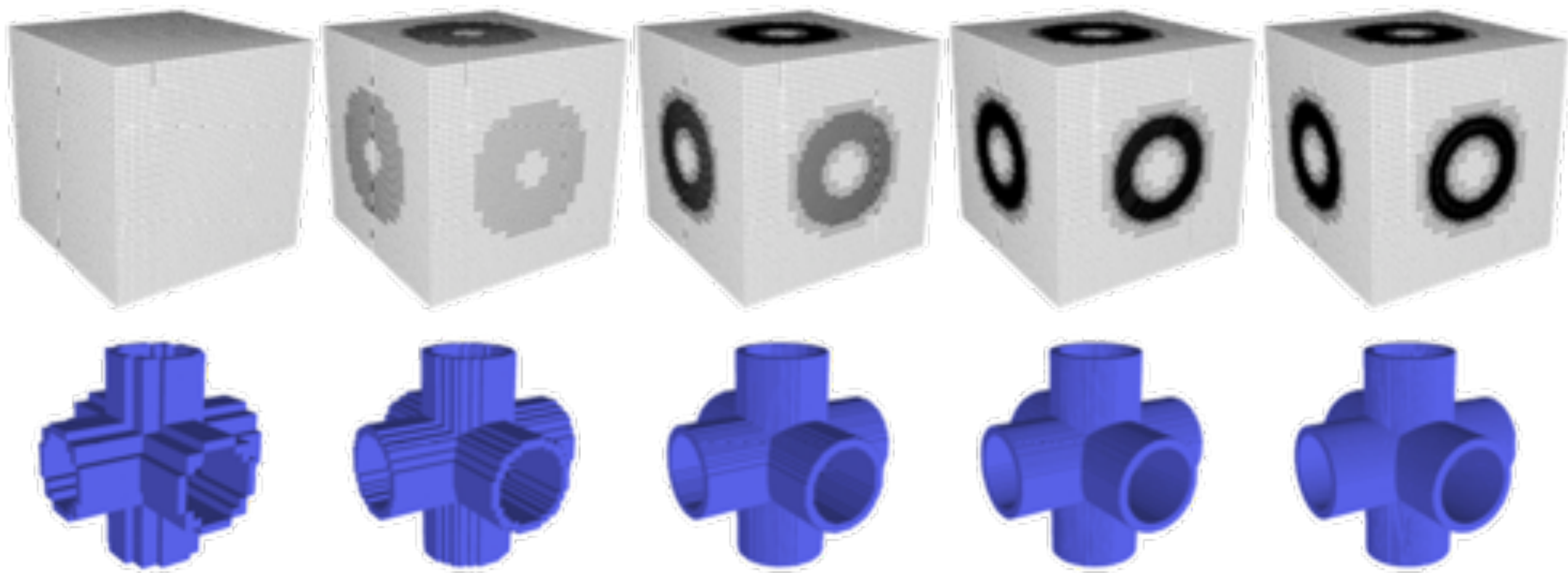




Goal: *create more accurate surrogate models that are (almost) as simple as existing ones.*

Our approach is to first sample the design space…

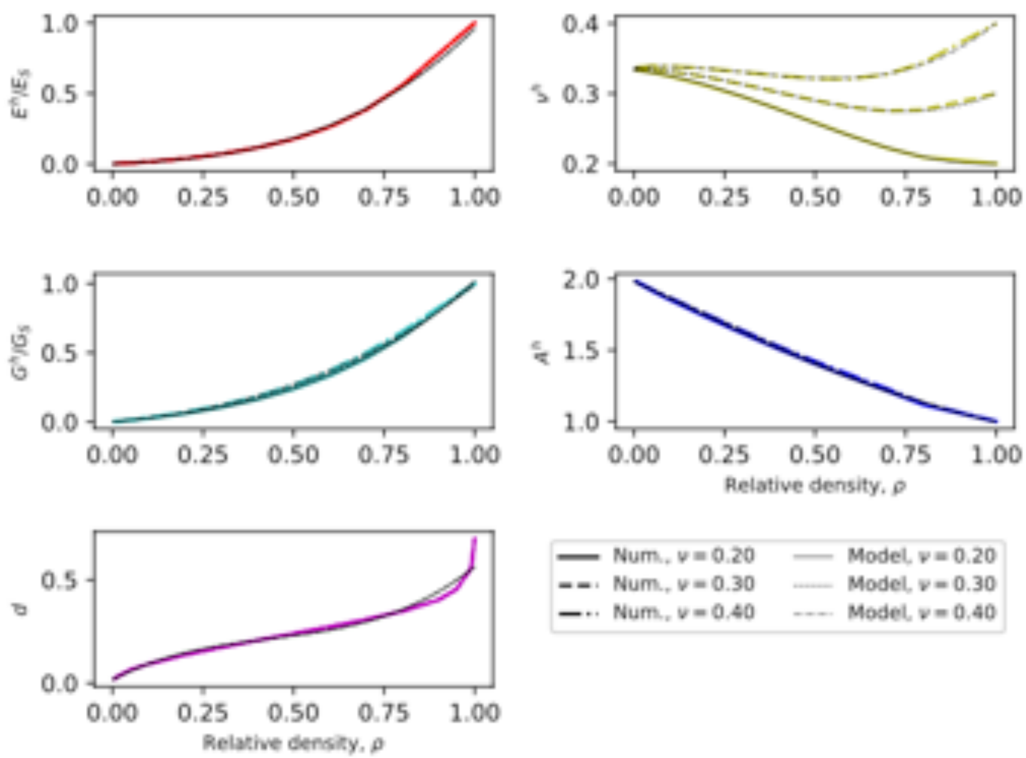
- Relative densities 0.5% to 90%, Poisson's ratio 0.2, 0.3, 0.4
- Ersatz field recursively projected and adaptively refined
- Solve cell problems and extract homogenized properties in parallel

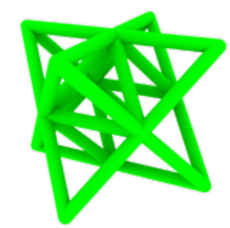


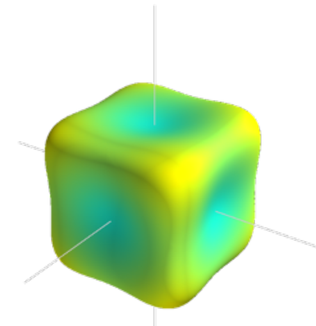
Homogenized elasticity tensor components converged to within 1% over final refinement.

… then to fit simple surrogate models to the data

- Low-dimensional polynomial basis chosen for simplicity and to avoid overfitting
- Linear least squares to minimize *relative* model error







$$\frac{E^h}{E_s} = (0.13627 - 0.01222\, \nu_s)\, \rho + (0.08580 + 0.06637\, \nu_s)\, \rho^2 + (0.73989 - 0.06261\, \nu_s)\, \rho^3$$

$$\nu^h = (0.32953 + 0.01860\, \nu_s) - (0.14216 - 0.45781\, \nu_s)\, \rho - (0.32984 + 0.05598\, \nu_s)\, \rho^2 + (0.14123 + 0.47270\, \nu_s)\, \rho^3$$

Across all model fits, $R^2 > 0.95$. Modeled responses are generally accurate to within ~5%.

The paper contains all the sample data if you want to create a different model

- Splines, linear interpolants, different bases…

Appendix 2. Tabulated data for octet truss

Constituent Poisson's ratio ν_S	Relative density ρ	Rod diameter d	Relative Young's modulus E^h/E_S	Poisson's ratio ν^h	Relative shear modulus G^h/G_S	Zener ratio A^h
0.2	0.005	0.01960	0.001	0.333	0.001	1.981
	0.010	0.02786	0.001	0.333	0.002	1.972
	0.050	0.06430	0.007	0.330	0.012	1.915
	0.100	0.09308	0.015	0.325	0.026	1.851
	0.200	0.13673	0.038	0.311	0.060	1.731
	0.300	0.17331	0.070	0.296	0.105	1.616
	0.400	0.20709	0.115	0.278	0.163	1.506
	0.500	0.23978	0.177	0.258	0.237	1.403
	0.600	0.27292	0.264	0.239	0.334	1.306
	0.700	0.30805	0.385	0.222	0.458	1.212
	0.800	0.34804	0.556	0.209	0.616	1.115
	1.000	0.70000	1.000	0.200	1.000	1.000
0.3	0.005	0.01960	0.001	0.335	0.001	1.983
	0.010	0.02786	0.001	0.335	0.002	1.975

Across all model fits, R^2 values were never below 0.95, and the average value was >0.99.

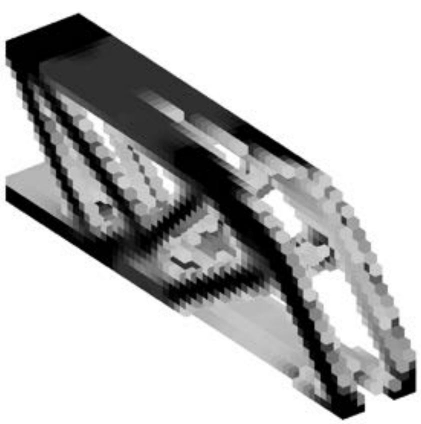
These models can be used in topology optimization codes for multiscale TO design

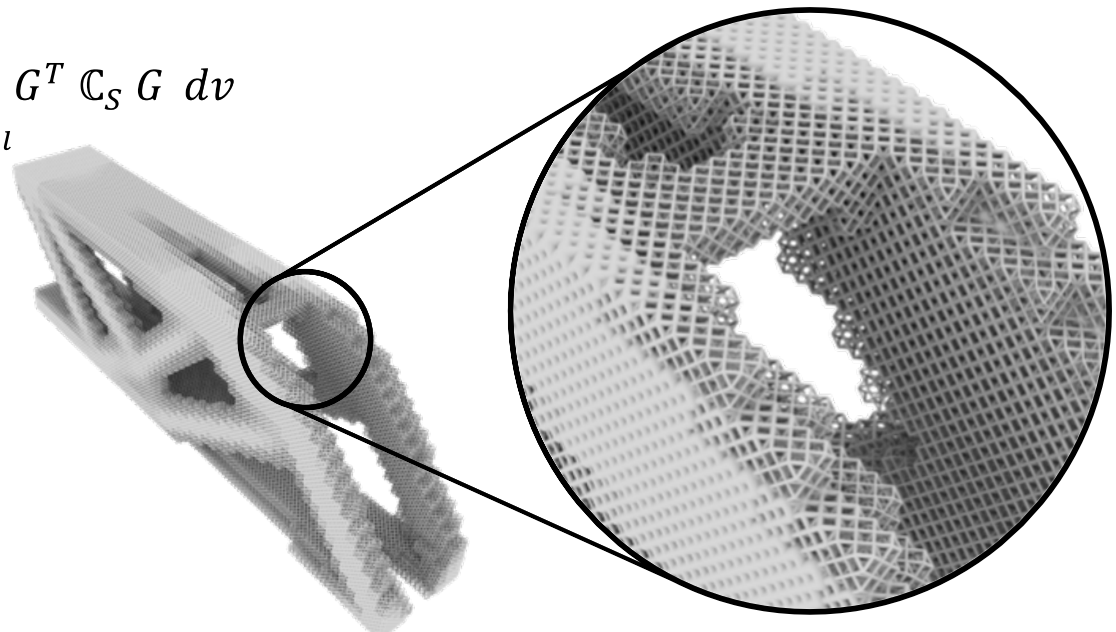
- Paper modifies the 99-line code to use surrogate models
- Lattices can be recovered from the macro density solution

$$K_{el} = \int_{\Omega_{el}} G^T \mathbb{C}^h(\rho)\, G \; dv$$

$$K_{el} = \int_{\Omega_{el}} G^T \mathbb{C}^h \left(E^h(\rho), \nu^h(\rho), G^h(\rho) \right) G \; dv$$

$$K_{el} = \rho^p \int_{\Omega_{el}} G^T \, \mathbb{C}_S \, G \; dv$$





On a Cartesian design mesh, recovery of the lattice is trivial given the unit cell definition.

Inclusion of a micro-architecture *can* but does not *guarantee* improvement of the design

- In the paper we show improvements in compliance up to 10%
- Simply including a micro-geometry does not improve compliance, and can in fact make it substantially worse, depending on problem specifics
- Truss lattice micro-architectures are generally anisotropic
  - Orientation of the lattice to the design should be considered
  - Different unit cell designs can perform better than others
- Enlarging the design space can improve performance
  - Hollow tubes decouple density, stiffness, and isotropy
  - Independent rod/tube diameters will break symmetry and should improve performance in engineering components

There are always tradeoffs in *generality* and *cost* of the model and the resulting *performance*.

Multiscale design with surrogate models…

- … relieves the need to ensure convergence to a 0/1 design
- … can ensure by construction the continuity of a design and (at least to first order) its manufacturability
- … has comparable cost to single-scale design (once models are available)
- … has demonstrated modest performance improvements with additional potential given more sophisticated models
- … can be applied to other physics (thermal, fluids, etc.)

Thanks for your attention! I am happy to answer questions now or by email: watts24@llnl.gov

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