Solving stochastic, fractional PDEs with MFEM with applications to random field generation and topology optimization

MFEM community workshop 2022

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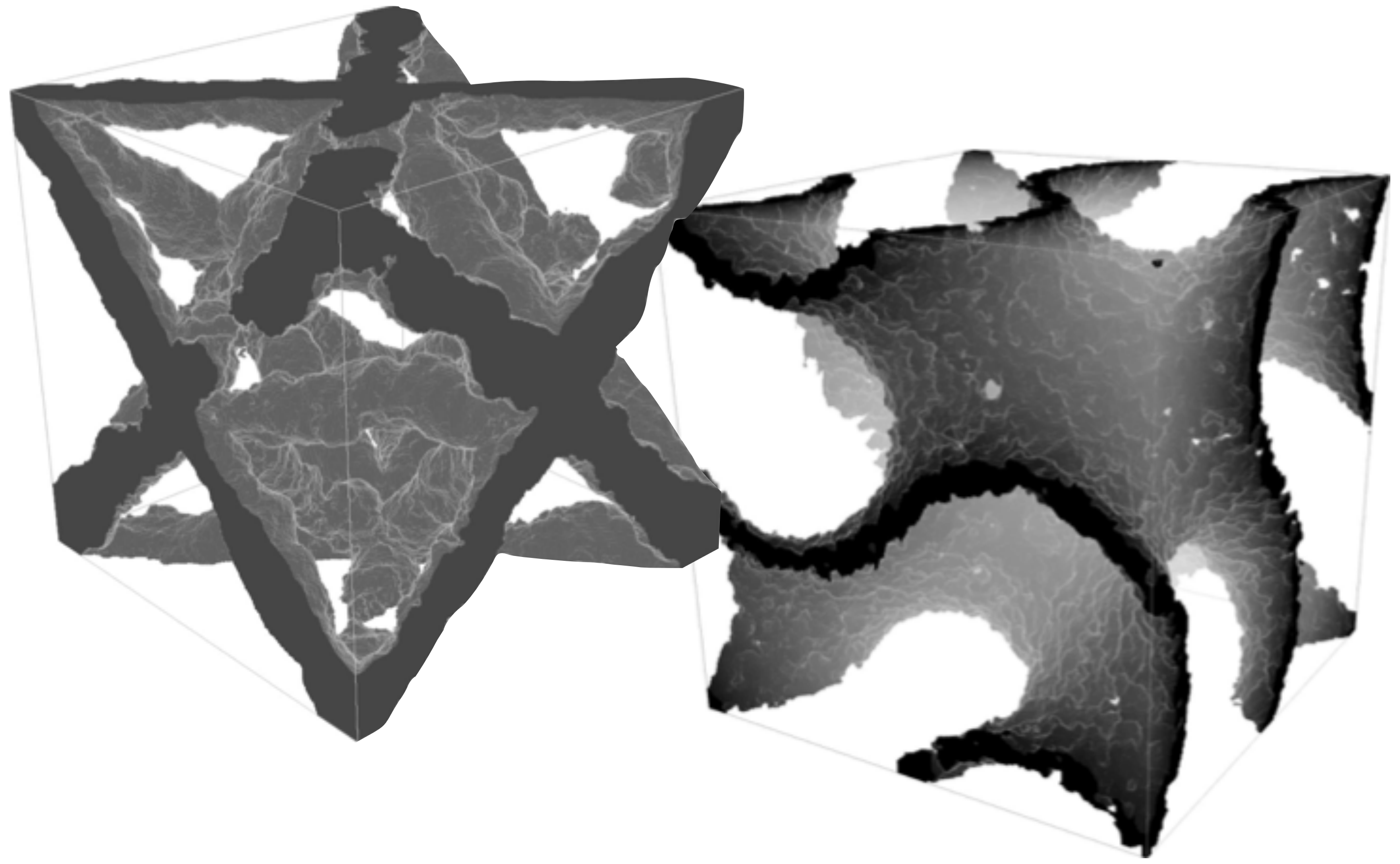
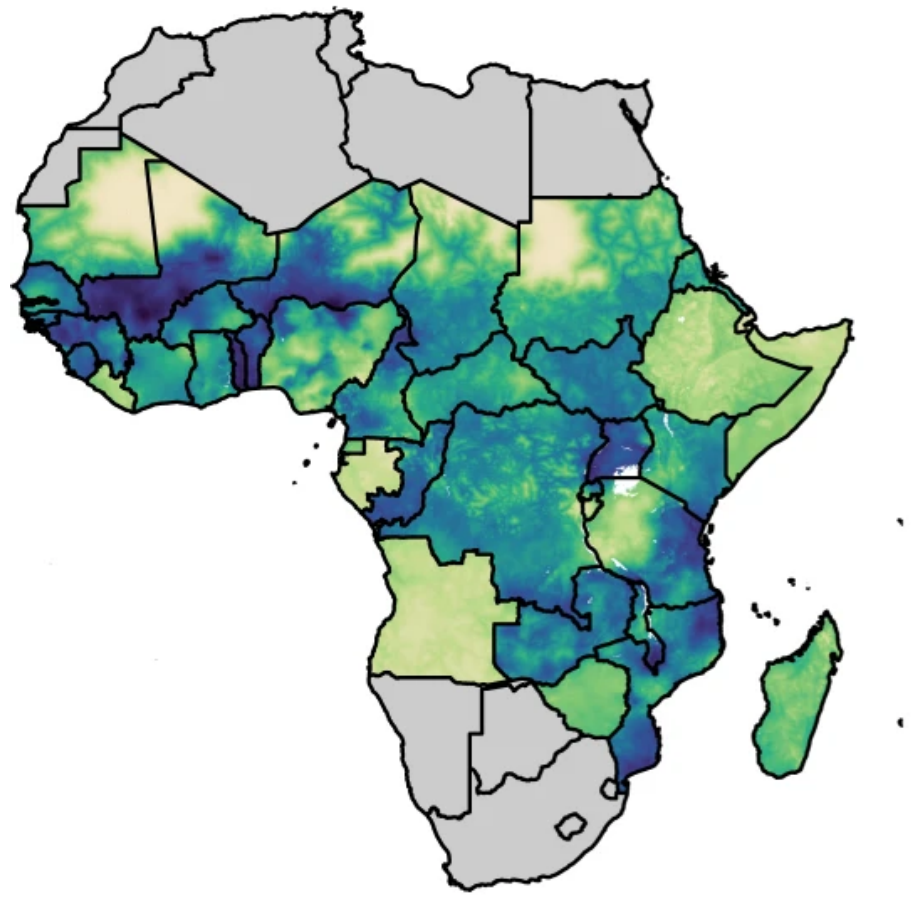
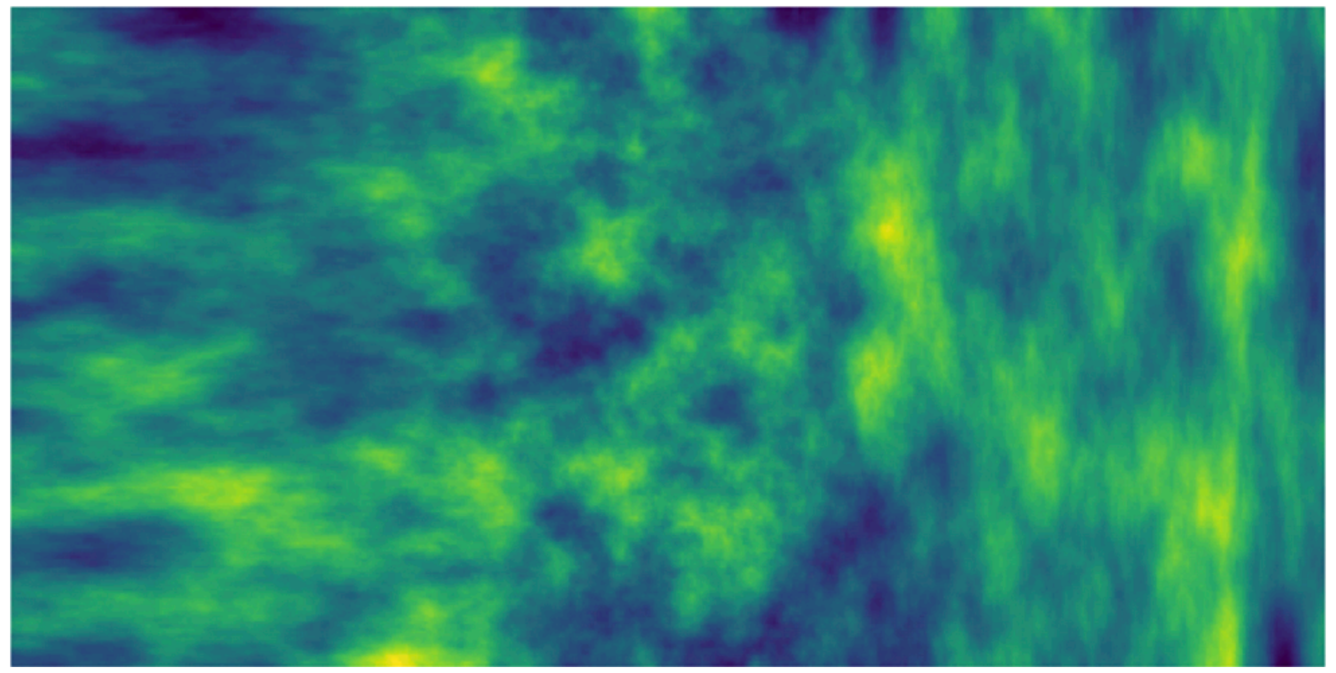
Random fields



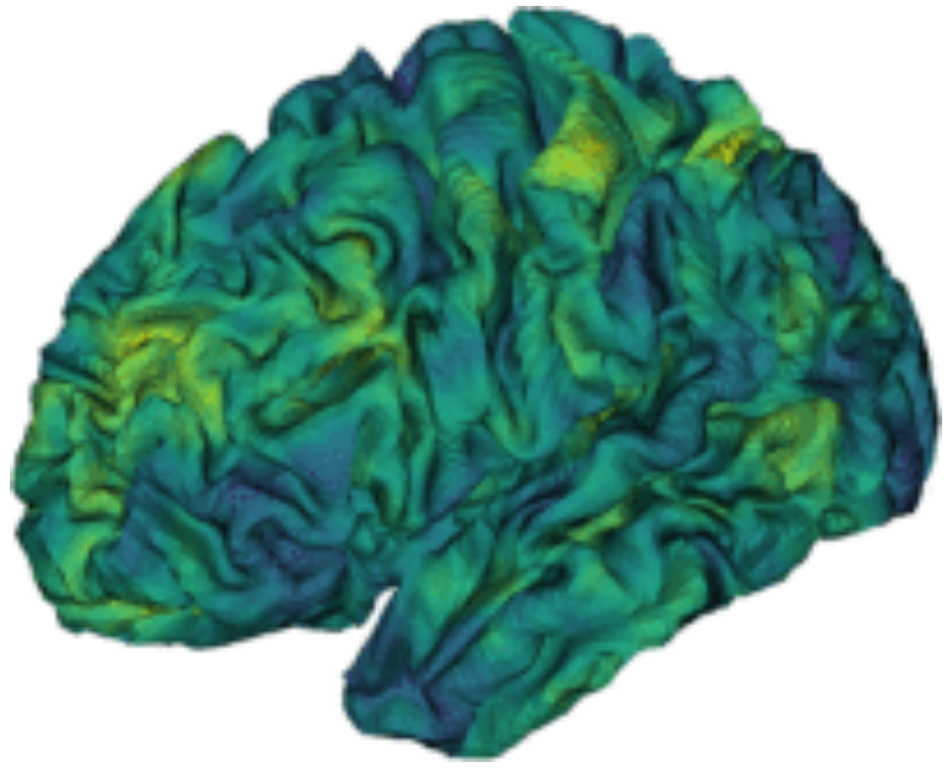
Khristenko, U., Constantinescu, A., Tallec, P. le, & Wohlmuth, B. (2021). *Statistically equivalent surrogate material models and the impact of random imperfections on elasto-plastic response*.



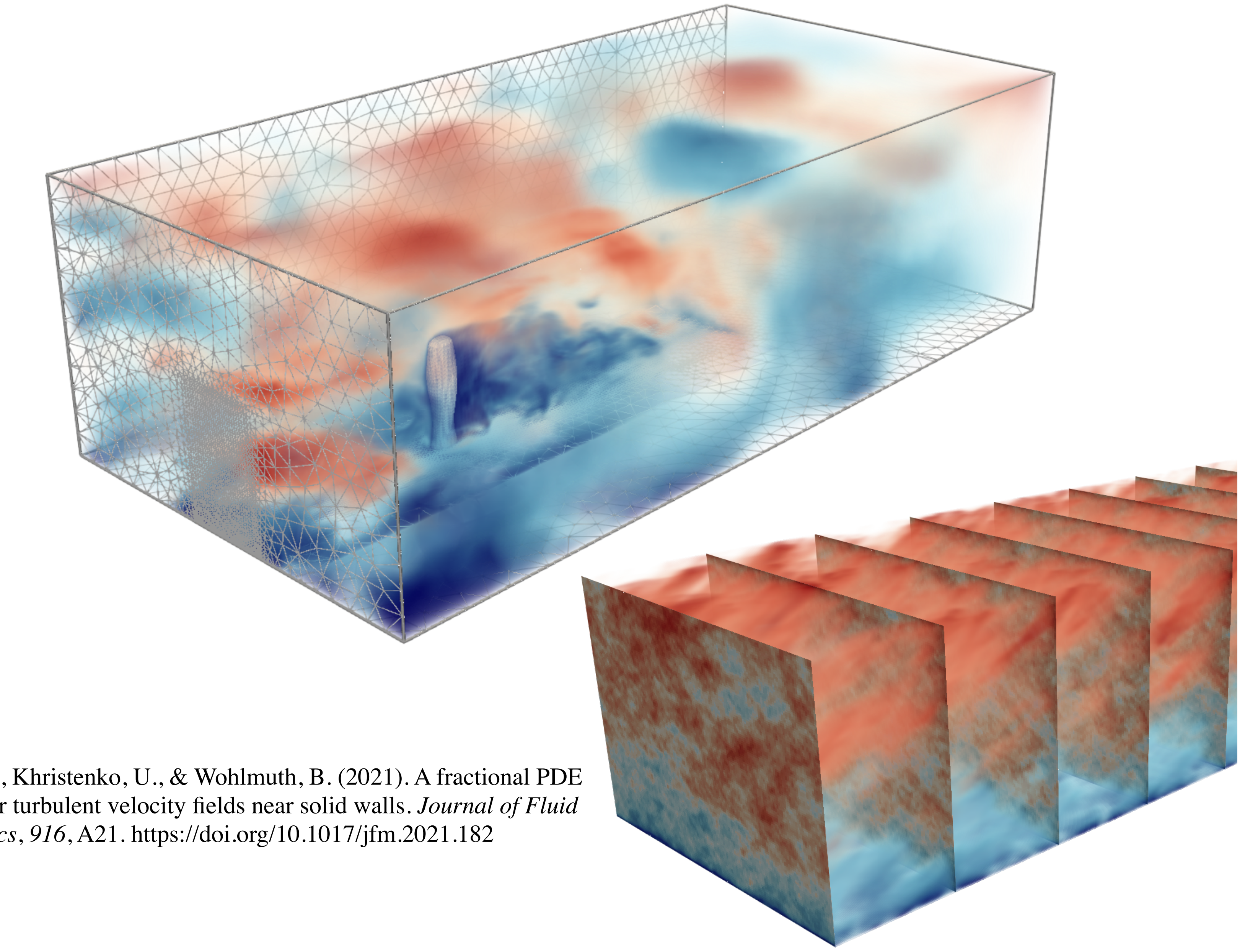
Bertozzi-Villa et. al (2021). Maps and metrics of insecticide-treated net access, use, and nets-per-capita in Africa from 2000-2020. *Nature Communications*, *12*(1), 3589. https://doi.org/10.1038/s41467-021-23707-7



Bakka, H., Rue, H., Fuglstad, G., Riebler, A., Bolin, D., Illian, J., Krainski, E., Simpson, D., & Lindgren, F. (2018). Spatial modeling with R-INLA: A review. *WIREs Computational Statistics*, *10*(6). https://doi.org/10.1002/wics.1443



Lindgren, F., Bolin, D., & Rue, H. (2022). The SPDE approach for Gaussian and non-Gaussian fields: 10 years and still running. *Spatial Statistics*, *50*, 100599. https://doi.org/10.1016/j.spasta.2022.100599



Keith, B., Khristenko, U., & Wohlmuth, B. (2021). A fractional PDE model for turbulent velocity fields near solid walls. *Journal of Fluid Mechanics*, *916*, A21. https://doi.org/10.1017/jfm.2021.182

Agenda

25th October, 2022

(I) Random fields
(II) Fractional PDEs and how to treat them
(III) Stochastic PDEs and how to treat white noise with FE / MFEM
(IV) The SPDE method for random field generation
(V) Application: topology optimization under uncertainty

What is the fractional Laplacian?

Fractional PDEs

Example

$$-\Delta^{\alpha/2} u = 1$$
$$\alpha \in [0,2]$$
$$u(x) = 0 \ \forall x \in \partial\Omega$$

Definition

We follow the *spectral definition* of the fractional laplacian. For regular Laplacian:

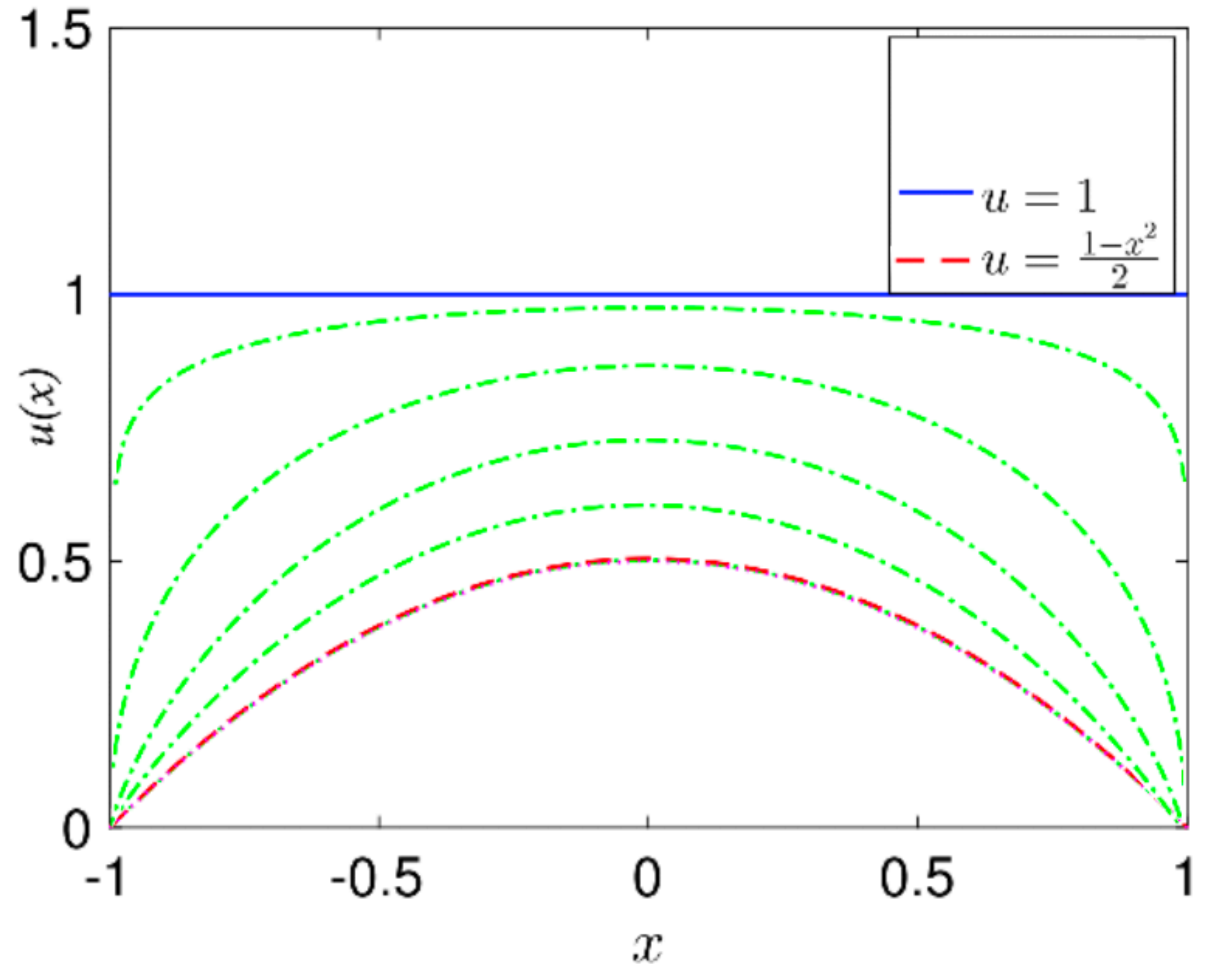
$$-\Delta e_k = \lambda_k e_k \qquad e_k(x) = 0 \, \forall x \in \partial\Omega$$

$$\Rightarrow -\Delta u(x) = \sum_k \lambda_k (u, e_k)_{L^2_\Omega} e_k$$

For fractional Laplacian:

$$\Rightarrow -\Delta^{\alpha/2} u(x) = \sum_k \lambda_k^{\alpha/2} (u, e_k)_{L^2_\Omega} e_k$$

Intuition

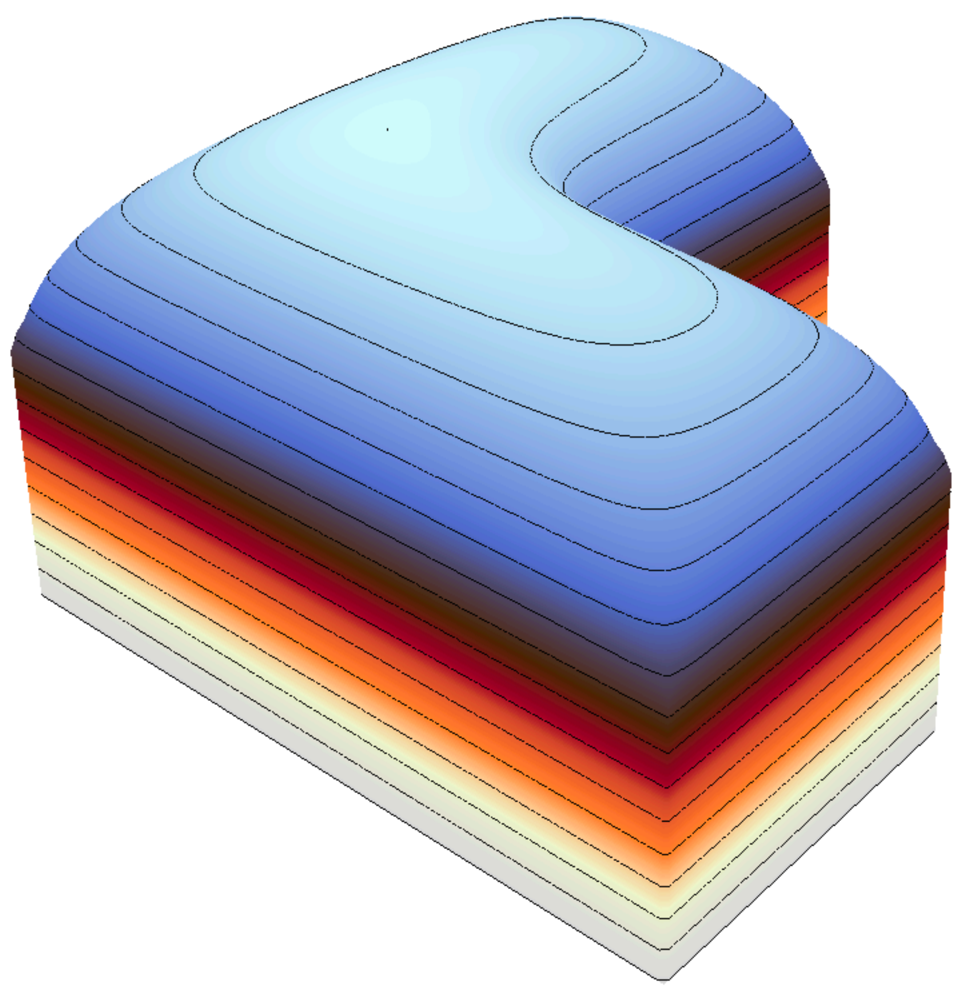


Solution for different fractional exponents.
Blue: $\alpha = 0$
Green (top to bottom): $\alpha \in \{0.1, 0.5, 1.0, 1.5\}$
Red: $\alpha = 2$

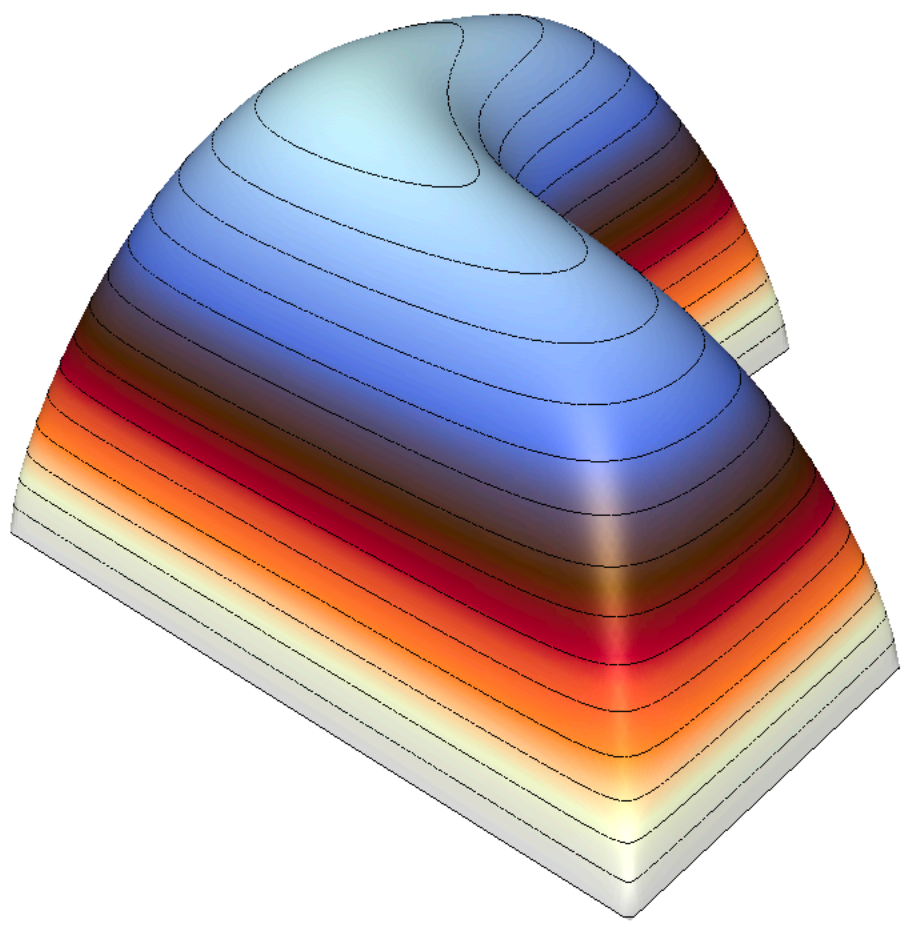
Lischke, A., Pang, G., Gulian, M., Song, F., Glusa, C., Zheng, X., Mao, Z., Cai, W., Meerschaert, M. M., Ainsworth, M., & Karniadakis, G. E. (2020). What is the fractional Laplacian? A comparative review with new results. *Journal of Computational Physics*, *404*, 109009. https://doi.org/10.1016/j.jcp.2019.109009

The fractional Laplacian with MFEM

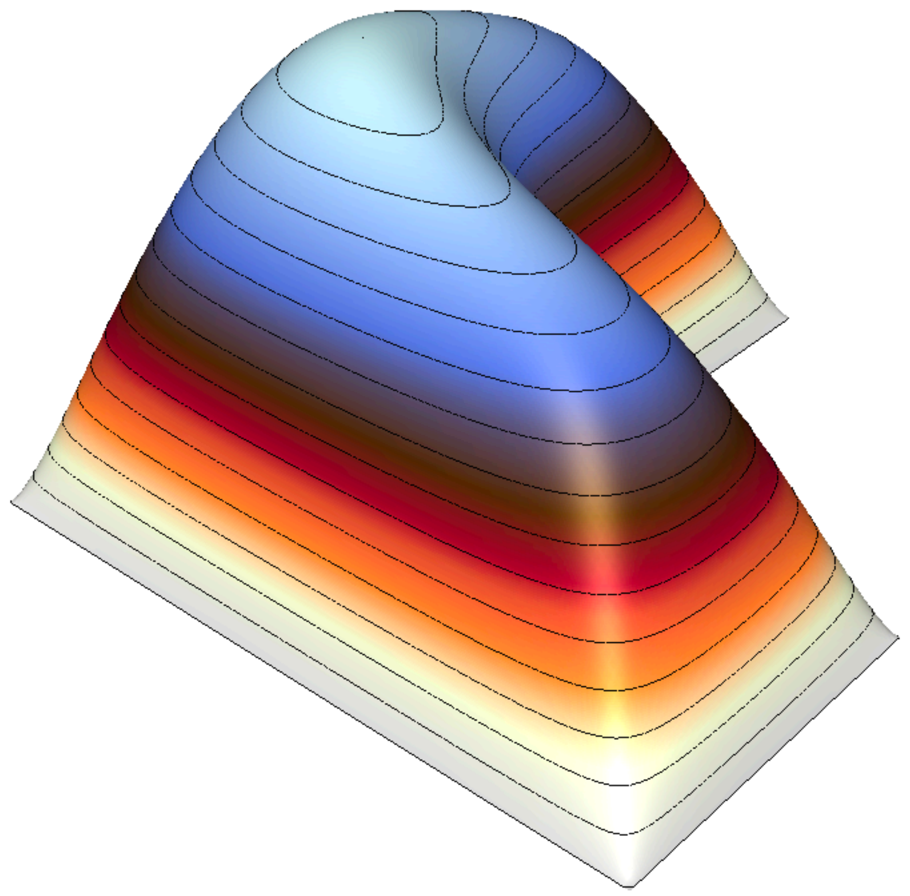
examples/ex33p



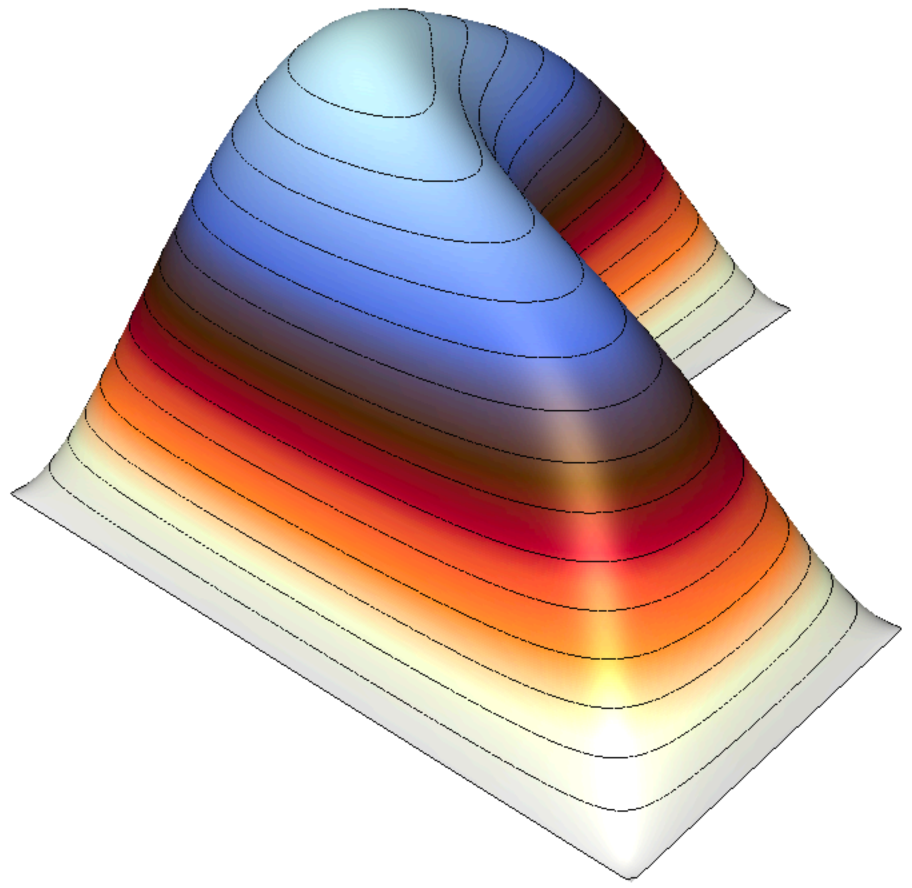
$\alpha = 0.2$



$\alpha = 0.8$



$\alpha = 1.4$



$\alpha = 2.0$

```
make ex33p && mpirun -np 4 ex33p -m ../data/l-shape.mesh -alpha <your-alpha/2.0> -o 3 -r 5
```

Rational approximation

.. via the AAA algorithm

$$-\Delta^{\alpha} u = b \quad \Rightarrow \quad u = -\Delta^{-\alpha} b$$

$$x^{-\alpha} \approx \sum_{k=1}^{N} \frac{c_k}{\left(x - p_k\right)} \quad \Leftrightarrow \quad (-\Delta)^{-\alpha} \approx \sum_{k=1}^{N} c_k \left((-\Delta) - p_k\right)^{-1}$$

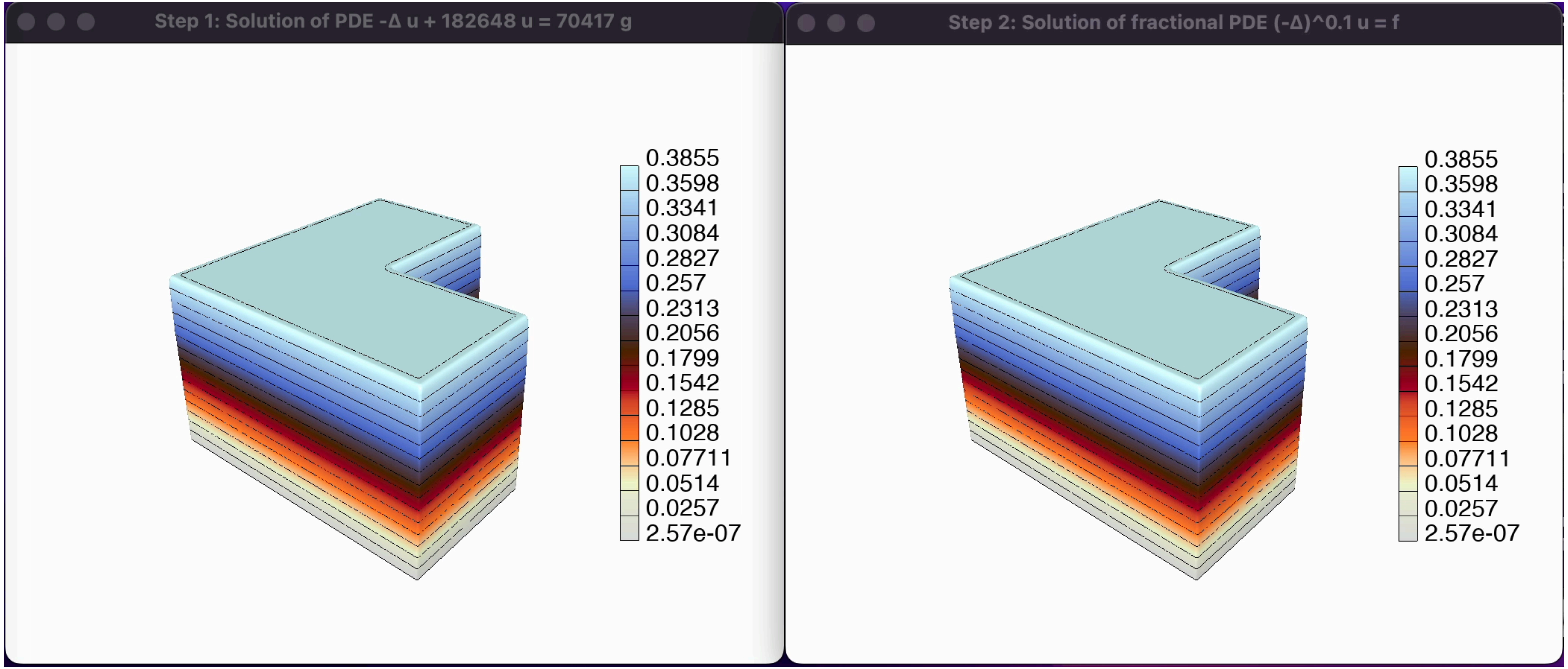
$$u = \sum_{k=1}^{N} u_k \quad \text{with} \quad ((-\Delta) - p_k) u_k = c_k b$$

- Apply a *rational approximation* to the inverse of the operator
- Equivalence holds due to central results of the *spectral theory* for normal operators
- Ultimately, we solve N independent *reactio-diffusion equations* and sum them up

Harizanov, S., Lazarov, R., Margenov, S., Marinov, P., & Vutov, Y. (2018). Optimal solvers for linear systems with fractional powers of sparse SPD matrices. *Numerical Linear Algebra with Applications*, *25*(5), e2167. https://doi.org/10.1002/nla.2167
Nakatsukasa, Y., Sète, O., & Trefethen, L. N. (2018). The AAA Algorithm for Rational Approximation. *SIAM Journal on Scientific Computing*, *40*(3), A1494–A1522. https://doi.org/10.1137/16M1106122

The fractional Laplacian with MFEM

examples/ex33p




```
make ex33p && mpirun -np 4 ex33p -m ../data/l-shape.mesh -alpha 0.1 -o 3 -r 5
```

What are stochastic PDEs?

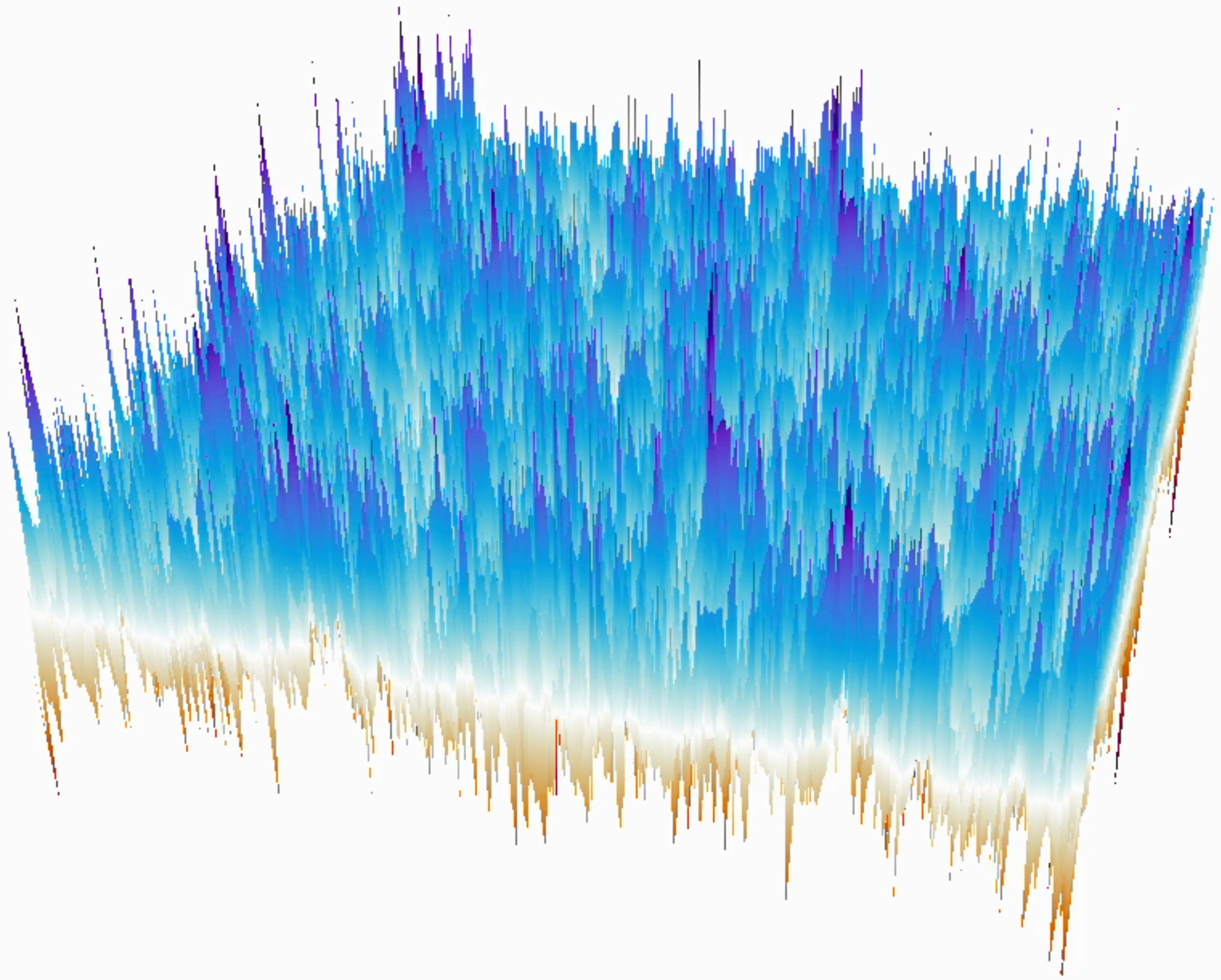
Some examples

I. Stochastic Coefficients

$$\left(\frac{\partial}{\partial t} - \nabla \cdot D(\omega)\nabla\right)u = f$$

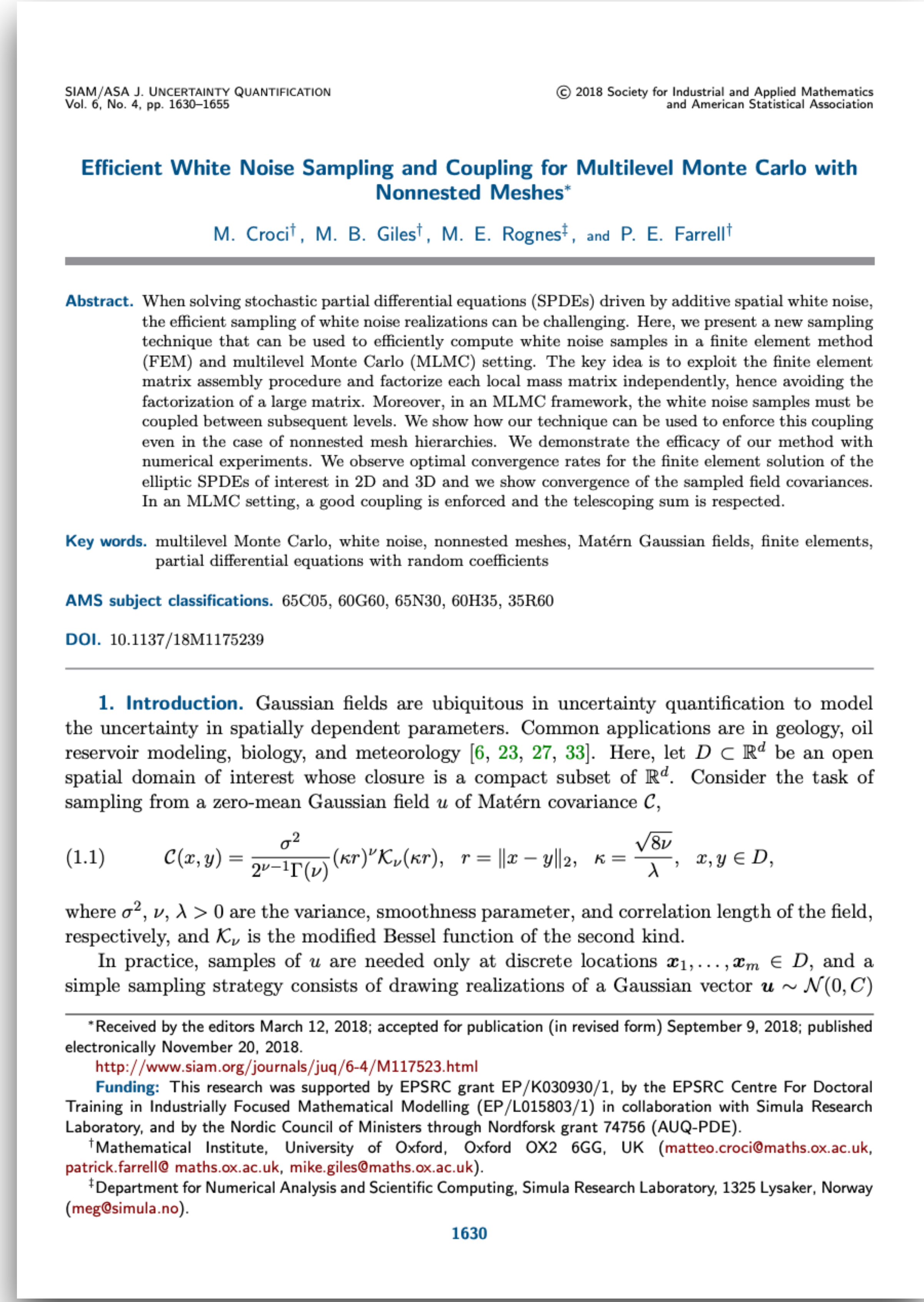
II. Stochastic Load

$$\left(\frac{\partial}{\partial t} - \nabla \cdot D\nabla\right)u = W(\omega)$$



White noise in MFEM

WhiteNoiseIntegrator



SIAM/ASA J. UNCERTAINTY QUANTIFICATION
Vol. 6, No. 4, pp. 1630–1655

Efficient White Noise Sampling and Coupling for Multilevel Monte Carlo with Nonnested Meshes*

M. Croci[†], M. B. Giles[†], M. E. Rognes[‡], and P. E. Farrell[†]

Abstract. When solving stochastic partial differential equations (SPDEs) driven by additive spatial white noise, the efficient sampling of white noise realizations can be challenging. Here, we present a new sampling technique that can be used to efficiently compute white noise samples in a finite element method (FEM) and multilevel Monte Carlo (MLMC) setting. The key idea is to exploit the finite element matrix assembly procedure and factorize each local mass matrix independently, hence avoiding the factorization of a large matrix. Moreover, in an MLMC framework, the white noise samples must be coupled between subsequent levels. We show how our technique can be used to enforce this coupling even in the case of nonnested mesh hierarchies. We demonstrate the efficacy of our method with numerical experiments. We observe optimal convergence rates for the finite element solution of the elliptic SPDEs of interest in 2D and 3D and we show convergence of the sampled field covariances. In an MLMC setting, a good coupling is enforced and the telescoping sum is respected.

Key words. multilevel Monte Carlo, white noise, nonnested meshes, Matérn Gaussian fields, finite elements, partial differential equations with random coefficients

AMS subject classifications. 65C05, 60G60, 65N30, 60H35, 35R60

DOI. 10.1137/18M1175239

1. Introduction. Gaussian fields are ubiquitous in uncertainty quantification to model the uncertainty in spatially dependent parameters. Common applications are in geology, oil reservoir modeling, biology, and meteorology [6, 23, 27, 33]. Here, let $D \subset \mathbb{R}^d$ be an open spatial domain of interest whose closure is a compact subset of $\mathbb{R}^d$. Consider the task of sampling from a zero-mean Gaussian field u of Matérn covariance $\mathcal{C}$,

$$\mathcal{C}(x,y) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(\kappa r)^\nu \mathcal{K}_\nu(\kappa r), \quad r = \|x-y\|_2, \quad \kappa = \frac{\sqrt{8\nu}}{\lambda}, \quad x,y \in D, \tag{1.1}$$

where $\sigma^2, \nu, \lambda > 0$ are the variance, smoothness parameter, and correlation length of the field, respectively, and $\mathcal{K}_\nu$ is the modified Bessel function of the second kind.

In practice, samples of u are needed only at discrete locations $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in D$, and a simple sampling strategy consists of drawing realizations of a Gaussian vector $\boldsymbol{u} \sim \mathcal{N}(0, C)$

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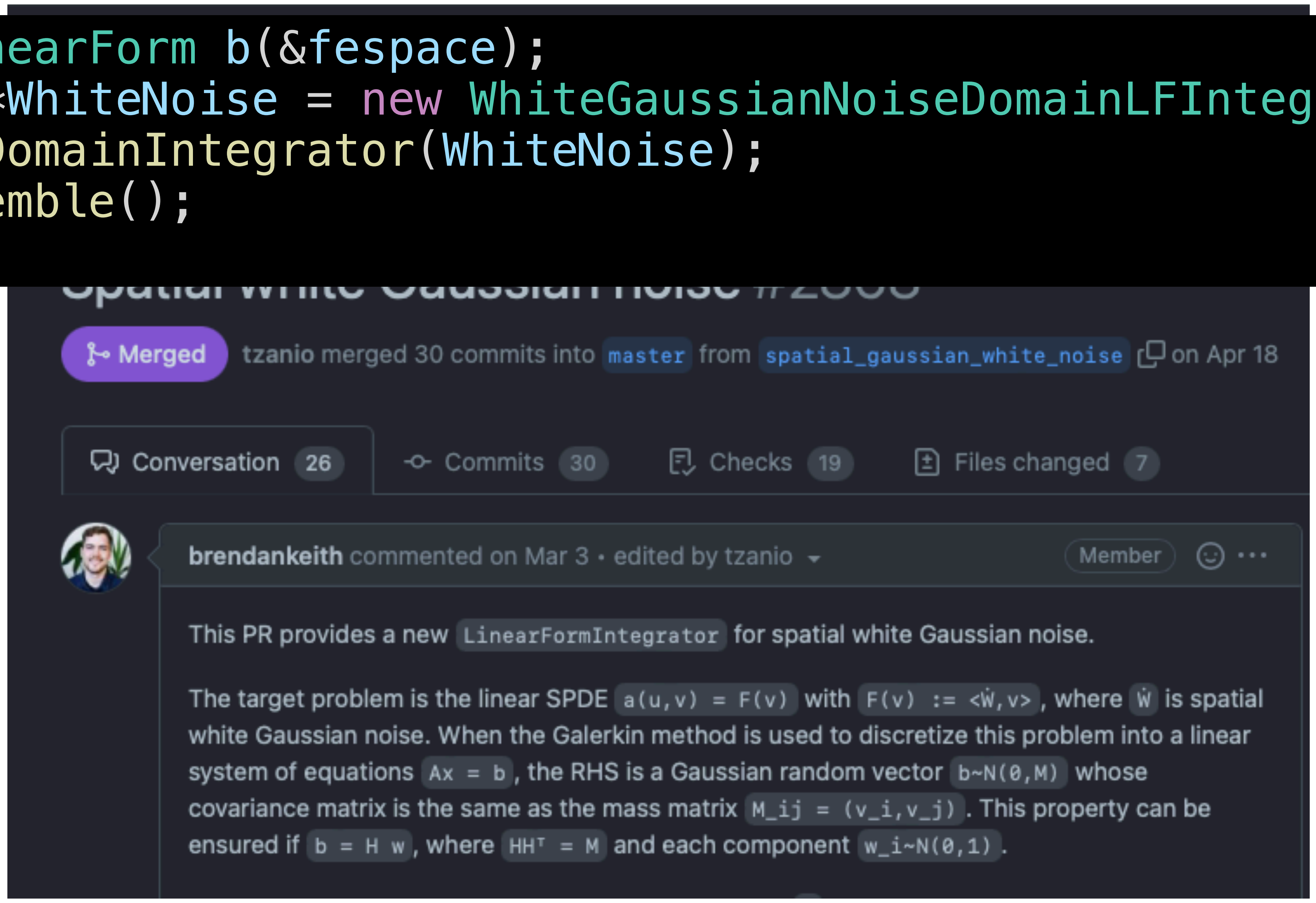
[‡]Department for Numerical Analysis and Scientific Computing, Simula Research Laboratory, 1325 Lysaker, Norway (meg@simula.no).

Croci, M., Giles, M. B., Rognes, M. E., & Farrell, P. E. (2018). Efficient White Noise Sampling and Coupling for Multilevel Monte Carlo with Nonnested Meshes. *SIAM/ASA Journal on Uncertainty Quantification*, *6*(4), 1630–1655. https://doi.org/10.1137/18M1175239

How to apply a stochastic load with MFEM?

```
ParLinearForm b(&fespace);
auto *WhiteNoise = new WhiteGaussianNoiseDomainLFIntegrator(seed);
b.AddDomainIntegrator(WhiteNoise);
b.Assemble();
```



The SPDE method

Generating Gaussian random fields with Matérn Covariance

$$\left(-\frac{1}{2\nu}\nabla\cdot\left(\boldsymbol{\Theta}\,\nabla\right)+1\right)^{\frac{2\nu+d}{4}} u(\overrightarrow{x},\omega)=\eta W(\overrightarrow{x},\omega)$$

Whittle, P. (1954). On Stationary Processes in the Plane. *Biometrika*, *41*(3/4), 434. https://doi.org/10.2307/2332724
Whittle, P. (1963). Stochastic processes in several dimensions. *Bull. Inst. Internat. Statist.*, *40*, 974–994
Lindgren, F., Rue, H., & Lindström, J. (2011). An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, *73*(4), 423–498. https://doi.org/10.1111/j.1467-9868.2011.00777.x

The SPDE method

Generating Gaussian random fields with Matérn Covariance

Equation

$$\left(-\frac{1}{2\nu}\nabla\cdot\left(\boldsymbol{\Theta}\,\nabla\right)+1\right)^{\frac{2\nu+d}{4}} u(\overrightarrow{x},\omega)=\eta W(\overrightarrow{x},\omega)$$

Normalization

$$\eta=\left(\frac{(2\pi)^{\frac{d}{2}}\sqrt{\det(\boldsymbol{\Theta})}\,\Gamma(\nu+\frac{d}{2})}{\nu^{\frac{d}{2}}\Gamma(\nu)}\right)^{\frac{1}{2}}$$

Domain: arbitrary **Boundaries:** arbitrary

Theoretical results:

- The solution to the PDE is a *Gaussian random field with Matérn covariance and zero mean*
- The parameter ν determines the *smoothness* of the field.
- The parameter $\boldsymbol{\Theta}$ determines the *spatial structure* of the random field.

Whittle, P. (1954). On Stationary Processes in the Plane. *Biometrika*, *41*(3/4), 434. https://doi.org/10.2307/2332724

Whittle, P. (1963). Stochastic processes in several dimensions. *Bull. Inst. Internat. Statist.*, *40*, 974–994

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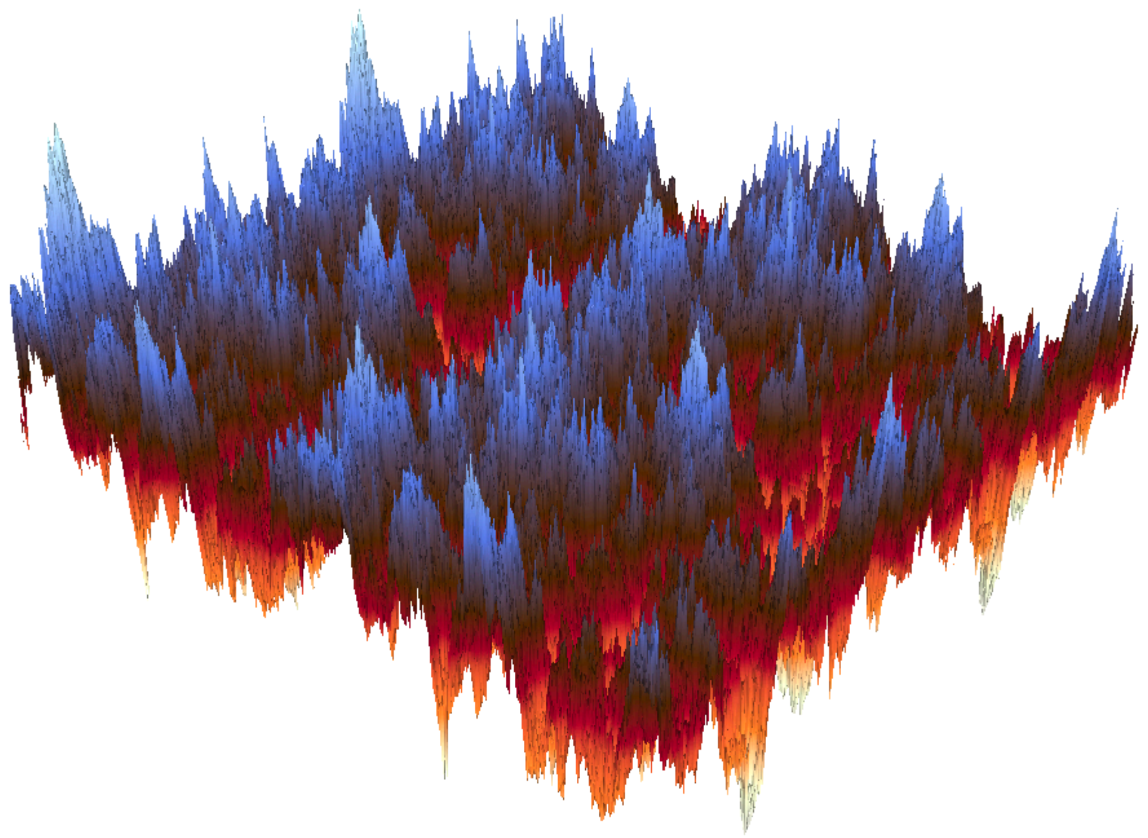
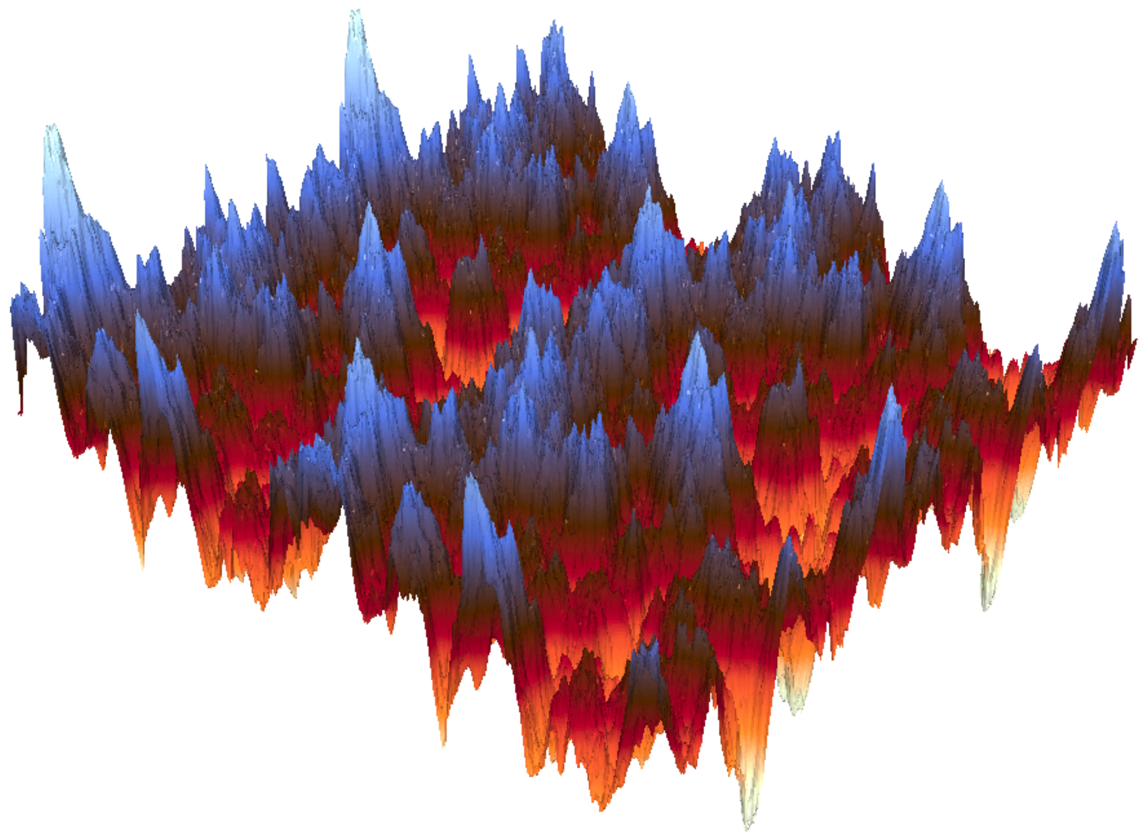
The SPDE method with MFEM

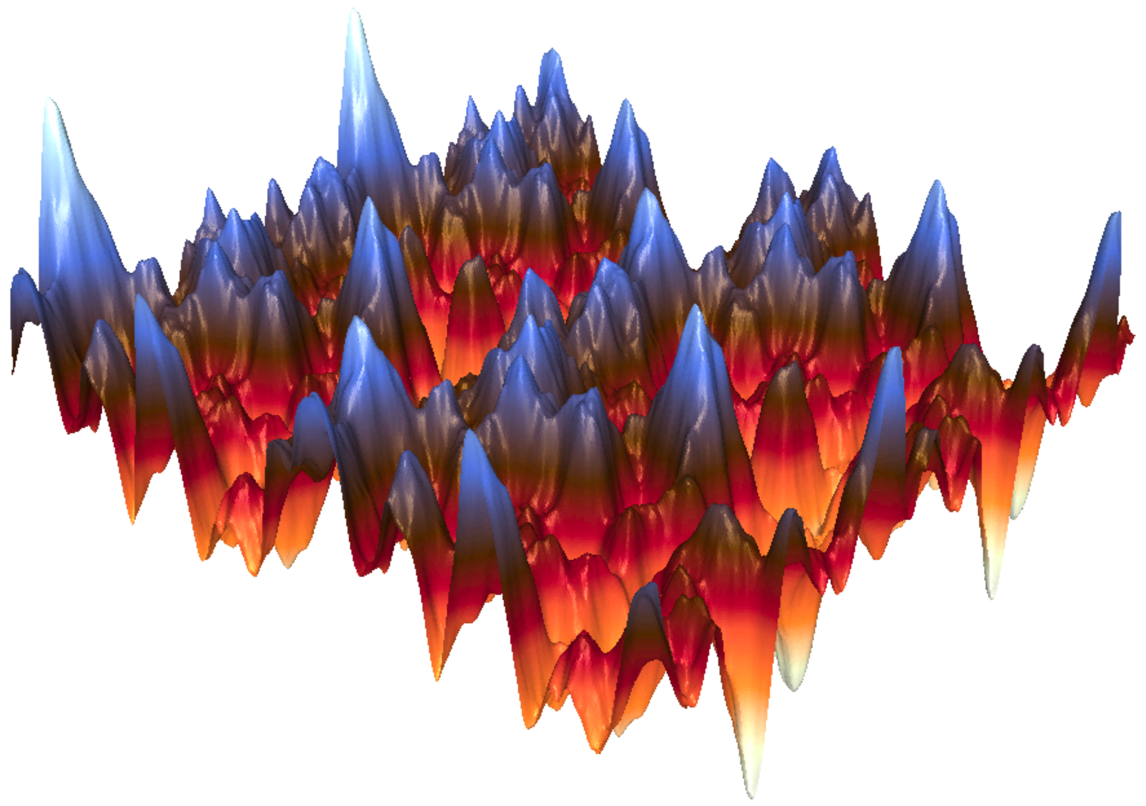
miniapps/materials



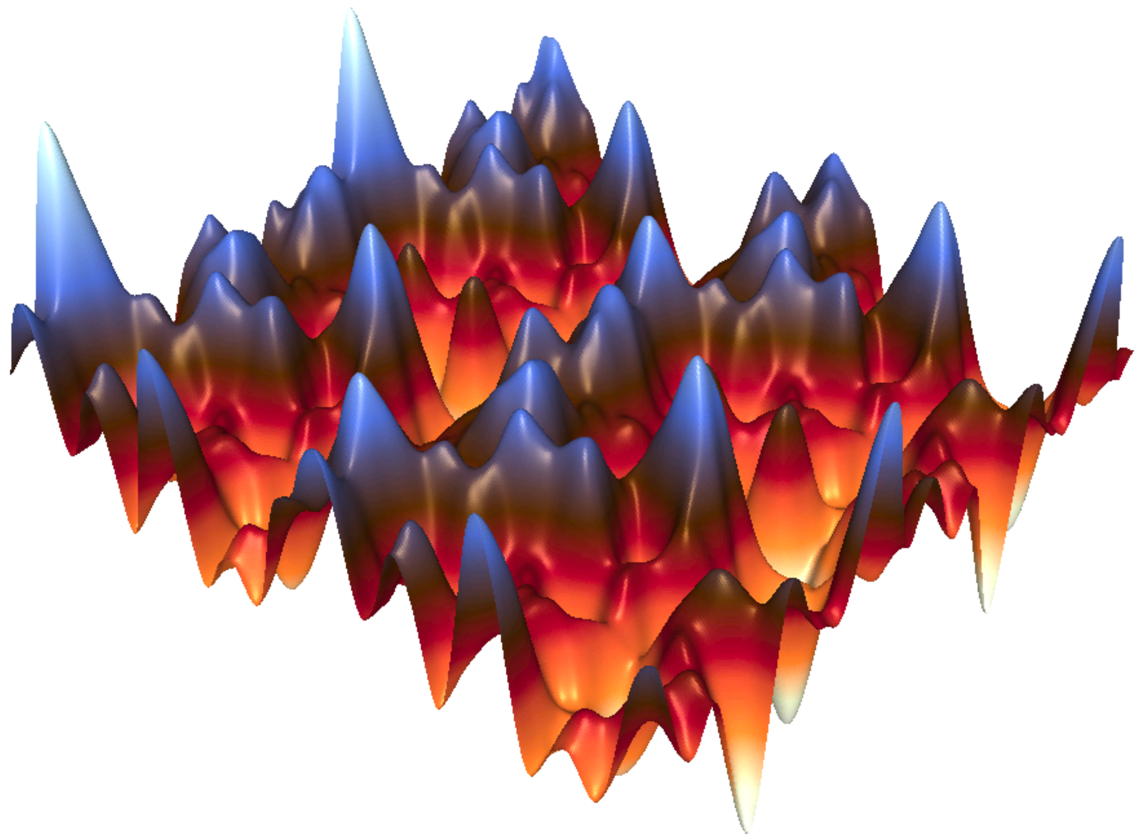
$\nu = 0.5$



$\nu = 1.0$



$\nu = 2.0$



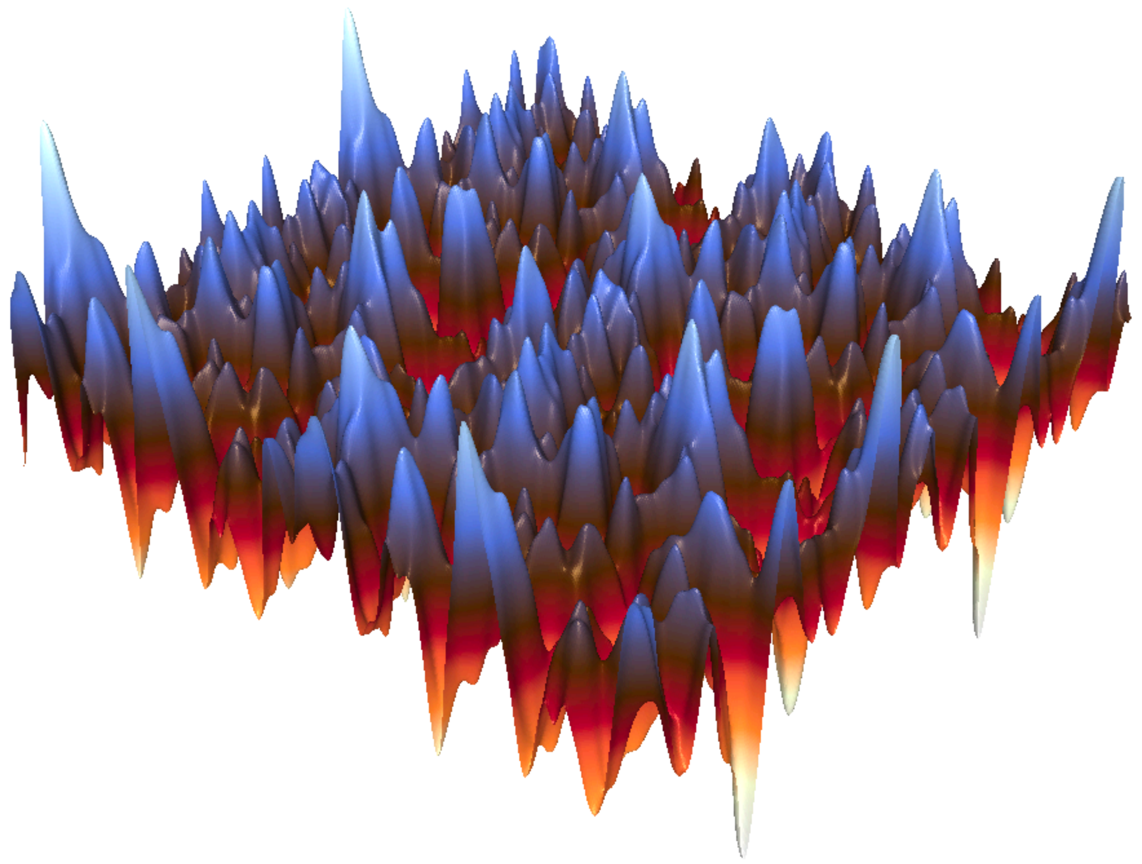
$\nu = 4.0$

```
make && mpirun -np 4 main -o 1 -r 3 -rp 6 -nu <your-nu> -l1 0.05 -l2 0.05 -no-rs
```

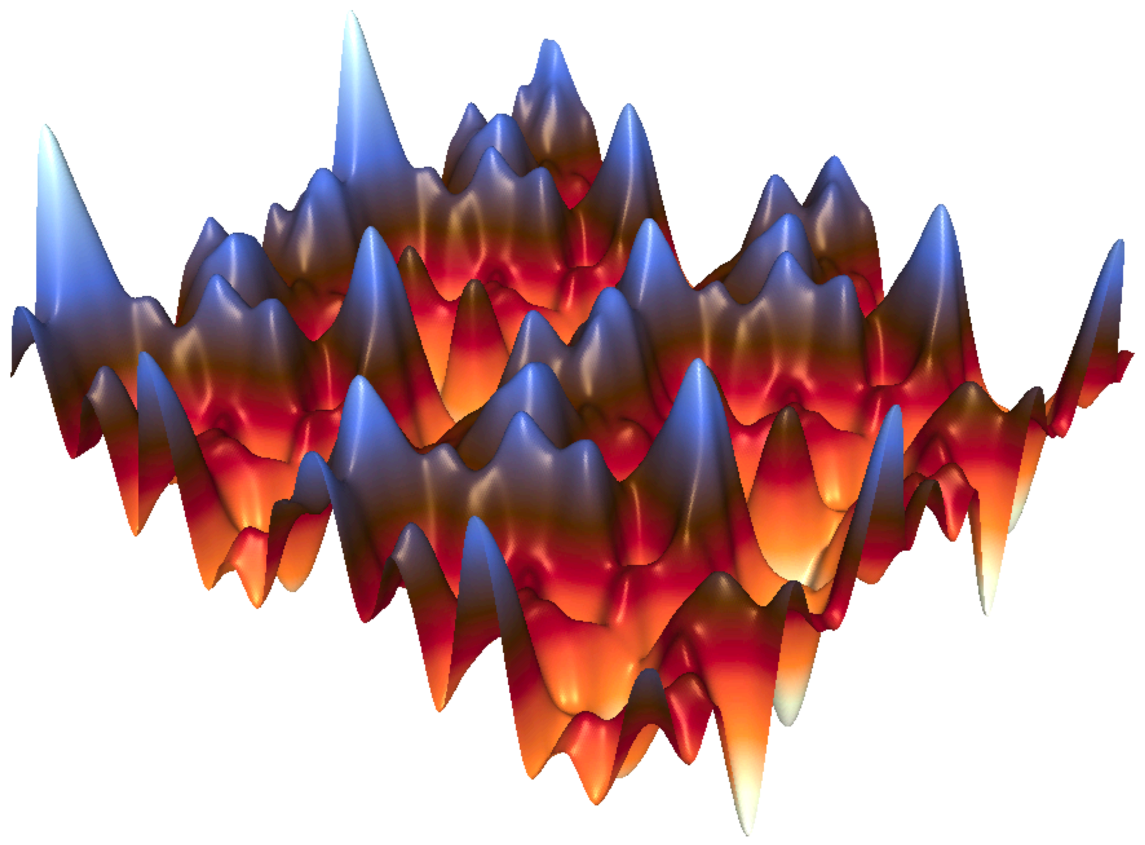
The SPDE method with MFEM

miniapps/materials

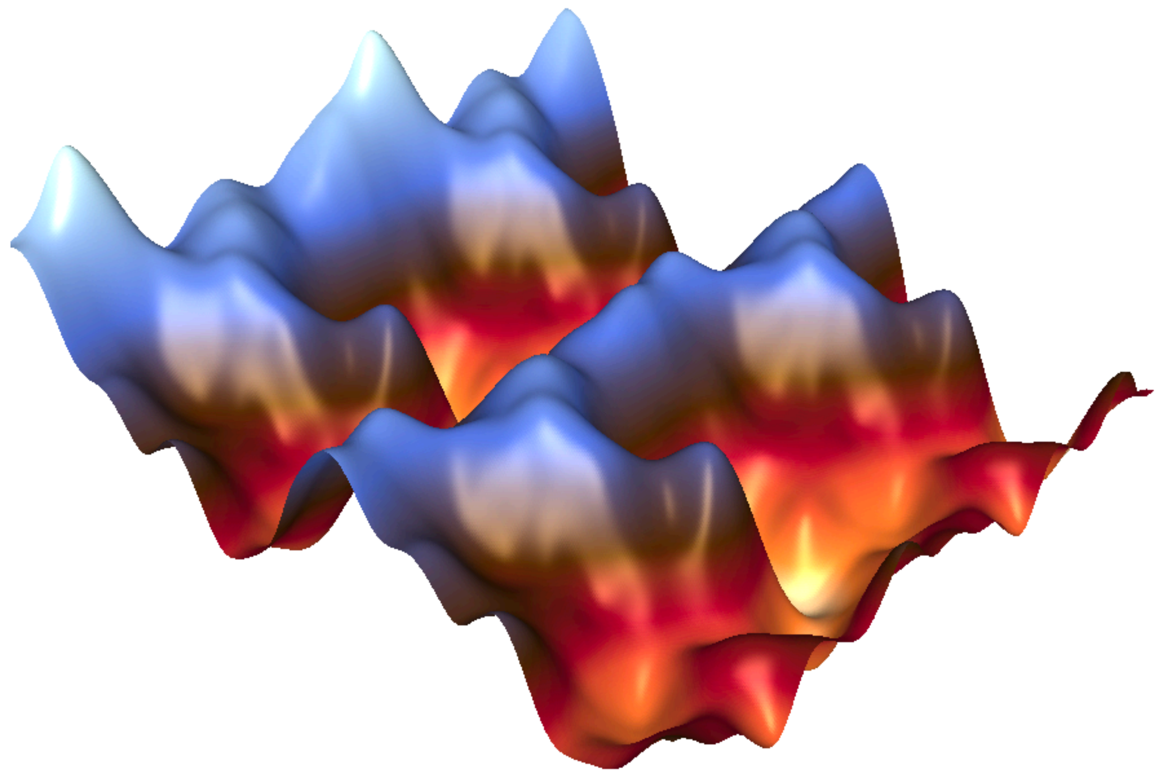
$$\Theta = \frac{1}{2\nu}\begin{pmatrix} (l_1)^2 & 0 \\ 0 & (l_2)^2 \end{pmatrix}$$



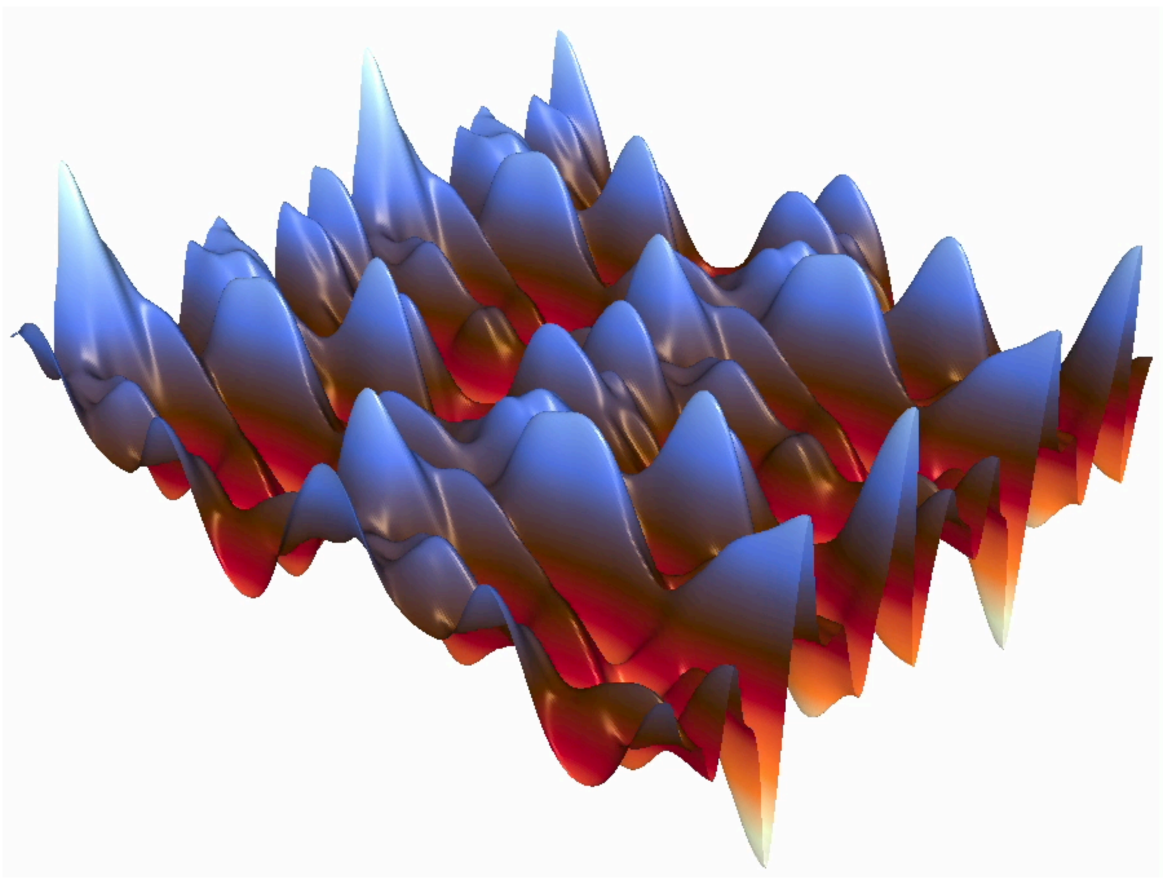
$l_1 = l_2 = 0.025$



$l_1 = l_2 = 0.050$



$l_1 = l_2 = 0.100$



$l_1 = 0.09,\ l_2 = 0.03$

```
make && mpirun -np 4 main -o 1 -r 3 -rp 6 -nu 4.0 -l1 <your-l1> -l2 <your-l2> -no-rs
```

What is topology optimization?

minimize $$\min_{\rho \in L^2(\Omega)} \int_\Omega u f \, dx$$

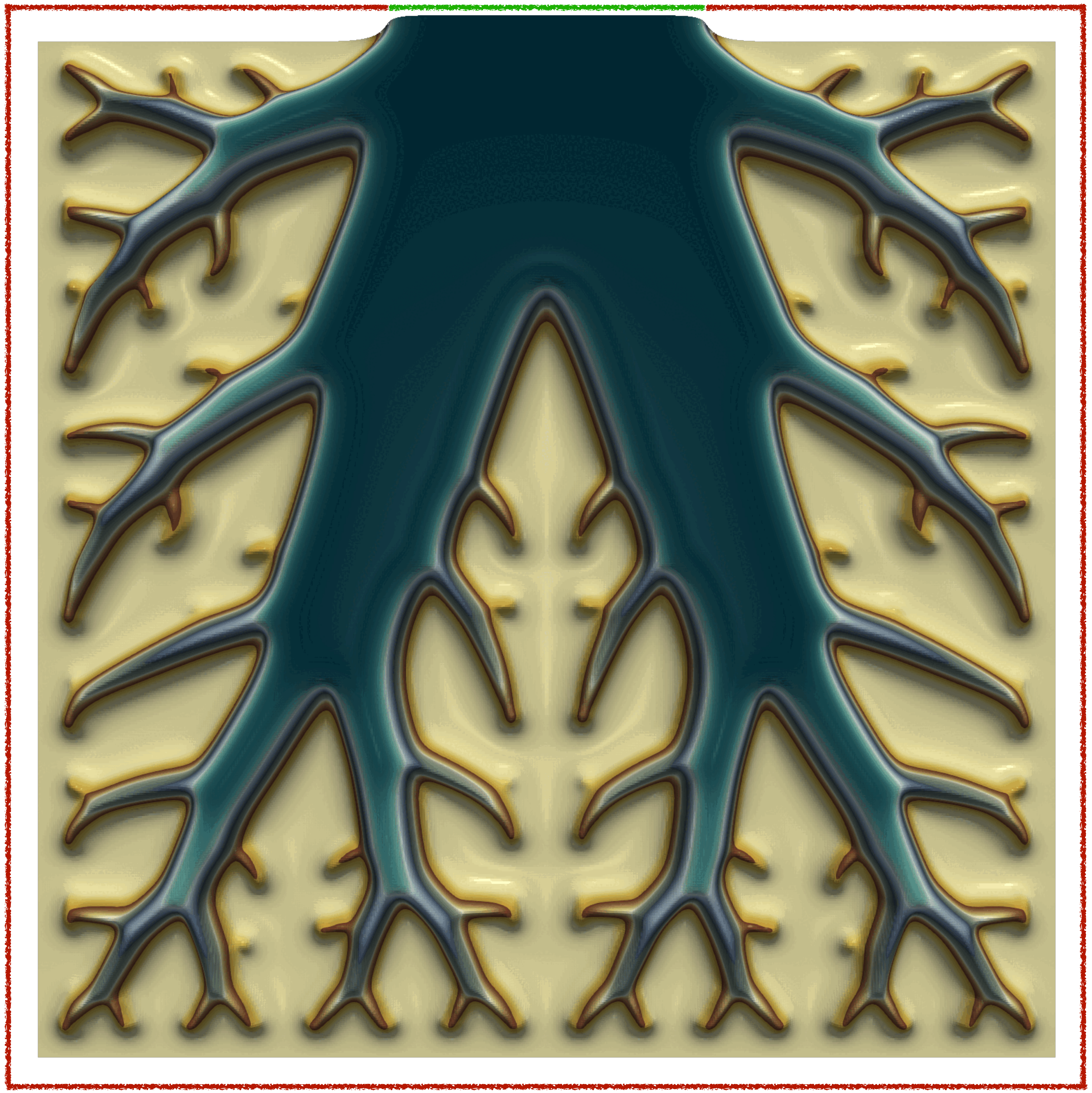
subject to $$-\operatorname{div} r(\tilde{\rho}) \nabla u = f$$

$$-\epsilon^2 \Delta \tilde{\rho} + \tilde{\rho} = \rho$$

$$\int_\Omega \rho(x) dx \leq V$$

$$0 \leq \rho \leq 1$$

$$r(\tilde{\rho}) = \rho_{\min} + \tilde{\rho}^3 (1 - \rho_{\min})$$

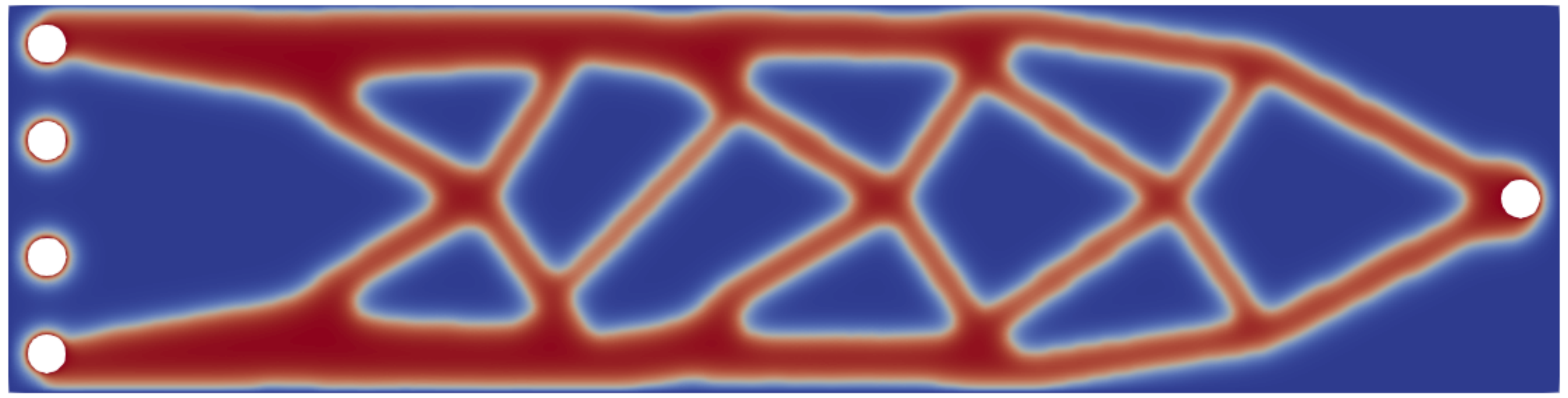


$\rho_{\min} = 0.001$ $\epsilon = 0.01$

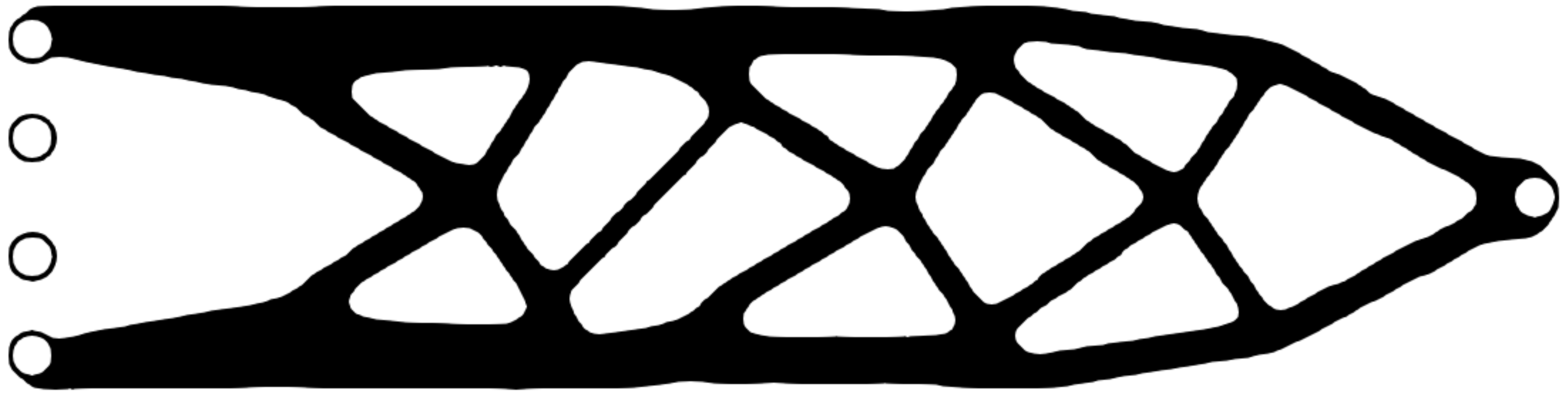
Homogeneous Neumann   Inhomogeneous Dirichlet

Examples

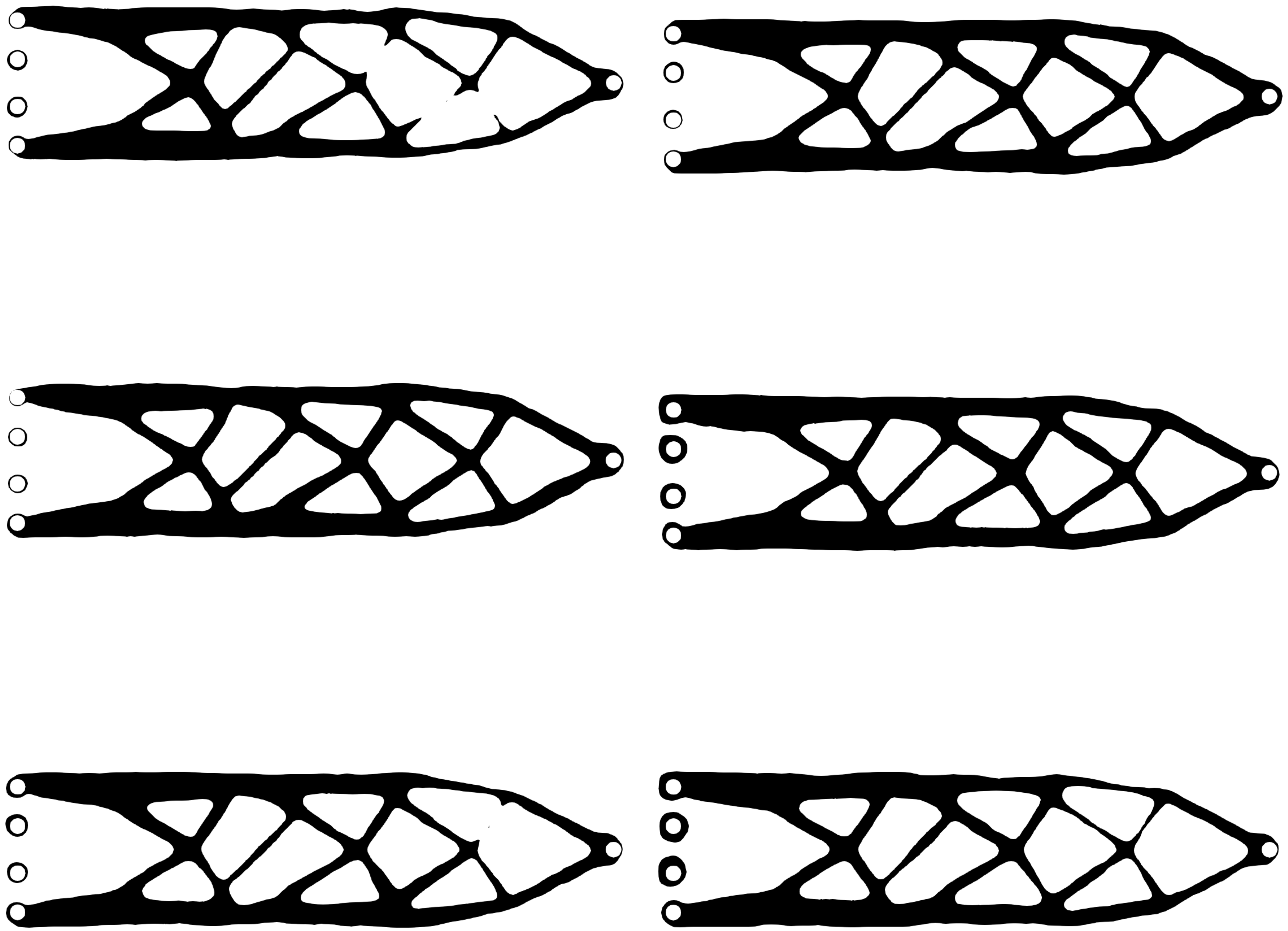
Unprojected filtered density



Blueprint



Realizations



Topology optimization under uncertainty

Lazarov, B. S., Wang, F., & Sigmund, O. (2016). Length scale and manufacturability in density-based topology optimization. *Archive of Applied Mechanics*, *86*(1–2), 189–218. https://doi.org/10.1007/s00419-015-1106-4

The end / Q&A