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Bayesian Nonlocal Operator Regression (BNOR): Towards the Characterization of Uncertainty in Heterogeneous Materials

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Introduction

- **Consider the modeling of heterogeneous materials.**

- Material properties (microstructure, interfacial conditions, environments, etc.) cause variability in material response.

- Non-trivial to provide quantitative characterization for each sample.

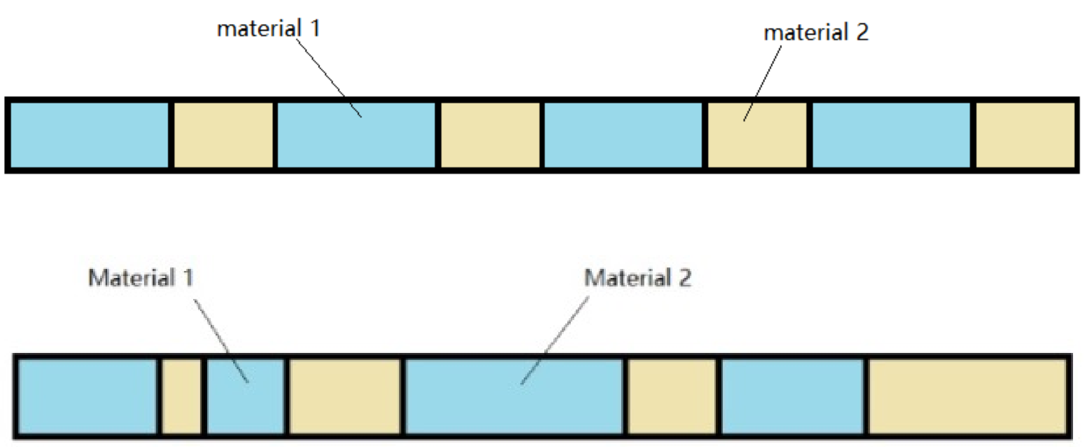


Figure: One-dimensional bar with periodic microstructure and disordered microstructure.

Why use nonlocal model?

Local model:

- Characterized by differential operators,
- Interactions happen at contact,
- Regularity requirements on the solution.

- Local Poisson's equation

$$-\triangle \mathbf{u}(\mathbf{x}) = \mathbf{f}(\mathbf{x})$$

Nonlocal model:

- Characterized by integral operators,
- Long-range interactions of size δ (horizon),
- No regularity requirements on the solution.

- Nonlocal Poisson's equation [3]

$$-2\int_{B(\mathbf{x},\delta)} K(\mathbf{x},\mathbf{y})\big(\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x})\big)d\mathbf{y} = \mathbf{f}(\mathbf{x})$$

[1] Du, Q., Gunzburger, M., Lehoucq, R. B., & Zhou, K. (2013). A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws. *Mathematical Models and Methods in Applied Sciences*, 23(03), 493-540.

Introduction

- Objective: Develop a Bayesian framework to characterize the uncertainty in using a nonlocal model to describe material response.
- Approach: Bayesian Nonlocal Operator Regression (BNOR) technique. To be specific, an MCMC Bayesian inference method, to identify the probability distribution of the nonlocal constitutive law that embeds the material properties.
- Application: Wave propagation through a heterogeneous bar, with disordered microstructure layers.

- [2] You, H., Yu, Y., Silling, S., & D'Elia, M. (2020). Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws. AAAI Spring Symposium MLPS 2021.

High-Fidelity Data

- Define a set of materials parameterized by the disorder parameter $\mathcal{D} \in [0,1]$ such that each layer material 1 or 2 has size $w \sim \mathcal{U}((1-\mathcal{D})w_i, (1+\mathcal{D})w_i)$, where $i = 1,2$ and $w_1 = (1-\phi)\lambda$, $w_2 = \phi\lambda$, where λ is the mean period of the microstructure. In our experiments we set L=0.2 (the bar length), E_1=1, E_2=0.25 (the Young's Moduli), ρ=1 (the density), and $\Omega = (-\mathrm{b}, \mathrm{b})$ (the spatial domain representing the bar).

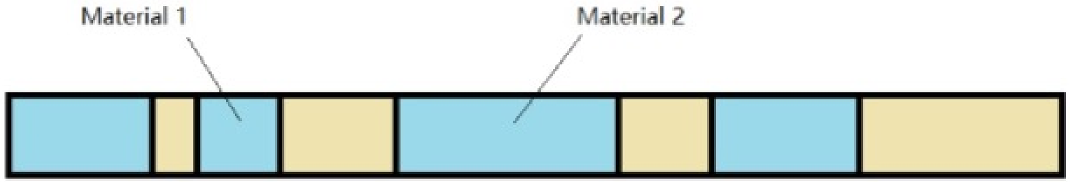


Figure: One-dimensional bar with disordered microstructure.

High-Fidelity Data

- Both training and validation datasets are generated via high-fidelity (HF) simulations of the propagation of stress wave through a one-dimensional heterogeneous bar. The HF model is a classical wave equation: find $u(x,t)$ such that, for $(x,t) \in \Omega \times [0,T]$,

$$\frac{\partial^2 u_{\mathrm{HF}}}{\partial t^2} - \mathcal{L}_{HF}[u_{\mathrm{HF}}](x,t) = f(x,t)$$

with force loading term $f(x,t)$, provided some initial conditions at $t = 0$ and boundary conditions on $\partial\Omega$.

- The HF-model is numerically solved using a Direct Numerical Solver (DNS) in [2], which guarantees that the wave velocity is computed exactly.

- [3] Silling, S. A. (2021). Propagation of a Stress Pulse in a Heterogeneous Elastic Bar. Journal of Peridynamics and Nonlocal Modeling, 1-21.

High-Fidelity Data

- Three types of data are generated where type 1 and type 2 are used for training, and type 3 is used for validation. In what follows, *v* presents the velocity.

- Type 1: Oscillating source. We set b=50, *T*=2, $v(x,0)=u(x,0)=0$,

$$f(x,t) = e^{-\left(\frac{2x}{(5kL)}\right)^2} e^{-\left(\frac{t-t_0}{t_p}\right)} \cos^2\left(\frac{2\pi x}{kL}\right), k = 1,2,\ldots,20, t_0 = t_p = 0.8.$$

- Type 2: Plane wave with ramp. For b=50, *T*=2, $f(x,t)=0$ and $u(x,0)=0$,

we prescribe $v(-b,t) = \begin{cases} \cos(\omega t)\sin^2(\frac{\pi t}{30}), & \text{if } t \le 15 \\ \cos(\omega t), & \text{if } t > 15 \end{cases}$, for $\omega =$ $0.35, 0.7, \ldots, 3.85.$

- Type 3: Wave packet. b=133.3, *T*=100 , $f(x,t)=0$ and $v(-b,t) =$ $\sin(\omega t)\, e^{\{-(\frac{t}{5}-3)^\wedge 2\}}$, for $\omega = 1.0, 2.0, 3.0, 4.0.$

Nonlocal Operator Regression (NOR)

- Following the method in [1], we proposed a nonlocal model to approximate the HF-model at large scales:

$$\frac{\partial^2 u_{NL}}{\partial t^2} - \mathcal{L}_{\mathcal{K}}[u_{NL}](x,t) = \mathrm{f}(x,t)$$

where

$$\mathcal{L}_{\mathcal{K}}[u](x,t) = \int_{\Omega} K(|x-y|)\big(u_{NL}(y,t) - u_{NL}(x,t)\big)dy$$

- We represent the kernel K as a linear combination of Bernstein basis polynomials:

$$K(|x-y|) = \sum_{m=0}^{M} \frac{C_m}{\delta^{d+2}} B_{m,M}\left(\left|\frac{x-y}{\delta}\right|\right)$$

where

$$B_{m,M}(x) = \binom{M}{m} x^m (1-x)^{M-m}$$

for $0 \le x \le 1$ and $C_m \in \mathbb{R}$.

- [2] You, H., Yu, Y., Silling, S., & D'Elia, M. (2020). Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws. AAAI Spring Symposium MLPS 2021.

Nonlocal Operator Regression (NOR)

- From now on, denote K_C and $u_{NL,C}$ as the nonlocal kernel and nonlocal solution corresponding to a specific set of kernel parameters $C := \{C_m\}_{m=0}^{M}$.

- Using central-difference scheme in time

$$u_{NL,C}(x_i, t_{n+1}) = 2u_{NL,C}(x_i, t_n) - u_{NL,C}(x_i, t_n - 1) + \mathrm{d}t^2 \left(\mathcal{L}_{\mathcal{K}_{\mathcal{C}},\hbar}[u_{\mathrm{NL,C}}](x_i, t_n) + f(x_i, t_n)\right)$$

- Learning procedure: minimize the following cost function with regularization

$$\sum_{s=1}^{S} \frac{\left|\left|u_{NL,C}^{s} - u_{DNS}^{s}\right|\right|_{l_2(\Omega\times[0,t])}^{2}}{\left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}^{2}} + \lambda\left|\left|C\right|\right|_{l_2}^{2}$$

- $u_{NL,C}$ satisfies the central difference equation and K_C satisfies physical-based constraints[1].

- [2] You, H., Yu, Y., Silling, S., & D'Elia, M. (2020). Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws. arXiv preprint arXiv:2012.04157.

- Note1: NOR is a purely deterministic approach. It cannot quantify the uncertainty in using a nonlocal model to describe material response.

- Note2: We can use this preliminary result as prior knowledge in Bayesian inference.

Bayesian Inference: likelihood

- In this work, we take ground truth u_{HF} as the numerical solution u_{DNS} generated from the DNS solver.
- Denote the nonlocal solution corresponding to a specific set of kernel parameters $\{C_m\}$ as $u_{\{C_m\}}(x,t)$, model the error between the nonlocal solution and the ground truth as a Gaussian variable

$$u_{DNS}^{s}(x,t) = u_{NL,C}^{s}(x,t) + \epsilon(x,t), \epsilon \sim N(o, \sigma_{s}^{2})$$

where $\sigma_s = \sigma \left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}^{2}$, σ is a constant independent of s.

- The negative log-likelihood reads

$$\sum_{s=1}^{S}\left(\frac{\left|\left|u_{NL,C}^{s} - u_{DNS}^{s}\right|\right|_{l_2(\Omega\times[0,T])}^{2}}{\left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}} + N\log(\sigma\left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}^{2})\right)$$

Bayesian Inference: prior

- Assume $C = \{C_m\}$ has a Gaussian prior, i.e. $C_m, m = 0, \dots, M$ are independent Gaussian variables with $C_m \sim N\left(C_{0,m}, \frac{\sigma_0^2}{\lambda}\right)$. Here $\{C_{0,m}\}$ is the set of parameters of the kernel learnt from the deterministic NOR, and σ_0 is the standard deviation calculated using the current nonlocal solution associated with $\{C_m\}$.
- The negative log-prior reads

$$\lambda \frac{\left|\left|C - C_0\right|\right|^2}{2\sigma_0^2}$$

- Combining the negative log-likelihood and the negative log-prior, we have the negative log posterior

$$\sum_{s=1}^{S}\left(\frac{\left|\left|u_{NL,C}^{s} - u_{DNS}^{s}\right|\right|_{l_2(\Omega\times[0,T])}^{2}}{\left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}} + \mathrm{Nlog}(\sigma\left|\left|u_{NL,C}^{s}\right|\right|_{l_2(\Omega\times[0,t])}^{2})\right) + \lambda\frac{\left|\left|C - C_0\right|\right|_{l_2}^{2}}{2\sigma_0^2}$$

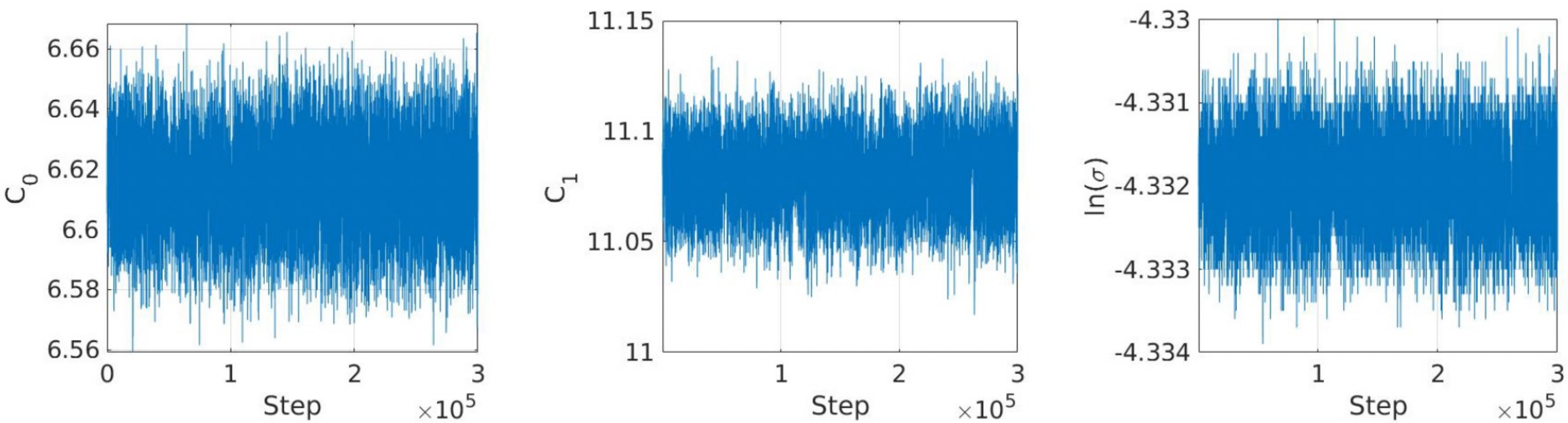
MCMC: algorithm and evaluation

- We adopt the adaptive MCMC algorithm proposed in [4]. In practice, we couple PyUQTk [5] with our nonlocal model to apply the MCMC algorithm.
- Inspect the trace plot visually and evaluate the acceptance rate (the percentage of the accepted proposal states) of MCMC.
- Effective sample size (ESS) is a guidance on sub-sampling, also a criterion which could tell us how long an MCMC chain we need. In this work, the ESS is computed following the multivariate extension defined in [6].
- Plot the probability density function (PDF) based on equally spaced samples of the chain, where the number of the subsamples is determined by the ESS.

- [4] Haario, H., Saksman, E., & Tamminen, J. (1999). Adaptive proposal distribution for random walk Metropolis algorithm. Computational statistics, 14(3), 375-395.
- [5] Sargsyan, K., Safta, C., Boll, L., Johnston, K., Khalil, M., Chowdhary, K., ... & Debusschere, B. (2022). UQTk Version 3.1. 2 User Manual (No. SAND2022-0377). Sandia National Lab.(SNL-NM), Albuquerque, NM (United States).
- [6] Vats, D., Flegal, J. M., & Jones, G. L. (2019). Multivariate output analysis for Markov chain Monte Carlo. *Biometrika*, *106*(2), 321-337.

Results on Disordered Material

MCMC Trace Plot

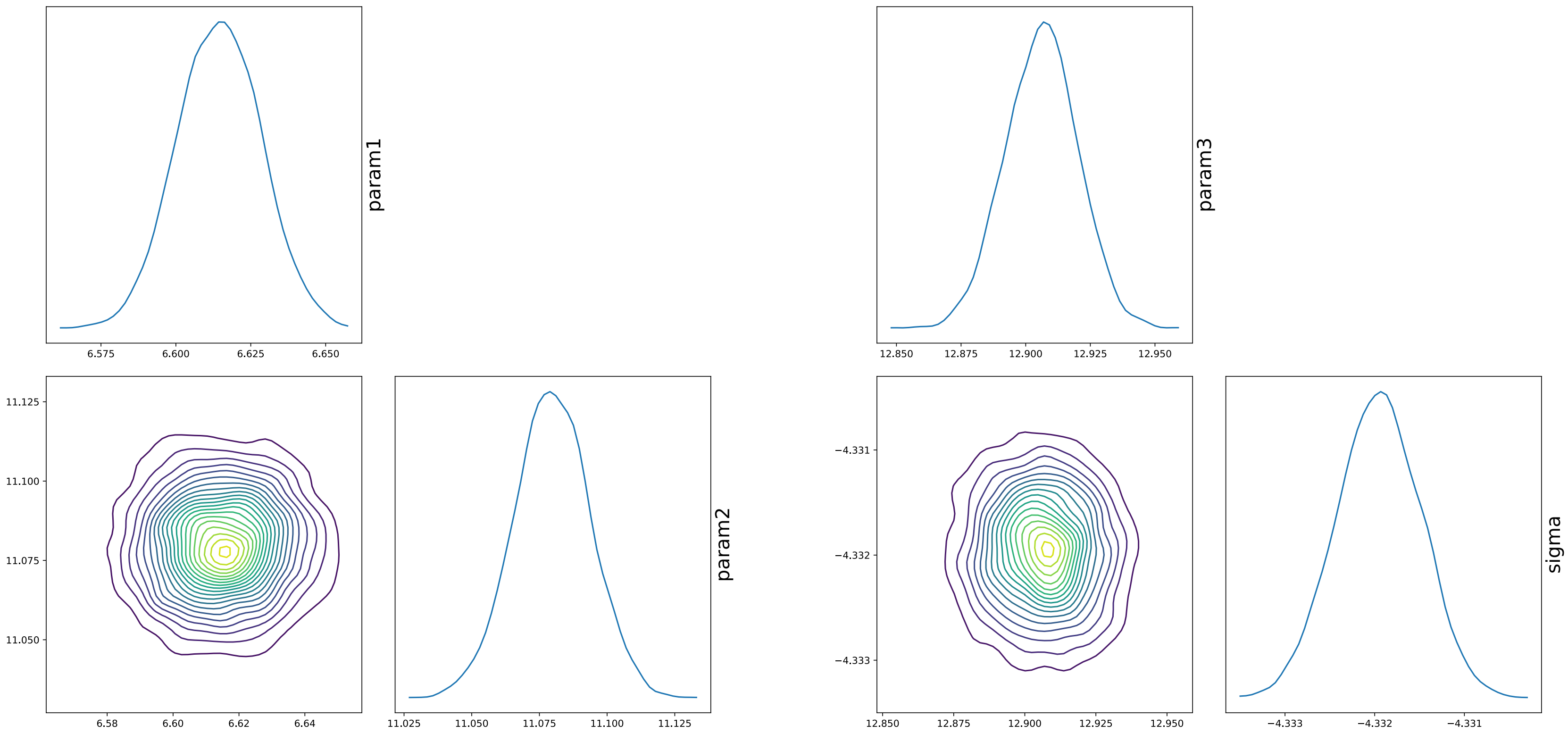


(a) Parameter 1 (b) Parameter 2 (c) $\ln(\sigma)$

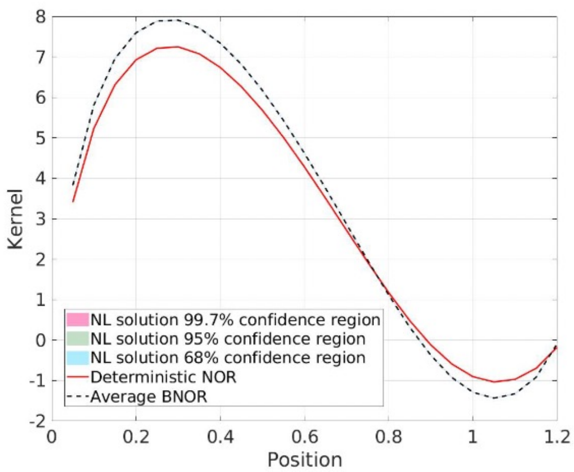
- Chain length = 300,000, acceptance rate = 0.31, ESS=4212.

Results on Disordered Material

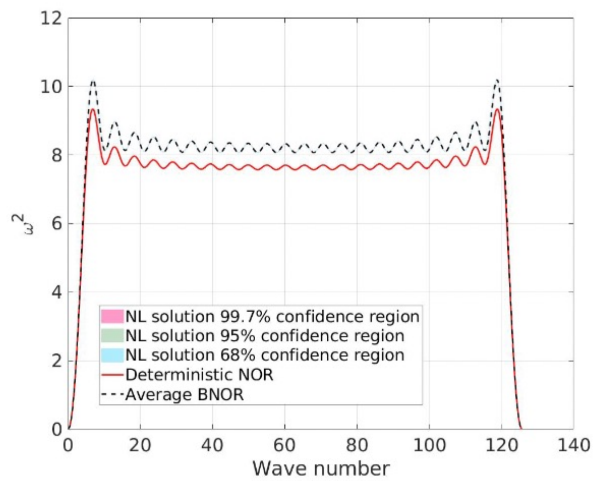
Density Plot



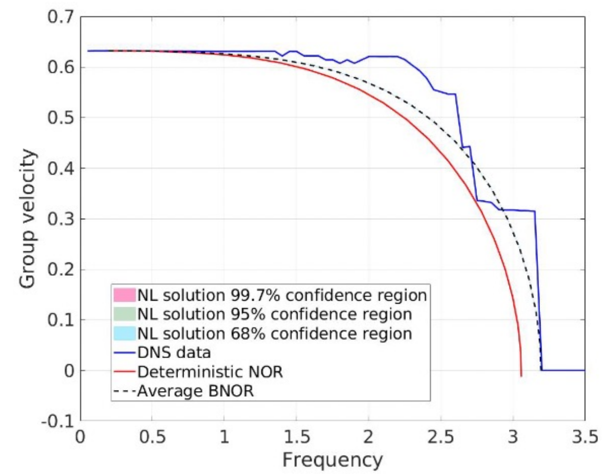
Results on Disordered Material



(a) Optimal kernel



(b) Dispersion curve



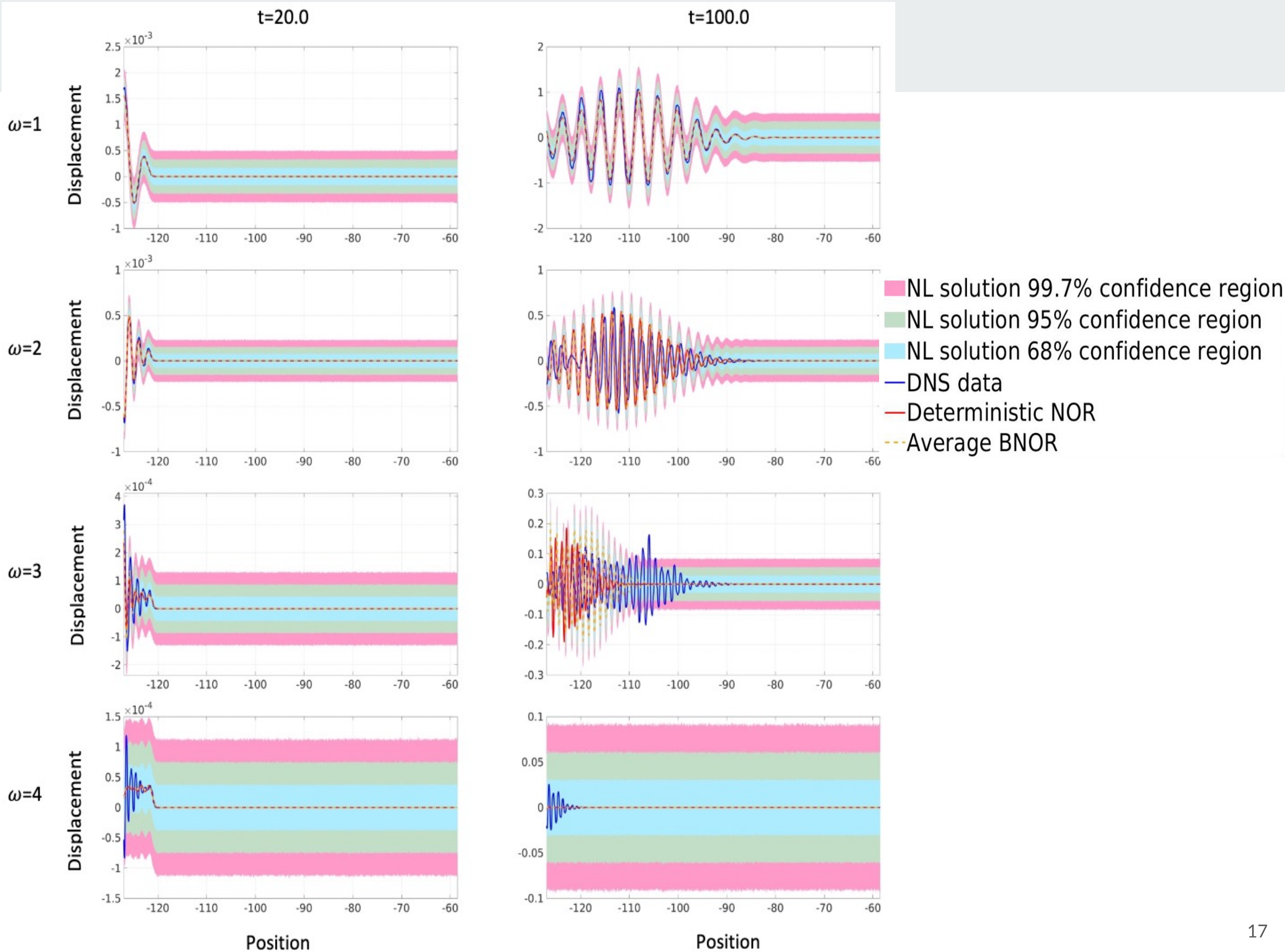
(c) Group velocity

- Positive dispersion curves indicate physically stable material models
- The group velocity matches the one computed with DNS both at low frequencies and at the band stop.

Validation on wave packet through a disordered material

- Validation on the wave packet with ω=2.0 at t=20.0s (short time prediction) and t=100.0s (long time prediction). 4 different frequencies (ω=1.0,2.0,3.0,4.0) are considered. For each sample in ESS, we calculate the nonlocal kernel C and the corresponding nonlocal solution $u_{NL,C}$. Then plot the 68%-95%-99.7% confidence region for $u_{NL,C} + \epsilon$, where

$$\epsilon \sim \mathcal{N}\left(0, \sigma^2 \left|\left|u_{NL,C}(x,t)\right|\right|^2_{l_2([-b,b]\times[0,T])}\right)$$


t=20.0
t=100.0
ω=1
ω=2
ω=3
ω=4
Displacement
Position
NL solution 99.7% confidence region
NL solution 95% confidence region
NL solution 68% confidence region
DNS data
Deterministic NOR
Average BNOR

Conclusion

We proposed a Bayesian nonlocal operator regression technique, which

- captures the nonlocal constitutive law that embeds the material properties,
- characterizes the uncertainty in using a nonlocal model for predicting wave propagation through heterogeneous materials,
- Provides models that reproduce high-fidelity data that are substantially different from the training data

Future work

- Noisy data,
- More sophisticated error model, etc.

Acknowledgement

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Reference

- [1] Du, Q., Gunzburger, M., Lehoucq, R. B., & Zhou, K. (2013). A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws. Mathematical Models and Methods in Applied Sciences, 23(03), 493-540.
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Thank you! Q & A