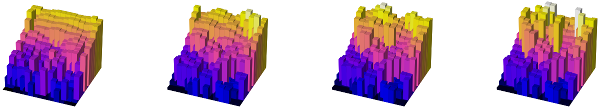
# Scientific Machine Learning for Exact Recovery of Nonlinear PDEs



Aleksei Sorokin[123], Fred Hickernell[1], Pieterjan Robbe[2], Mohamed Wahib[3], Houman Owhadi[4], Aras Bacho[4], Xianjin Yang[4], Matthieu Darcy[4], Theo Bourdais[4], Edo Calvello[4], Bamdad Hosseini[5], Alexandre Hsu[5]

[1]Illinois Tech, Department of Applied Math, Chicago IL, USA
[2]Sandia National Laboratories, Livermore CA, USA
[3]RIKEN Center for Computational Science, Tokyo Japan
[4]California Institute of Technology, Pasadena, California
[5]University of Washington, Seattle, Washington

# Background

PhD Student in Applied Math at Illinois Tech in Chicago IL, advisor Fred J Hickernell

- (Quasi-)Monte Carlo for fast high dimensional integration
- Gaussian Process Modeling with structure-exploits for scalable UQ
- Scientific Software Development for distribution of efficient algorithms

US DOE SCGSR Fellow[1] at Sandia National Laboratories in Livermore CA

- Multilevel (Quasi-)Monte Carlo for multi-fidelity or infinite-dimensional problems
- Scientific machine learning (SciML) for solving nonlinear PDEs

Intern in the RIKEN CCS AI-HPC Research Team in Tokyo Japan

- SciML for Exact PDE Recovery focused on applications to inverse problems
- HPC Compatible Implementations supporting multi-GPU parallelism

[1] Department of Energy Office of Science Graduate Student Research Program

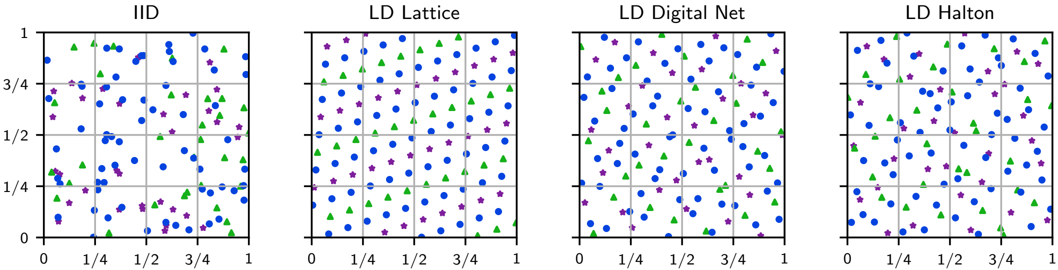
# Quasi-Monte Carlo Methods

Efficient algorithms for high dimensional numerical integration [Choi et al., 2022, Hickernell et al., 2025]

$$\mu = \int_{\mathcal{T}} g(\boldsymbol{t})\lambda(\mathrm{d}\boldsymbol{t}) = \int_{[0,1]^d} f(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \approx \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i), \qquad \boldsymbol{x}_1,\dots,\boldsymbol{x}_n \in [0,1]^d$$

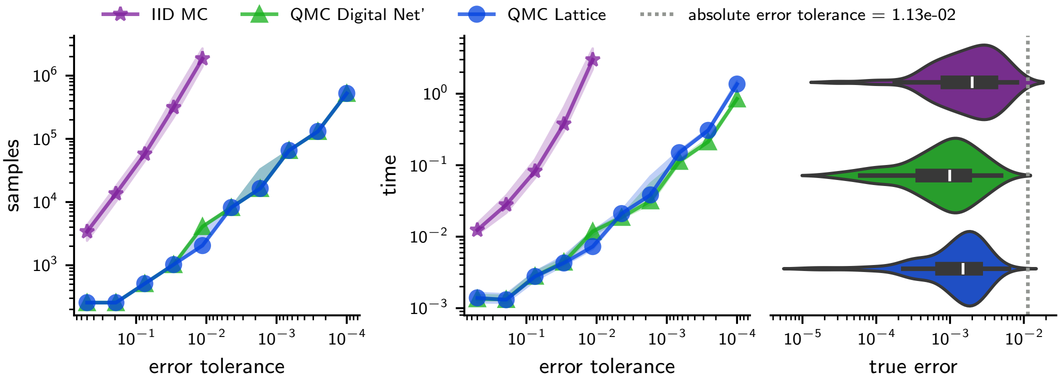
Classic Monte Carlo has error like $\mathcal{O}(1/\sqrt{n})$ using IID points $[\boldsymbol{x}_i]_{i=1}^n$

QMC has errors like $\mathcal{O}(1/n)$ using low discrepancy (LD) points with greater uniformity



# Adaptive QMC Stopping Criterion

Automatically choose sample size $n$ to meet user specified error tolerances [Sorokin and Rathinavel, 2022]



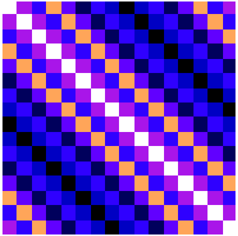

`pip install qmcpy`: QMC Python software qmcsoftware.github.io/QMCSoftware

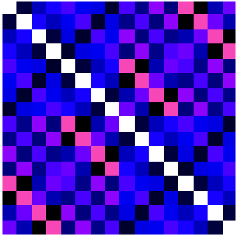
# Gaussian Process Regression with Structure-Exploits

Scalable kernel interpolation with built in uncertainty quantification (UQ) [Rathinavel and Hickernell, 2019, 2022]

$$f(\boldsymbol{x}) \approx \boldsymbol{K}(\boldsymbol{x})^T \mathsf{K}^{-1} \boldsymbol{f}$$

- SPD kernel $K(\cdot,\cdot)$
- Points $[\boldsymbol{x}_i]_{i=1}^n$
- Values $\boldsymbol{f} = [f(\boldsymbol{x}_i)]_{i=1}^n$
- Basis $\boldsymbol{K}(\cdot) = [K(\cdot,\boldsymbol{x}_i)]_{i=1}^n$
- Gram matrix $\mathsf{K} = [K(\boldsymbol{x}_i,\boldsymbol{x}_j)]_{i,j=1}^N$



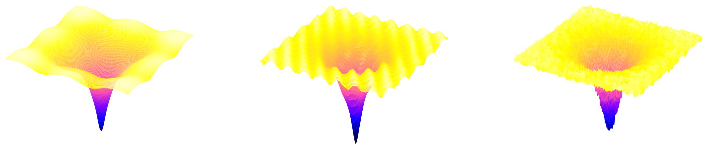

Classic GPR costs $\mathcal{O}(n^3)$ as we must compute the matrix inverse $\mathsf{K}^{-1}$

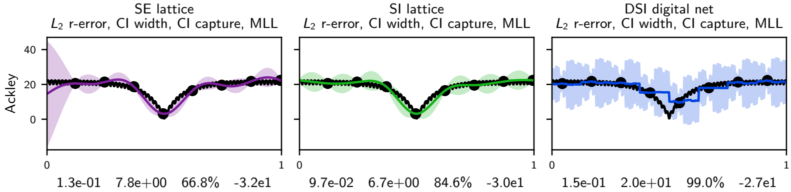
Fast GPR cost only $\mathcal{O}(n \log n)$ by pairing (SI/DSI) kernels $K$ to LD points $[\boldsymbol{x}_i]_{i=1}^n$

- Exploit structure in the Gram matrix $\mathsf{K}$: diagonalizable by fast Fourier transforms

# Fast Gaussian Process Regression

| SE grid | SI lattice | DSI digital net |
|---|---|---|
| error = 3.7e-2 | error = 2.8e-2 | error = 2.6e-2 |
| time = 1.6e0 | time = 8.0e-4 | time = 1.5e-3 |
| MLL = 6.3e3 | MLL = -3.8e2 | MLL = -4.5e3 |






`pip install fastgps`: Scalable GPR Python software alegresor.github.io/fastgps

# Nonlinear PDEs with Random Coefficients

## Applications in Fluid Mechanics, Geophysics, Medical Imaging, ...

Nonlinear PDE $F(v^\star|c) = 0$, solution $v^\star$, random coefficient $c$

**Nonlinear Elliptic PDE**

$$F(v|c) = -\Delta v + \kappa v^3 - c$$

**Burgers' Equation** with an implicit time stepping scheme (step size $h_t$, constant $\kappa > 0$)

$$F(v|c) = v - h_t(\kappa \nabla^2 v - v \nabla v) - c$$

**Nonlinear Darcy flow** with forcing term $f$

$$F(v|c) = -e^c[\nabla c . \nabla v + \nabla^2 v] + \kappa v^3 - f$$

**Full Waveform Inversion** sets $F(v|c) = P(v) - c$ where $P$ a numerical forward solver

# The Newton–Kantorovich Iteration

A relaxed Gauss–Newton algorithm for root finding in Hilbert spaces of functions [Polyak, 2006]

Nonlinear PDE $F(v^\star|c) = 0$, solution $v^\star$, random coefficient $c$

Given $c$ and a relaxation parameter $\lambda > 0$, an optimal update $\delta^\star(v)$ is

$$\underset{\delta}{\operatorname{argmin}} \left(\|F(v+\delta)\|^2 + \lambda \|\delta|^2\right) \approx -\left[\frac{\partial F^T}{\partial v}(v)\frac{\partial F}{\partial v}(v) + \lambda \mathsf{I}\right]^{-1} \frac{\partial F^T}{\partial v}(v)F(v) =: \delta^\star(v)$$

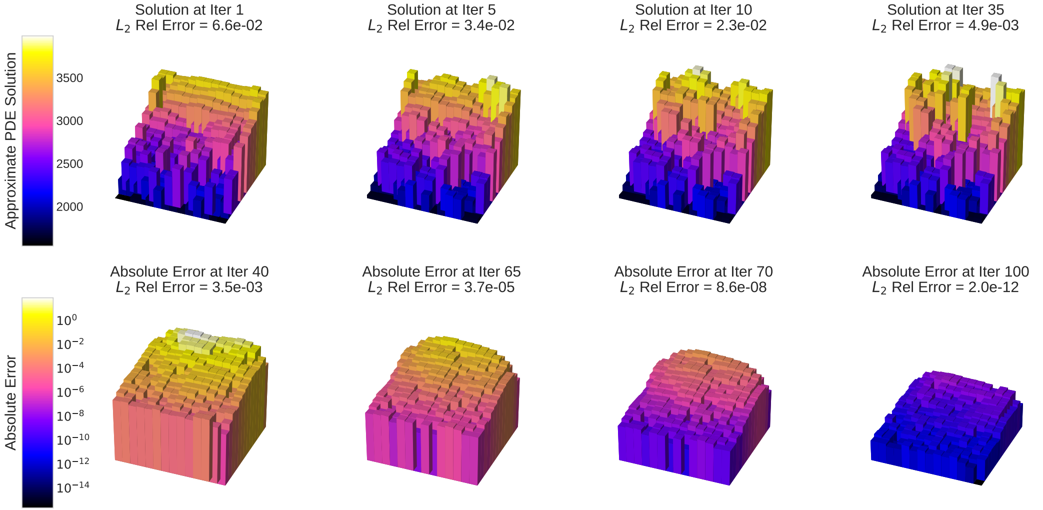
The Newton–Kantorovich iteration with learning rate $\alpha > 0$ sets

$$v_{n+1} = v_n + \alpha \delta^\star(v_n)$$

Relaxation $\lambda$ interpolates between gradient descent and Gauss–Newton updates

# Newton–Kantorovich Iteration for Full Waveform Inversion

Finds subsurface velocity from a surface acoustic signal [Deng et al., 2022, Virieux and Operto, 2009]



# SciML for Exact Recovery of Nonlinear PDEs

Learning the approximate Hessian operator enables sciML to converge to machine precision

$$v_{n+1}(c) = v_n(c) - \alpha H^{-1}(v,c,\lambda)\frac{\partial F^T}{\partial v}(v,c)F(v,c)$$

$$H(v,c,\lambda) = L(v,c,\lambda)L^T(v,c,\lambda) = \frac{\partial F^T}{\partial v}(v,c)\frac{\partial F}{\partial v}(v,c) + \lambda \mathsf{I}$$

| | Existing sciML Methods | Novel CHONKNORIS Method |
|---|---|---|
| Learn to predict | a function (operator learning) | an operator (learning to learn) |
| Learned Map | $c \mapsto v_S$ | $(v,c,\lambda) \mapsto L(v,c,\lambda)$ |
| Input $\mapsto$ Output Sizes | $\mathcal{O}(N) \mapsto \mathcal{O}(N)$ | $\mathcal{O}(N) \mapsto \mathcal{O}(N^2)$ |
| Achievable Errors | $\approx \mathcal{O}(10^{-2})$ or $\mathcal{O}(10^{-3})$ | machine precision $\mathcal{O}(10^{-16})$ |

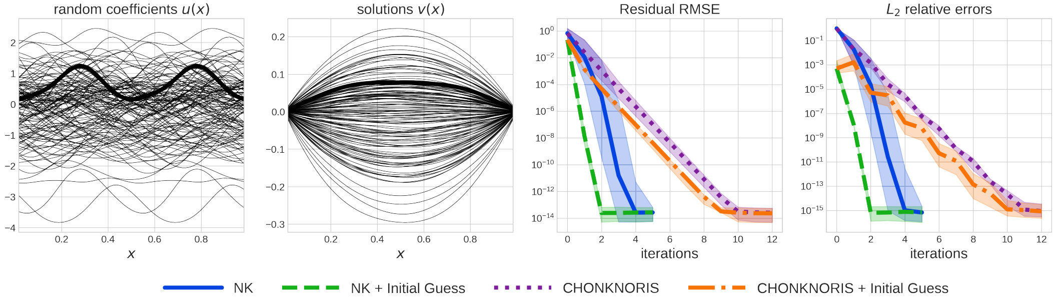
Existing sciML methods

- artificial neural networks [Li et al., 2020, Lu et al., 2021]
- kernel methods [Batlle et al., 2024, Kadri et al., 2016, Nelsen and Stuart, 2021]
- hybrid approaches [Mora et al., 2025, Owhadi, 2023, Owhadi and Yoo, 2019]

# Nonlinear Elliptic PDE

CHONKNORIS achieves machine precision recovery in 12 iterations

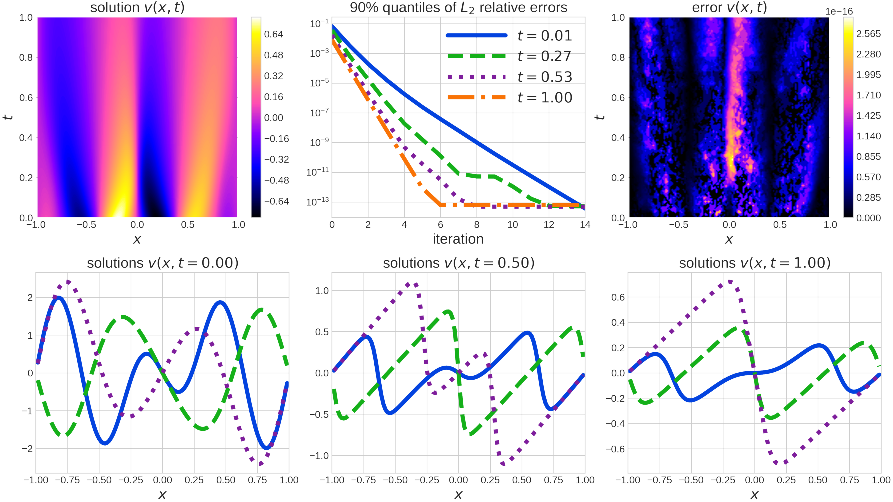
$$F(v|c) = -\Delta v + \kappa v^3 - c, \qquad \left[\frac{\partial F}{\partial v}(v)\right](h) = [-\Delta + 3\kappa v^2](h)$$




- CHONKNORIS requires more iterations but avoids cubic inversion cost in NK
- Initial guess from existing sciML method can accelerate convergence

# Burgers' Equation with Shocks via Implicit Time Stepping

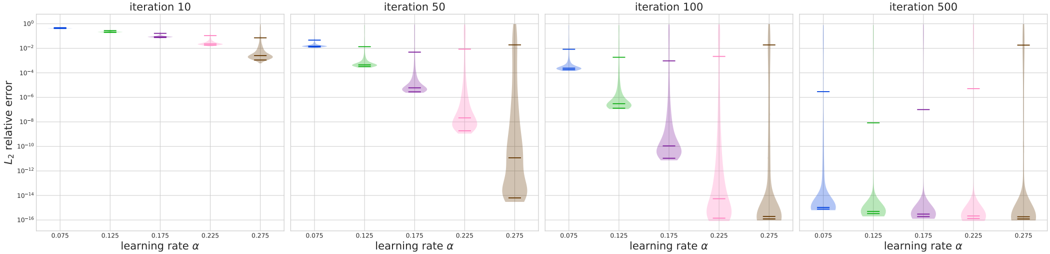
## CHONKNORIS (at each time step) recovers solutions $f$ to within $10^{-16}$ error



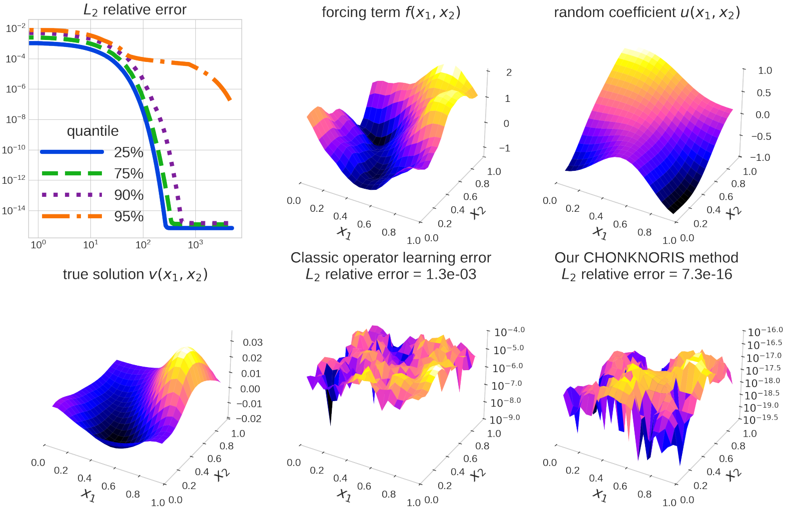
# CHONKNORIS Requires a Scalable Implementation and Careful Tuning

Darcy equation with $15 \times 15$ discretization requires predicting over $> 25$k outputs
Automatic selection of $(\lambda, \alpha)$ improve stability, e.g., using line search

- Relaxation $\lambda$ must be adaptively decreased for convergence to machine precision
- Learning rate $\alpha$ trades off convergence speed and robustness

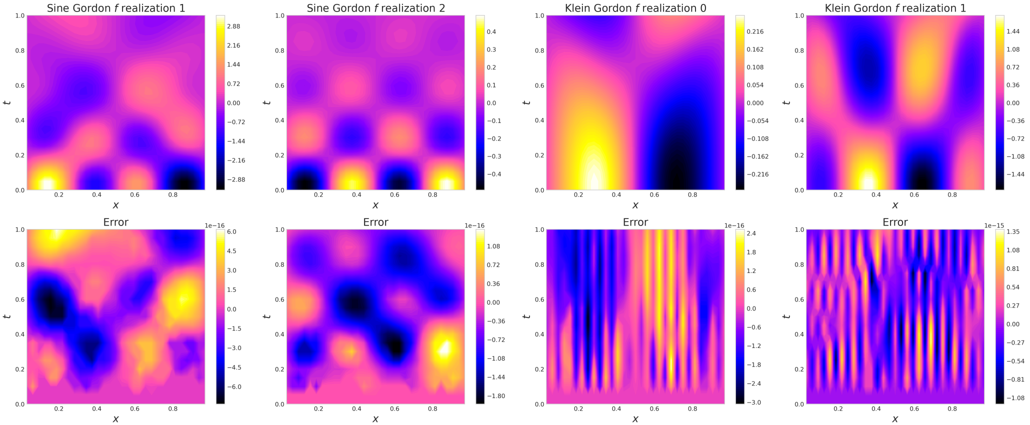


# Darcy Flow in Two Dimensions



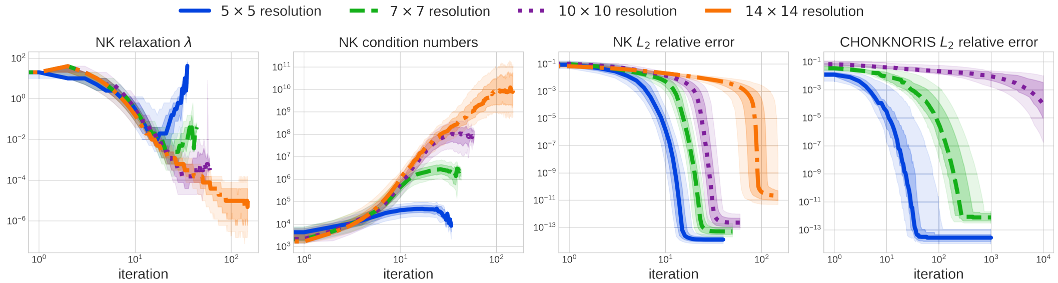
# Machine Precision Foundation Modeling for Common Jacobian Structures

## CHONKNORIS trained on 1D PDEs can exactly recover unseen Sine–Gordon and Klein–Gordon PDEs



# Full Waveform Inversion

## CHONKNORIS can exactly recover rough solutions at low resolutions




CHONKNORIS struggles to predict the ill conditioned matrices from

- fine discretizations
- rough coefficients
- near convergence perturbations

# RIKEN-CCS Experience

Thank you to Dr Wahib and the AI-HPC team!

- Everyone was engaging, helpful, and kind
- Smooth onboarding and supportive staff

Provided access to large-scale HPC machines

- Implemented multi-GPU acceleration
- Evaluated Jacobians with millions of entries
- Trained large scale AI models

Appreciated the culture in Tokyo

- Business professional atmosphere
- Respectful, clean, and safe

Benten Pond near Tokyo Tower

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**Thank you for listening!** Connect or follow my research at alegresor.github.io

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