Solving High Frequency and Multi-Scale PDEs with Gaussian Processes

Shikai Fang*, Madison Cooley*, Da Long*, Shibo Li, Robert M. Kirby, Shandian Zhe

KAHLERT SCHOOL OF COMPUTING
THE UNIVERSITY OF UTAH

ICLR

www.sci.utah.edu

Github Repo

➢ML-based PDE Solvers help scientific and engineering tasks

➢Canonical form of PINN family solvers

DNN as surrogate model: $\widehat{u}_{\boldsymbol{\theta}}(\mathbf{x}) \approx u_{\boldsymbol{\theta}}(\mathbf{x})$

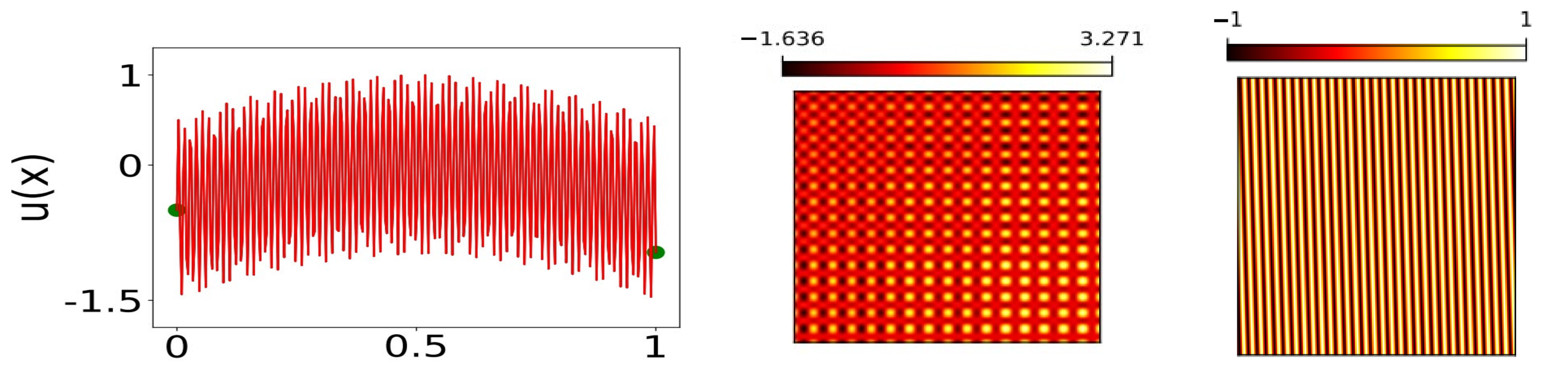
Loss func.: $\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} \; L_b(\boldsymbol{\theta}) + L_r(\boldsymbol{\theta})$,

where $L_b(\boldsymbol{\theta}) = \frac{1}{N_b}\sum_{j=1}^{N_b}\left(\widehat{u}_{\boldsymbol{\theta}}(\mathbf{x}_b^j) - g(\mathbf{x}_b^j)\right)^2$ **Boundary**

$L_r(\boldsymbol{\theta}) = \frac{1}{N_c}\sum_{j=1}^{N_c}\left(\mathcal{F}[\widehat{u}_{\boldsymbol{\theta}}](\mathbf{x}_c^j) - f(\mathbf{x}_c^j)\right)^2$ **Diff. terms**

➢Challenges: "Specturm bias" of DNN

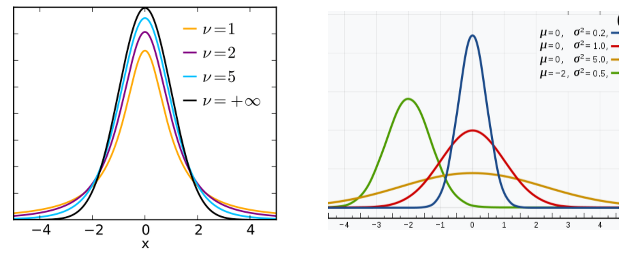
- Easy to learn low-frequency info, but hard to learn *high-frequency* info *[Rahaman et al. ICML 2019]*
- DNN-based solvers hard to handle PDEs with *high-frequency* components



➢GP-HM: model PDE solution in frequency domain

Assume solution's **power spectrum** is mixture of Student-t or Gaussian

$$S(s) = \sum_{q=1}^{Q} w_q \mathrm{St}(s; \mu_q, \rho_q^2, \nu), \qquad S(s) = \sum_{q=1}^{Q} w_q \mathcal{N}(s; \mu_q, \rho_q^2)$$



Wiener-Khinchin theorem & Inverse Fourier transform (IFT)

GP kernels!

$$k_{\mathrm{StM}}(x, x') = \sum_{q=1}^{Q} w_q \gamma_{\nu,\rho_q}(x, x') \cos(2\pi\mu_q(x - x')),$$

$$k_{\mathrm{GM}}(x, x') = \sum_{q=1}^{Q} w_q \exp\left(-\rho_q^2(x - x')^2\right) \cdot \cos(2\pi(x - x')\mu_q).$$

GP with Stm/GM kernel as **frequency-aware** surrogate model:

$$u(\cdot) \sim \mathcal{GP}(m(\cdot), \mathrm{cov}(\cdot,\cdot)) \qquad \mathrm{cov}\left(\partial_{x_1x_2}u(\mathbf{x}), u(\mathbf{x}')\right) = \partial_{x_1x_2}k(\mathbf{x}, \mathbf{x}')$$

➢Inference by maximizing log-joint prob

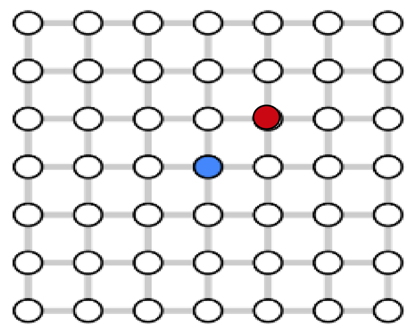
$$\mathcal{L}(\mathcal{U}, \Theta, \tau_1, \tau_2) = \log \mathcal{N}(\mathrm{vec}(\mathcal{U})|\mathbf{0}, \mathbf{C}) + \lambda_b \cdot \log \mathcal{N}(\mathbf{g}|\mathbf{u}_b, \tau_1^{-1}\mathbf{I}) + \log \mathcal{N}(\mathbf{0}|\mathrm{vec}(\mathcal{H}), \tau_2^{-1}\mathbf{I})$$

GP priors of the solution on grids — Likelihood of boundary conditions — Likelihood on the differential terms in domain

➢Structured kernel for efficient computation

For grids with reso. $M_1 \times \ldots \times M_d$, there are $M = \prod M_d$ allocation points:

GP-HM cost:
- Time: $\mathcal{O}\left(\sum M_d^3 + \left(\sum M_d\right) M\right)$
- Space: $\mathcal{O}\left(\sum M_d^2 + M\right)$



-Product kernel + Kronecker product structure of kernel matrix:

$$\mathrm{cov}(f(\mathbf{x}), f(\mathbf{x}')) = \kappa(\mathbf{x}, \mathbf{x}'|\Theta) = \prod_{j=1}^{d} k_{\mathrm{StM}}(x_j, x_j'|\boldsymbol{\theta}_q), \qquad \log|\mathbf{C}| = \sum_{j=1}^{d}\frac{M}{M_j}\log|\mathbf{C}_j|,$$

➢Numerical Results:

Method	Poission-1D					Poission-2D		1D Allen-cahn		2D Allen-cahn	1D Advection
	u_1	u_2	u_3	u_4	u_5	u_6	u_7	u_8	u_9	u_{10}	u_{11}
PINN	1.36e0	1.40e0	1.00e0	1.42e1	6.03e-1	1.63e0	9.99e-1	1.41e0	1.14e1	1.96e1	1.00e0
W-PINN	1.31e0	2.65e-1	1.86e0	2.60e1	6.94e-1	1.63e0	6.75e-1	1.34e0	1.45e1	2.03e1	1.01e0
RFF-PINN	4.97e-4	2.00e-5	7.29e-2	2.80e-1	5.74e-1	1.69e0	7.99 e-1	1.24e-3	2.46e-1	7.17e-1	9.96e-1
Rowdy	1.70e0	1.00e0	1.00e0	1.01e0	1.03e0	2.24e1	7.36e-1	1.30e0	1.31e0	1.18e0	1.03e0
Spectral method	2.36e-2	3.47e0	1.02e0	1.02e0	9.98e-1	1.58e-2	1.04e0	2.34e-2	2.45e1	2.45e1	2.67e0
Chebfun	**3.05e-11**	**1.17e-11**	**5.81e-11**	**1.14e-10**	**8.95e-10**	N/A	N/A	**1.39e-08**	**2.94e-10**	N/A	1.39e0
Finite Difference	5.58e-1	4.78e-2	2.34e-1	1.47e0	1.40e0	2.33e-1	1.75e-2	2.32e-01	2.36e-1	3.23e0	1.29e-1
GP-SE	2.70e-2	9.99e-1	9.99e-1	3.19e-1	9.75e-1	9.99e-1	9.53e-1	2.74e-2	1.06e-2	3.48e-1	9.99e-1
GP-Matérn	3.32e-2	9.8e-1	5.15e-1	1.83e-2	6.27e-1	6.28e-1	3.54e-2	3.32e-2	5.16e-2	2.96e-1	9.99e-1
GP-HM-GM	**3.99e-7**	2.73e-3	3.92e-6	1.55e-6	1.82e-3	**6.46e-5**	1.06e-3	**4.91e-6**	**4.24e-6**	5.78e-3	3.59e-3
GP-HM-StM	6.53e-7	**2.71e-3**	**3.17e-6**	**8.97e-7**	**4.22e-4**	6.87e-5	**1.02e-3**	7.71e-6	4.76e-6	**2.99e-3**	**9.08e-4**

Relative L_2 error. $u_1 = \sin(100x)$, $u_2 = \sin(x) + 0.1\sin(20x) + 0.05\cos(100x)$, $u_3 = \sin(6x)\cos(100x)$, $u_4 = x\sin(200x)$, $u_5 = \sin(500x) - 2(x-0.5)^2$, $u_6 = \sin(100x)\sin(100y)$, $u_7 = \sin(6x)\sin(20x) + \sin(6y)\sin(20y)$, $u_8 = \sin(100x)$, $u_9 = \sin(6x)\cos(100x)$, $u_{10} = (\sin(x) + 0.1\sin(20x) + \cos(100x)) \cdot (\sin(y) + 0.1\sin(20y) + \cos(100y))$ and $u_{11} = \sin(x - 200t)$.

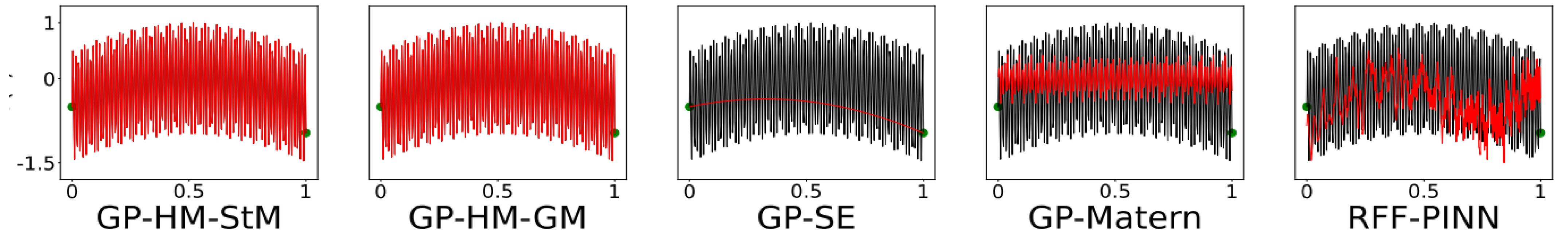


Figure 2: Prediction for the 1D Poisson equation with solution $\sin(500x) - 2(x - 0.5)^2$.

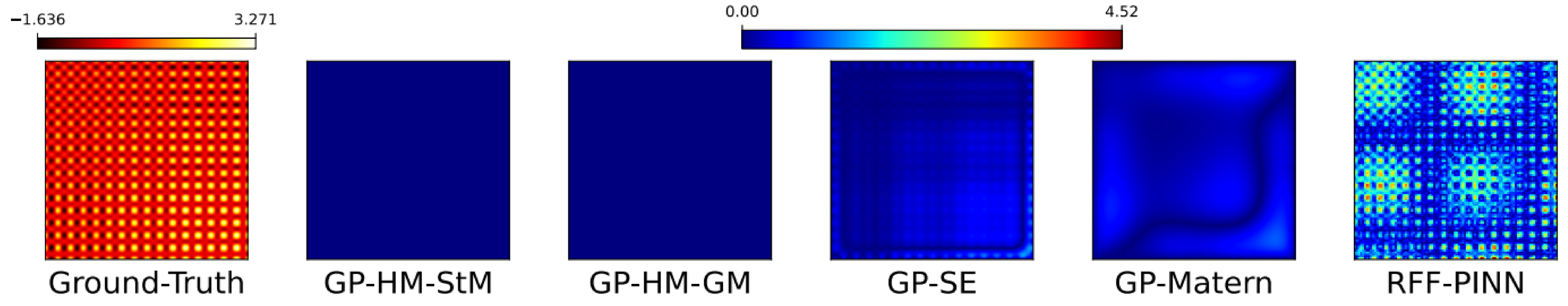
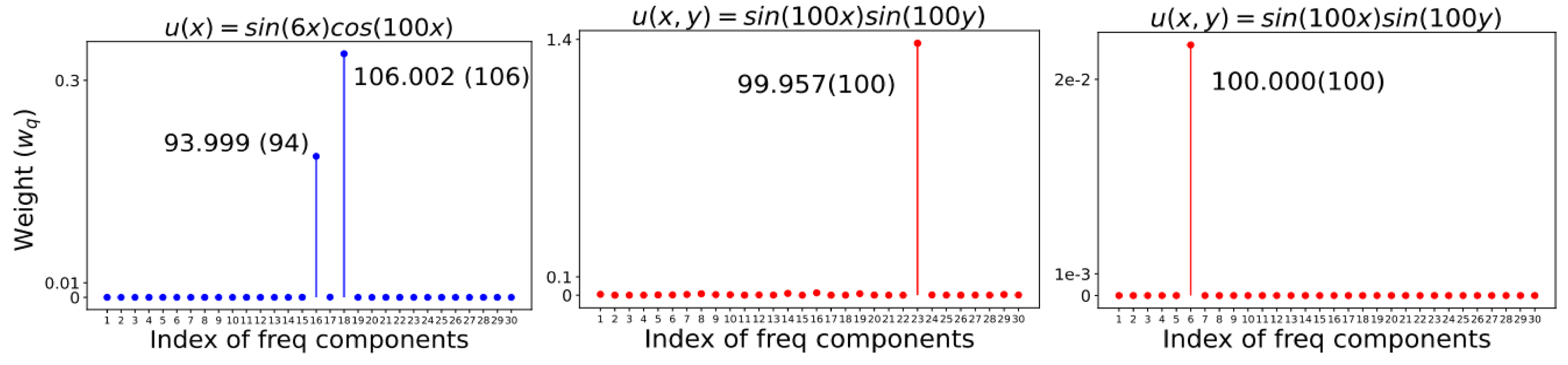


Figure 3: Point-wise solution error for 2D Allen-cahn equation, and the solution is $(\sin(x) + 0.1\sin(20x) + \cos(100x))(\sin(y) + 0.1\sin(20y) + \cos(100y))$.

➢Learned Frequency:



(a) Poisson-1D (b) Poisson-2D x-dim (c) Poisson-2D y-dim