Sobolev Cubatures Strengthen the Approximation Power of Physics Informed Neural Nets

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What are PINNs and why not use classic PDE solvers ?

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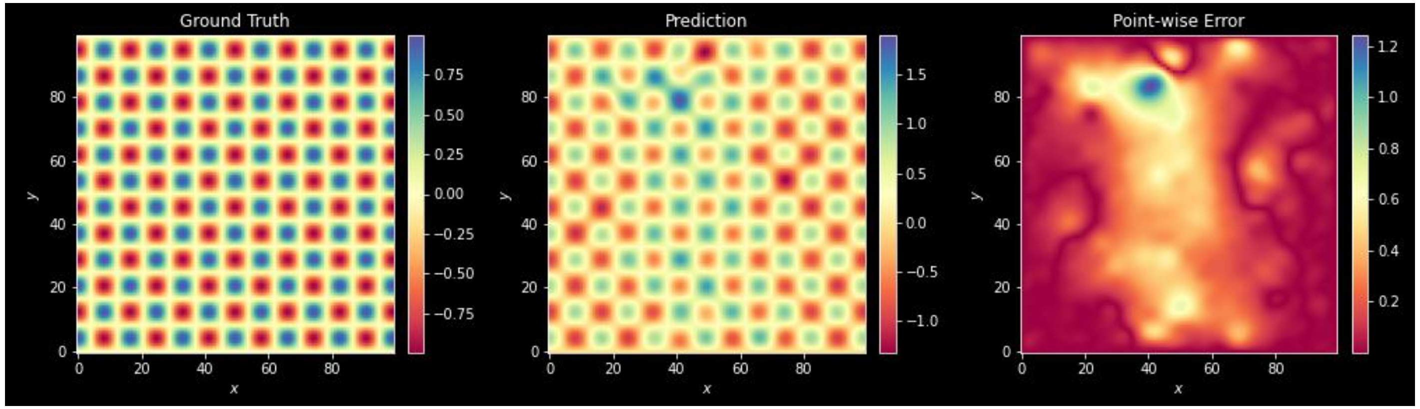
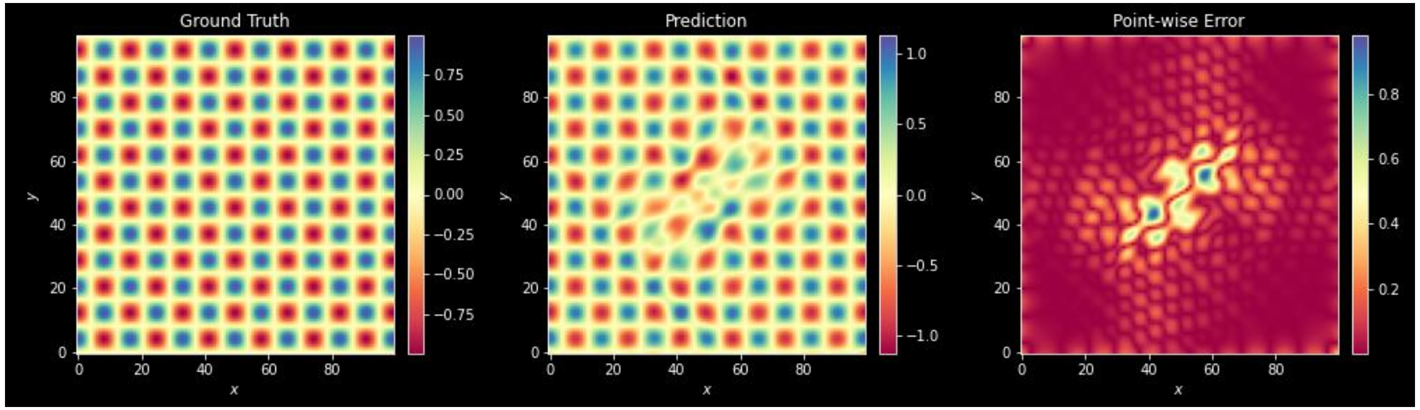
- Neural Networks with physics encoded by a PDE Loss
- Forward problem learning → surrogate models
- Inverse problem / Inferring parameters and governing equations

  → Costly for classic solvers
- Accuracy of PINNs → Challenge we want to tackle

- **2-D Poisson equation forward problem,** $N_{points} = 961, \omega = 6\pi$
- MSE Loss with Inverse Dirichlet [2] and A.D., $\epsilon_{L^\infty} = 1.24$, $t_{cpu} \approx 400$



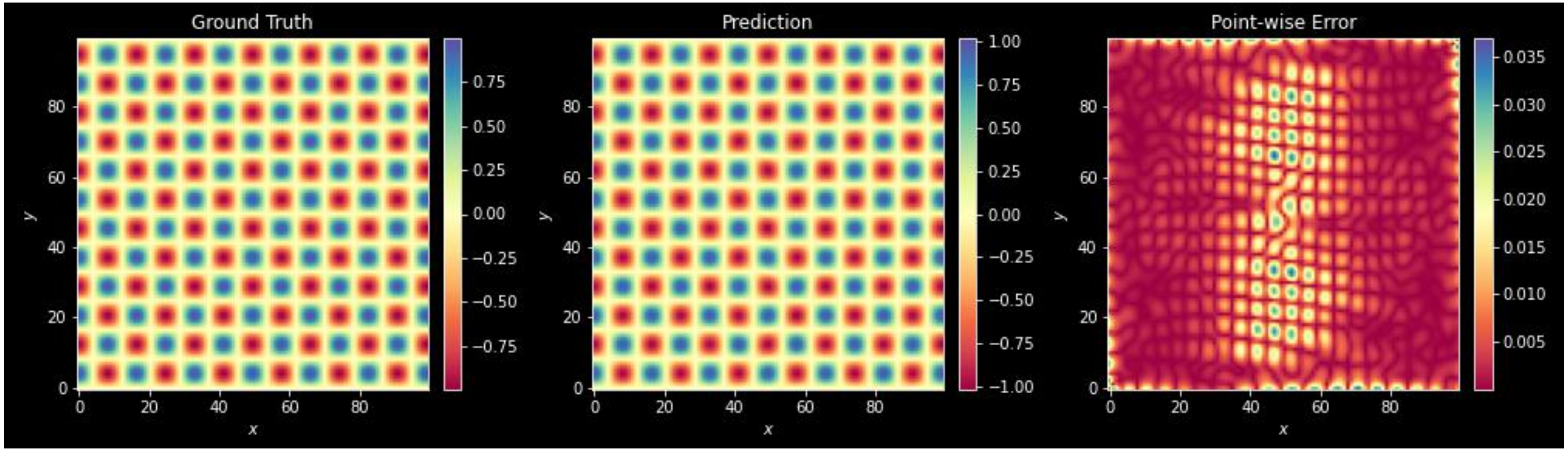
- Sobolev Loss ($\mathcal{L}_r = d_{L^2}, \mathcal{L}_b = d_{H^2}$) with A.D., $\epsilon_{L^\infty} = 9.78 \cdot 10^{-1}$, $t_{cpu} \approx 321$



[2] *Suryanarayana Maddu et al 2021 Mach. Learn.: Sci. Technol. in press https://doi.org/10.1088/2632- 2153/ac3712*

2-D Poisson equation forward problem, $N_{points} = 961$

- Sobolev Loss ($\mathcal{L}_r = d_{L^2}, \mathcal{L}_b = d_{H^2}$) without A.D., $\epsilon_{L^\infty} = 3.6 \cdot 10^{-2}$, $t_{cpu} \approx 190$



- Automatic differentiation is replaced by a discrete differential operator on a polynomial space.

Sobolev Spaces H^k

- $H^0 = L^2$ –Lebesgue space, $\Omega := (-1,1)^m \subset \mathbb{R}^m$

- The k-th Sobolev space $H^k(\Omega;\mathbb{R})$ is defined as:

$$H^k(\Omega;\mathbb{R}) \coloneqq \{f \in L^2(\Omega;\mathbb{R}) \mid \forall\, |\alpha| \le k, D^\alpha f \in L^2(\Omega;\mathbb{R})\}$$

- H^k is a Hilbert space with the norm:

$$||u-v||_{H^k}^2 \coloneqq ||u-v||_{L^2}^2 + \sum_{|\alpha|\le k} ||D^\alpha u - D^\alpha v||_{L^2}^2$$

- Sobolev Embedding Theorem: For $k > \frac{m}{2}, H^k(\Omega;\mathbb{R}) \subseteq C^0(\Omega;\mathbb{R})$

  If $||u-v||_{H^k} = 0 \longrightarrow u(x) = v(x)$, for all $x \in \Omega$

Variational Formulations (Example)

- Poisson equation with Dirichlet boundary conditions:

$$\begin{cases} -\Delta \mathrm{u} - f = 0 \ \text{ for } \mathrm{x} \in \Omega \\ \mathrm{u} = \mathrm{g} \ \text{ for } \mathrm{x} \in \partial\Omega \end{cases}$$

- We denote by **strong variational formulation**:

$$\int_{\Omega} (-\Delta \mathrm{u} - f)\phi \, dx = 0, \qquad \text{for } \mathrm{x} \in \Omega, \forall \phi \in C^{\infty}(\Omega; \mathbb{R})$$

- We denote by **weak variational formulation**:

$$\int_{\Omega} (\nabla \mathrm{u} \cdot \nabla \phi - f\phi) \, dx + \int_{\partial\Omega} (\phi \nabla u) \cdot \boldsymbol{n} \ dx = 0, \qquad \text{for } \mathrm{x} \in \Omega, \forall \phi \in C^{\infty}(\Omega; \mathbb{R})$$

- In practice we solve over a Polynomial space $\Pi_A \subset C^{\infty}(\Omega; \mathbb{R})$,spanned by the Lagrange basis $\{L_\alpha\}_{\alpha \in A}$

Computing Losses

- MSE Loss ⟶ Approximation of the L^2-integral

$$\int_\Omega (u-v)^2 dx \approx \frac{1}{N}\sum_{n\leq \mathrm{N}} \big(u(x_n)-v(x_n)\big)^2$$

- Gauss-Legendre cubature rules ⟶ Integrating polynomials exactly

$$\int_\Omega (u-v)^2 dx \approx \sum_{\alpha\in A} \big(u(P_\alpha)-v(P_\alpha)\big)^2 \omega_\alpha$$

- Generalize the Gauss-Legendere rule to Sobolev-Cubatures, *minterpy* [1]

$$\int_\Omega (D^\alpha u - D^\alpha v)^2 dx \approx \sum_{\alpha\in A} \big(u(P_\alpha)-v(P_\alpha)\big)^2 s_\alpha$$

MINTERPY

[1] minterpy Multi dimensional interpolation python 2021 *https://github.com/casus/minterpy/releases*

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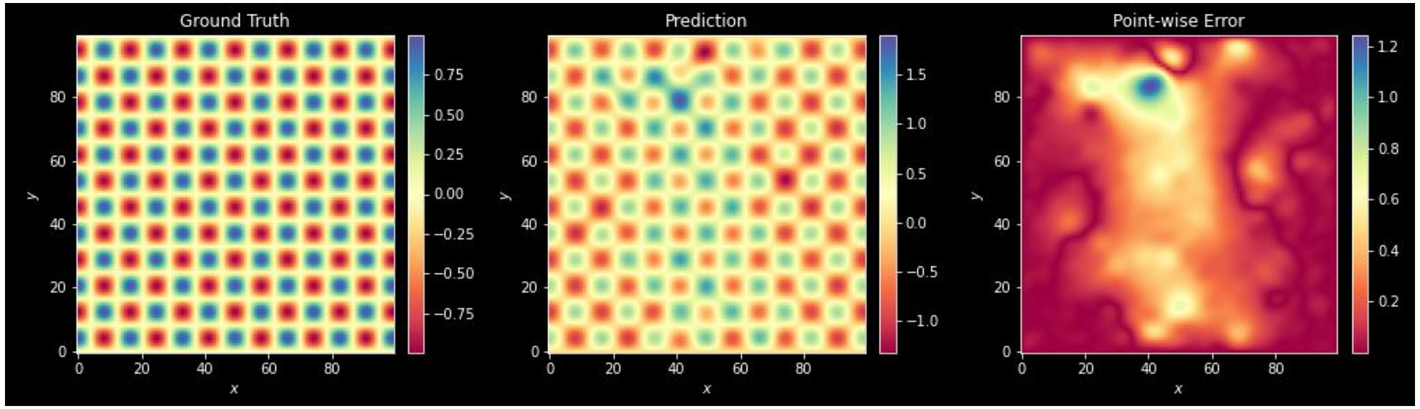

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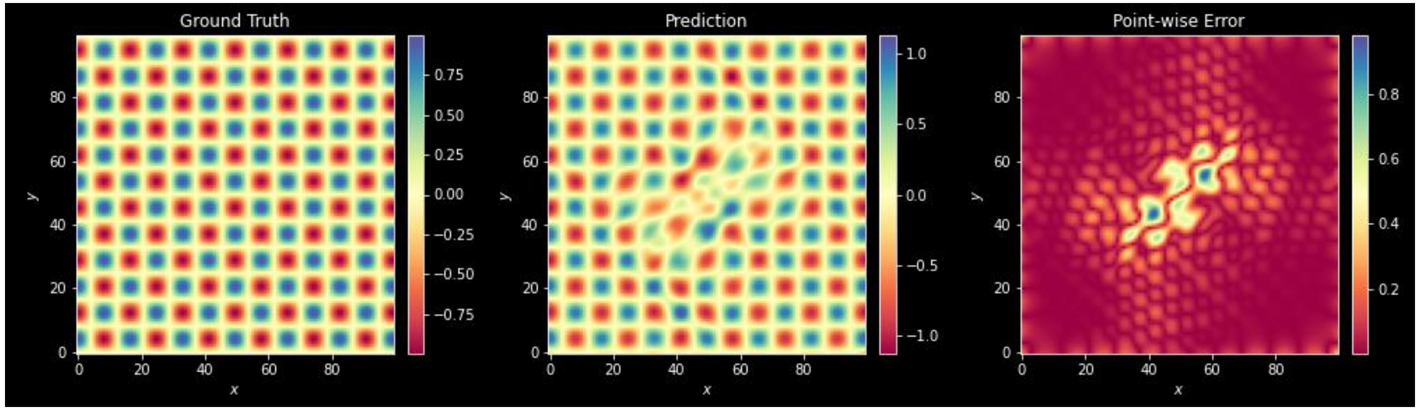

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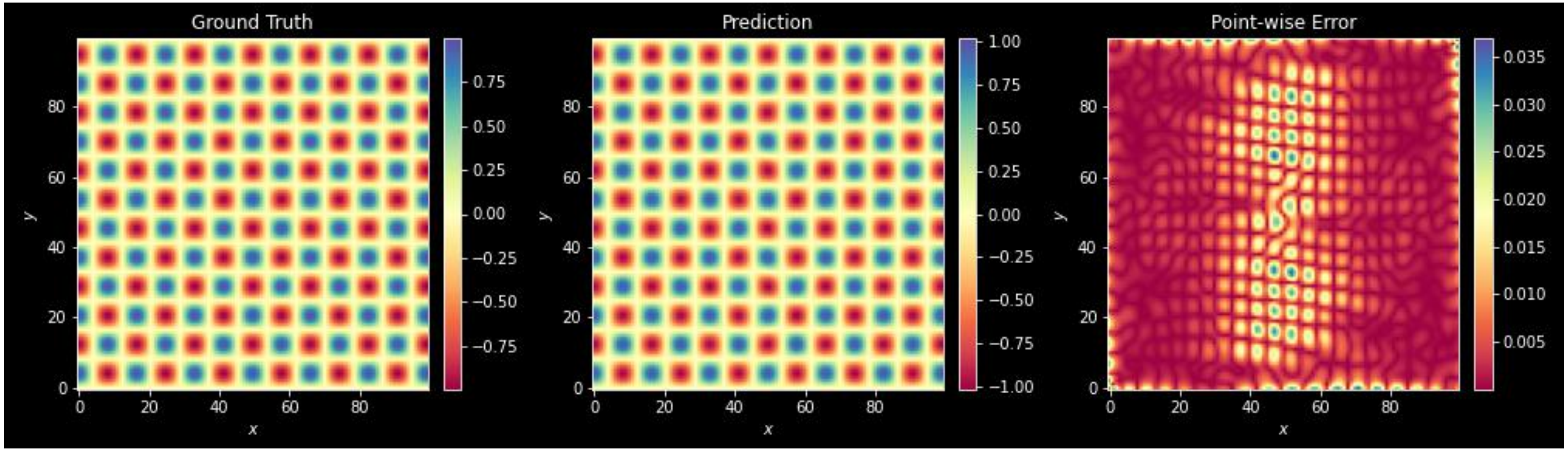

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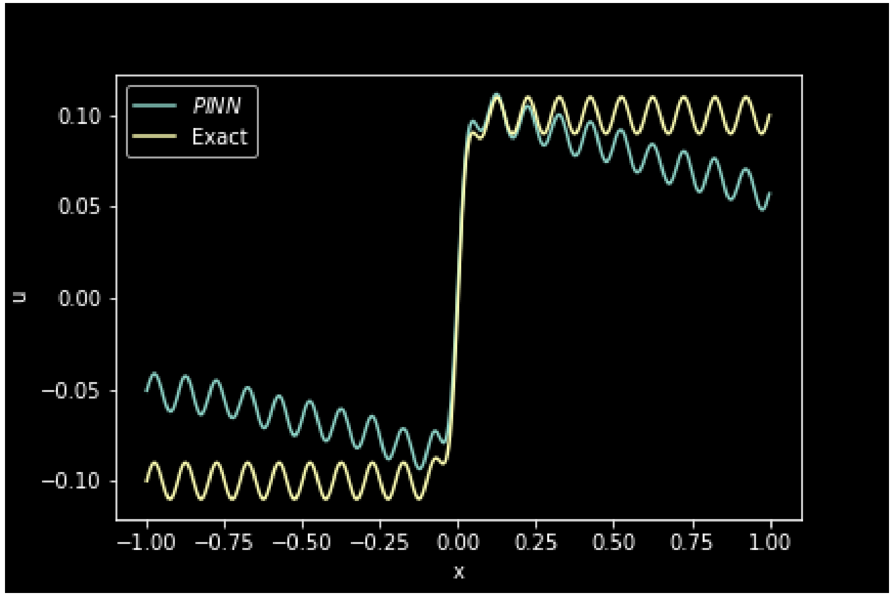
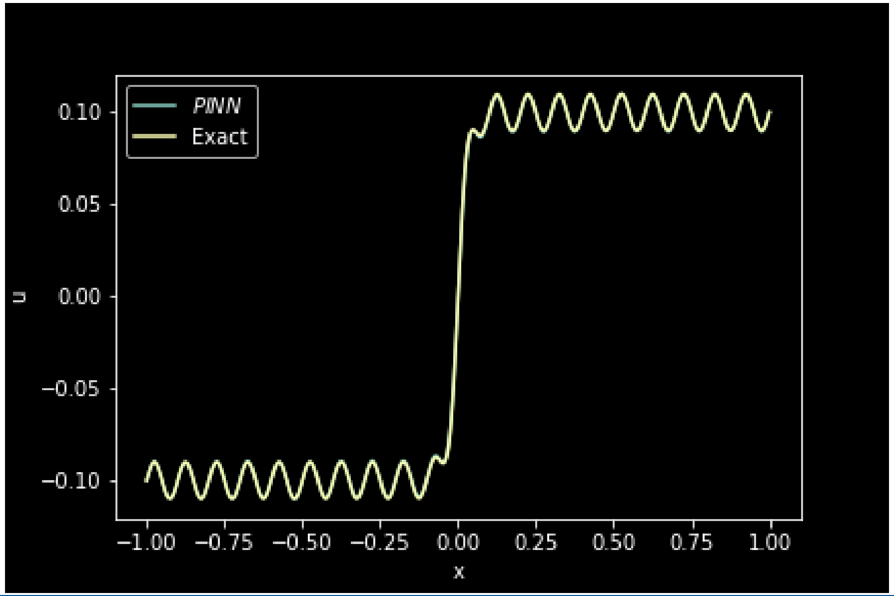
Other Numerical Results

- **1-D Poisson equation forward problem,** $\omega = 15\pi$ **,** $N_{points} = 100$

- Strong Sobolev Loss, $\epsilon_{L^\infty} = 0.049$

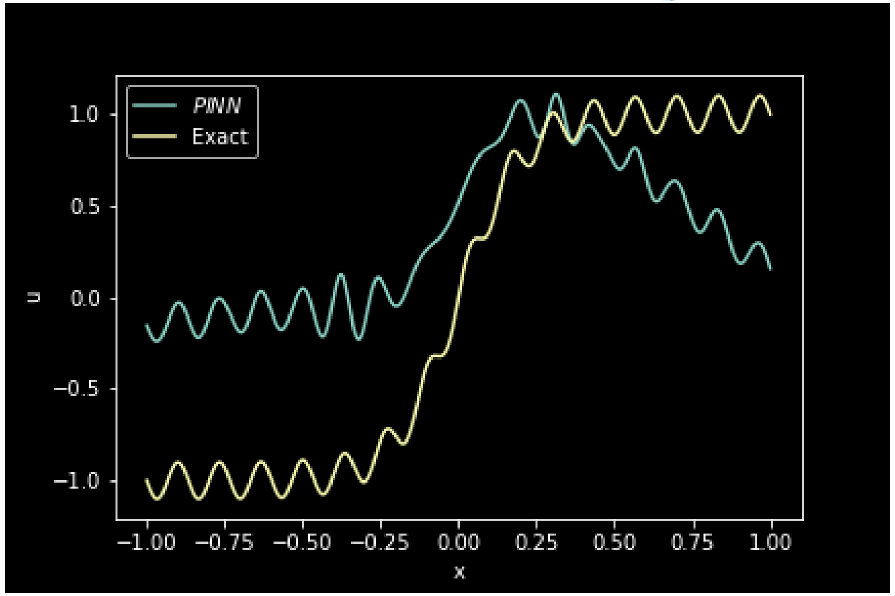


- Strong Variational Loss, $\epsilon_{L^\infty} = 0.002$

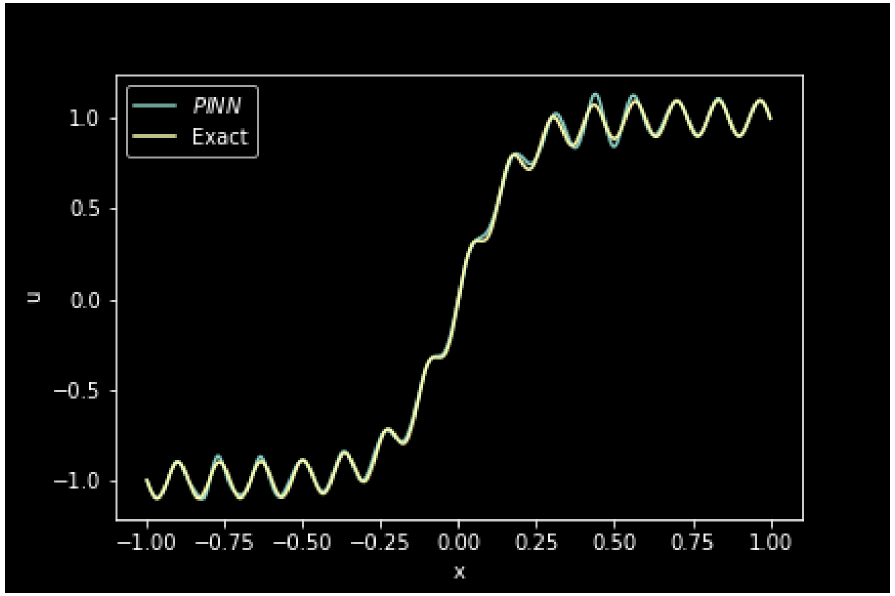


- **1-D Poisson equation forward problem,** $\omega = 15$ **,** $N_{points} = 50$

- Strong Sobolev Loss, $\epsilon_{L^\infty} = 1.002$



- Variational Loss, $\epsilon_{L^\infty} = 0.063$



1-D scaled Poisson equation forward problem, $\omega = 26.5\pi$, $N_{points} = 100$

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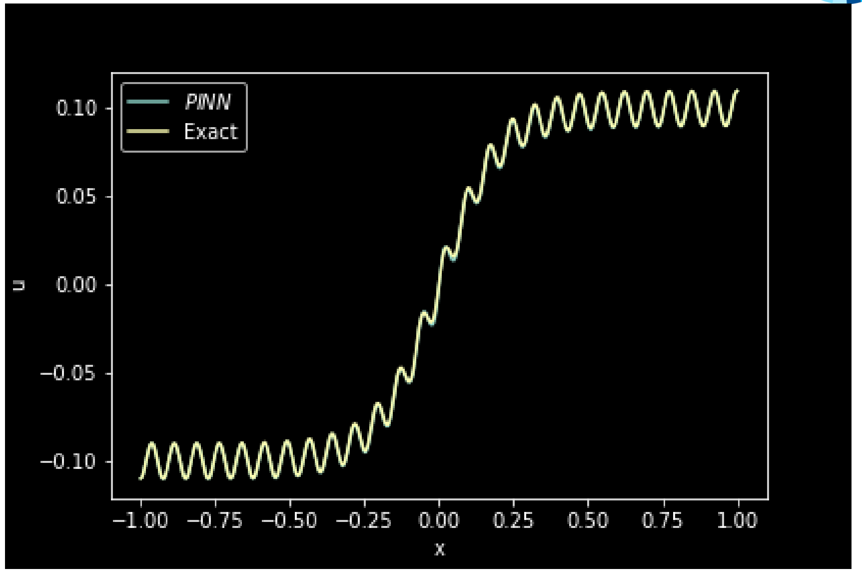
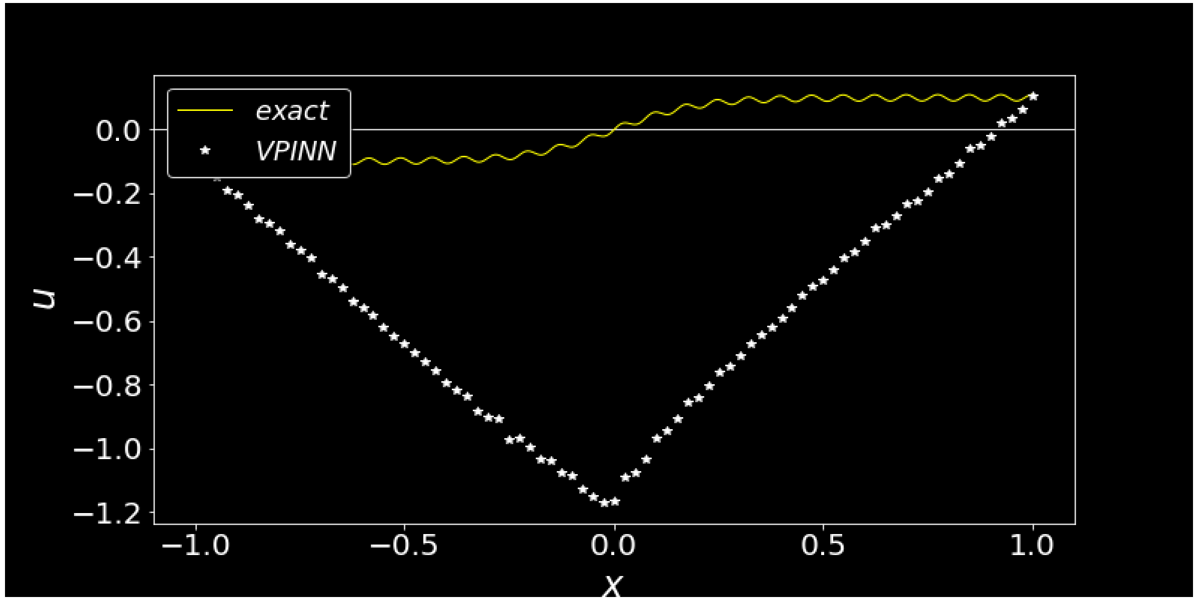


- Variational Loss, $\epsilon_{L^\infty} = 0.003$, $t_{cpu} \approx 130$



- VPINN [3], $\epsilon_{L^\infty} = 1.17$, $t_{cpu} \approx 144$

[3] Kharazmi E. et al 2021,
Computer Methods in Applied Mechanics and Engineering in press
https://doi.org/10.1016/j.cma.2020.113547

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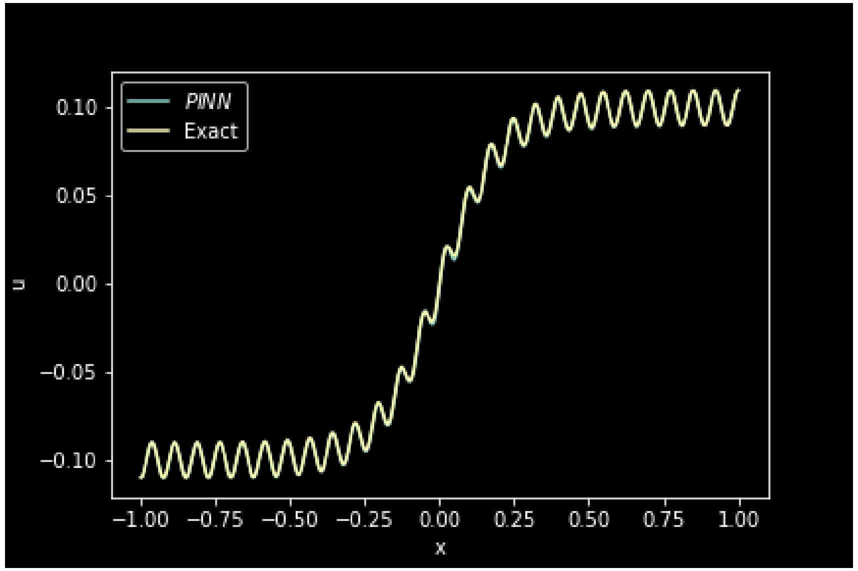
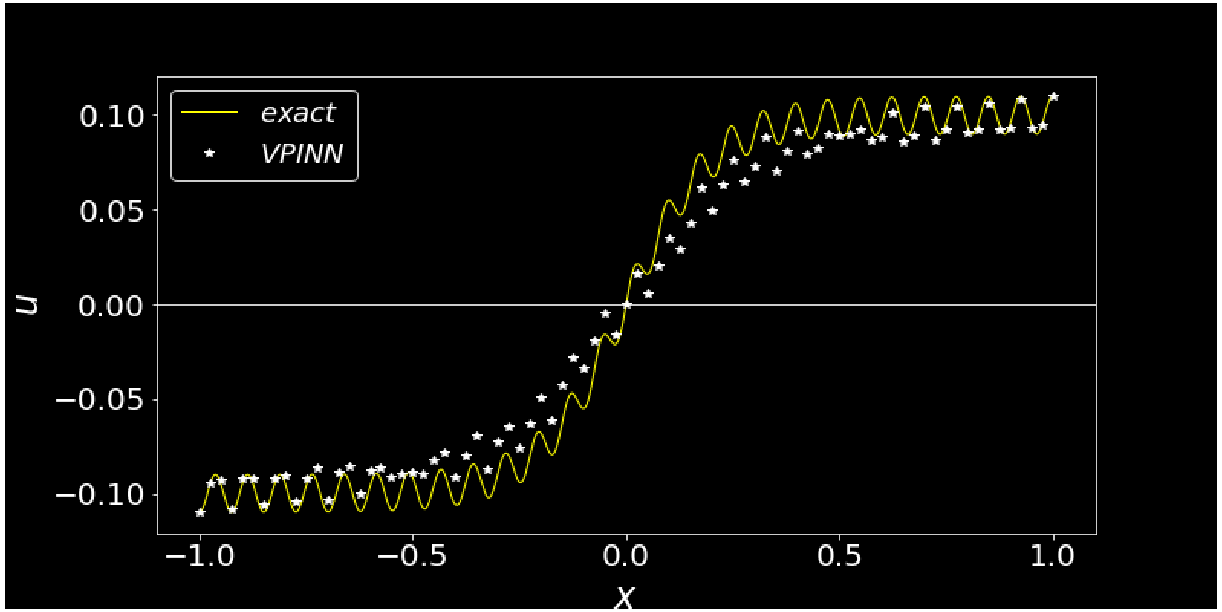


- VPINN [3], wit domain decomposition, $N_{dom} = 3$, $\epsilon_{L^\infty} = 0.02$, $t_{cpu} \approx 360$

- MSE with I.D. [2] becomes unstable



Overview

- This are preliminary results ⟶ we are working to scale it up, e.g. higher dimensions

- Sobolev Cubatures are expected to be included as feature on the Beta release of *minterpy*

- We want to extend the approach to complex geometries (Biological Systems)

- We want to apply the method to real problems in cooperation with:
  - Ivo Sbalzarini, MOSAIC group CSBD
  - Attila Cangi, Matter Under Extreme Conditions CASUS
  - Nico Hoffman, ML group HZDR

- Contact us if you are interested ! j.suarez-cardona@hzdr.de

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Thank you !

References

- [1] *minterpy Multi dimensional interpolation python 2021* *https://github.com/casus/minterpy/releases*

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