Neural operator preconditioning for accelerating the solution of the parametric Helmholtz equations

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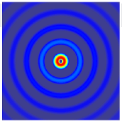
Parametric Helmholtz equations

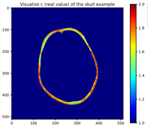
Helmholtz equation:

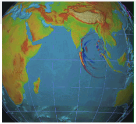
Parametric PDEs:
$$\begin{cases} \left[\nabla^2 + \left(\frac{\omega}{c(x)}\right)^2\right] u(x) = \rho(x) \\ \text{(subject to the Sommerfeld radiation condition at infinity)} \\ + \text{ Perfectly Matched Layer (PML) BCs on domain } \Omega \end{cases} \quad (1)$$

- let $x \in \mathbb{R}^d$ be the grid points in the d-dimensional Ω ($d = 1, 2, 3$);
- $u(x) : \mathbb{R}^d \to \mathbb{C}$ is the complex acoustic wavefield to be computed;
- $\rho(x) : \mathbb{R}^d \to \mathbb{C}$ is the source function (*could be fixed or not*);
- $c(x) : \mathbb{R}^d \to \mathbb{R}_+$ is a speed of sound distribution function (*could be fixed or not*) and $\omega = 1 \in \mathbb{R}_+$ is an angular frequency of the source.

Part of the Physical Applications:







Learning parametric Helmholtz operators

Transfer the differential expression to the discrete form:

$$\text{Parametric PDEs:} \begin{cases} \left[\nabla^2 + \left(\frac{\omega}{c(x)}\right)^2\right] u(x) = \rho(x) \\ + \text{ PML BCs on domain } \Omega \\ \quad \text{Discrete derivatives} \Downarrow \text{ FEM, FDM, } \textbf{FFT}, \ldots \\ A(\mathrm{c})\mathrm{u} = \mathrm{b}, \text{ with LinearOp } A(\mathrm{c}) \in \mathbb{C}^{n \times n}, \ \mathrm{u}, \ \mathrm{b} \in \mathbb{C}^n \end{cases} \tag{2}$$

After discretization, numerical linear algebra methods, like subspace methods, can be used to solve the parametric Eq. (2). However,

- simply using subspace methods without preconditioning is much less effective for solving the Helmholtz Eqs.[a];
- generate a properly algebraic preconditioner could be possible (if the n is not too big) but is as challenging as solve the system directly;
- generally, the algebraic preconditioning needs to be re-generated for each of the parametric Helmholtz Eqs. (2).

[a] Ernst and Gander. Why it is Difficult to Solve Helmholtz Problems with Classical Iterative Methods. 2012

Learning parametric Helmholtz operators

Transfer the differential expression to the discrete form:

$$\text{Parametric PDEs:} \begin{cases} \left[\nabla^2 + \left(\frac{\omega}{c(x)}\right)^2\right] u(x) = \rho(x) \\ + \text{ PML BCs on domain } \Omega \\ \quad \text{Discrete derivatives} \Downarrow \text{ FEM, FDM, } \textbf{FFT}, \ldots \\ A(c)\mathrm{u} = \mathrm{b}, \text{ with LinearOp } A(c) \in \mathbb{C}^{n\times n}, \ \mathrm{u}, \ \mathrm{b} \in \mathbb{C}^n \end{cases} \tag{2}$$

In recent decade, the thrived neural networks (NNs) solvers, like the physics-informed neural networks (PINNs)[a], is used to solve the parametric Eq. (2) without discretization. However, these NNs solvers

- are usually costly in training[b], and may fail to solve challenging PDEs if without finely tuning of the hyper-parameters of the NNs;
- solve the PDEs without the theoretical convergence guarantee;
- generally reach limited accuracy and exhibit limited or NO network generalizability, thus re-training is required even it is costly.

[a] Lu et al., Physics-Informed Neural Networks with Hard Constraints for Inverse Design. SISC. 2021

[b] Strubell et al., Energy and policy considerations for deep learning in NLP. ACL meeting, Italy. 2019

Learning parametric Helmholtz operators

Transfer the differential expression to the discrete form:

$$\text{Parametric PDEs:} \begin{cases} \left[\nabla^2 + \left(\frac{\omega}{c(x)}\right)^2\right] u(x) = \rho(x) \\ + \text{ PML BCs on domain } \Omega \\ \quad \text{Discrete derivatives} \Downarrow \text{ FEM, FDM, } \textbf{FFT}, \ldots \\ A(\mathrm{c})\mathrm{u} = \mathrm{b}, \text{ with LinearOp } A(\mathrm{c}) \in \mathbb{C}^{n\times n}, \ \mathrm{u}, \ \mathrm{b} \in \mathbb{C}^n \end{cases} \quad (2)$$

* **Goal of this work** $\Rightarrow$ To learn neural operator $\mathcal{F}_\theta$ that approximates

$$A(\mathrm{c})^{-1} \ \text{ by } \mathcal{F}_\theta([\mathrm{b}, \mathrm{c}, (\mathrm{BCs})]) \longrightarrow \mathrm{u}_\theta \sim A(\mathrm{c})^{-1}\mathrm{b}$$

The learned $\mathcal{F}_\theta$ can be used as a flexible preconditioner for the subspace methods (like FGMRES) to accelerate the solution of parametric Eq. (2) with varying c, varying b and varying domain Ω but **without re-training**.

* **Loss-function:**

$$\min_\theta \frac{\|A(\mathrm{c})\mathrm{u}_\theta - \mathrm{b}\|_2^2}{\|\mathrm{b}\|_2^2} \quad (3)$$

The generalized Arnoldi relation

Originally, the FGMRES method[a] have the generalized Arnoldi relation

$$AZ_m = V_{m+1}\bar{H}_m, \tag{4}$$

where $V_{m+1} = [v_1, ..., v_{m+1}]$ is the Krylov basis, and $Z_m = [z_1, ..., z_m]$ is the preconditioned Krylov basis.

In our FGMRES case, we have

$$z_i = \mathcal{F}_\theta(v_i), \; i = 1, \dots m, \tag{5}$$

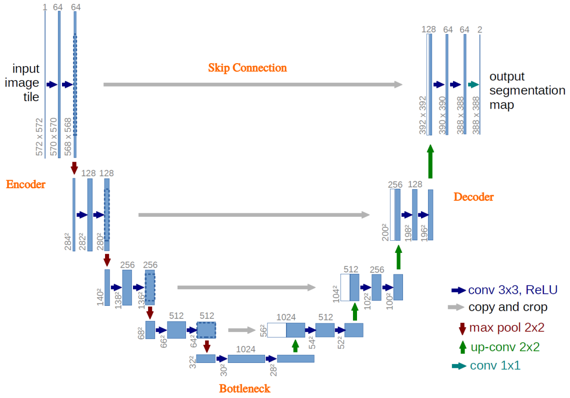
where $\mathcal{F}_\theta$ is the trained non-linear neural operator satisfies $\mathcal{F}_\theta \sim A^{-1}$. This part is computed with single machine precision (float 32), the one used in the training process, and other parts are in double precision.

$\Rightarrow$ Given there is no information about the data structure of the Krylov basis, the neural operator $\mathcal{F}_\theta$ is trained with randomly generated datasets.

[a] Y. Saad, A Flexible Inner-Outer Preconditioned GMRES Algorithm. SISC. 1993

U-Net architecture

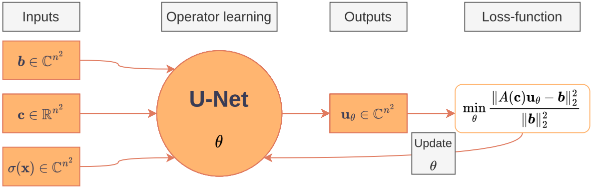
U-Net[a] architecture with 4 **depth**:



Each blue box corresponds to a multi-channel feature map. The number of channels is denoted on top of the box. The x-y-size is provided at the lower left edge of the box. White boxes represent copied feature maps. The arrows denote the different operations.

[a][Figure 1] Ronneberger et al., U-Net: Convolutional Networks for Biomedical Image Segmentation. 2015

U-Net with meshes in 2D (domain 64×64)



Training (on 2 V100 GPUs, depth $= 4$, train. time: 49.83min):

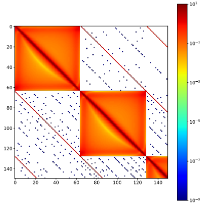
- Fixed grid point $\mathrm{x} \in \mathbb{R}^{\boldsymbol{n}^2}$ in the 2-dimensional domain ($n = 64$ for 2D case)
- Random source term $\mathrm{b} \in \mathbb{C}^{\boldsymbol{n}^2} \sim \mathcal{N}(0, 1)$ satisfying normally distr.
- Random speed of sound $\mathrm{c} \in \mathbb{R}^{\boldsymbol{n}^2}{}_+$ uniformly distributed on the interval [1, 2] and fixed frequency of the source $\omega = 1 \in \mathbb{R}_+$
- Function $\sigma(\mathrm{x}) : \mathbb{R}^{\boldsymbol{n}^2} \to \mathbb{C}^{\boldsymbol{n}^2}$ used in the definition of the PML boundary condition
- U-Net 2d: Training with single machine precision (float 32); Trainable params. - 832 K

Testing:

☺ Trained U-Net preconditioner can accelerate the solution of Eq. (2) with varying b c, domain size Ω (bcf. the discretisation invariance property from the convolution property)

Compare trained U-Net to algebraic preconditioner

Visualization of the first 150 sequential elements of a $64^2 \times 64^2$ matrix:

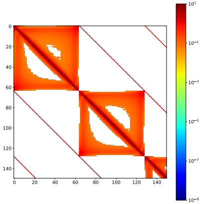


(a). Coefficient matrix A with $\frac{\text{nnz}}{n^2} \times \% = 33.38\%$

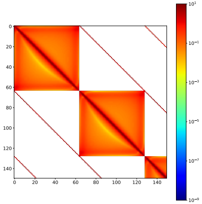
A with elements a_{ij} to be placed in matrix M.

$$(1).\ M(i,j) = \begin{cases} a_{ii}, & \text{if } \|a_{ii}\| \geq \texttt{thresh} \text{ for } i = j, \\ a_{ij}, & \text{if } \dfrac{\|a_{ij}\|}{\|a_{ii}\|\|a_{jj}\|} \geq \texttt{thresh} \text{ for } i \neq j. \end{cases}$$

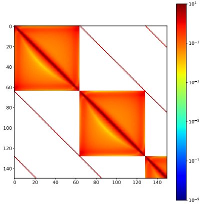
$$(2).\ \frac{\|A - M\|_F}{\|A\|_F} = \begin{cases} 5.41 \times 10^{-2} \text{ if } \texttt{thresh} = 10^{-3}, \\ 2.04 \times 10^{-3} \text{ if } \texttt{thresh} = 10^{-4}, \\ 1.81 \times 10^{-16} \text{ if } \texttt{thresh} = 10^{-5}. \end{cases}$$



(b). M with $\texttt{thresh}= 10^{-3}$, $\frac{\text{nnz}}{n^2} \times \% = 1.16\%$



(c). M with $\texttt{thresh}= 10^{-4}$, $\frac{\text{nnz}}{n^2} \times \% = 3.00\%$

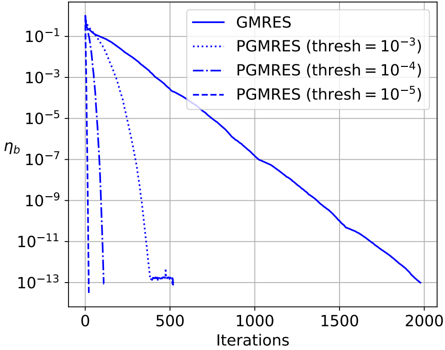


(d). M with $\texttt{thresh}= 10^{-5}$, $\frac{\text{nnz}}{n^2} \times \% = 3.10\%$

Compare trained U-Net to algebraic preconditioner

Solve $A(c)u = b$ on 2D domain 64×64 (i.e., $A(c) \in \mathbb{C}^{64^2 \times 64^2}$):

* All involved algorithms are run on the same CPUs/GPUs device with Python prototype.
* $\eta_b = \frac{\|A(c)u - b\|}{\|b\|}$. We stop the iteration when $\eta_b \leq \varepsilon$ with $\varepsilon = 10^{-13}$ by default.



PGMRES with varying `thresh`

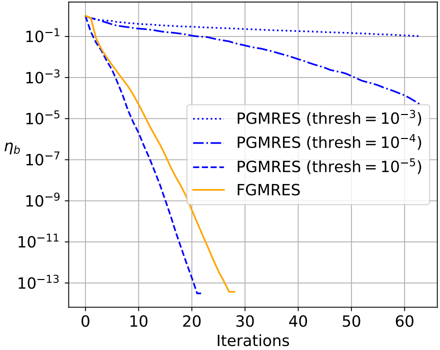
$$\frac{\|A - M\|_F}{\|A\|_F} = \begin{cases} 5.41 \times 10^{-2} & \text{if thresh} = 10^{-3}, \\ 2.04 \times 10^{-3} & \text{if thresh} = 10^{-4}, \\ 1.81 \times 10^{-16} & \text{if thresh} = 10^{-5}. \end{cases}$$

- PGMRES: GMRES preconditioned by `spilu`(M), which is realized by applying sparse `ilu` to the sparse matrix M with selected elements from coefficient matrix A

Compare trained U-Net to algebraic preconditioner

Solve $A(c)u = b$ on 2D domain 64×64 (i.e., $A(c) \in \mathbb{C}^{64^2 \times 64^2}$):

* FGMRES is GMRES preconditioned by the trained U-Net with depth = 4.
* FGMRES is implemented by the mixed-precision calculation.



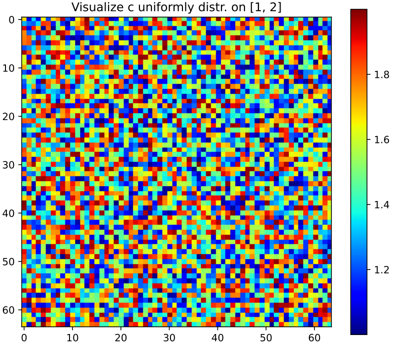
FGMRES and PGMRES

$$\frac{\|A - M\|_F}{\|A\|_F} = \begin{cases} 5.41 \times 10^{-2} \text{ if thresh} = 10^{-3}, \\ 2.04 \times 10^{-3} \text{ if thresh} = 10^{-4}, \\ 1.81 \times 10^{-16} \text{ if thresh} = 10^{-5}. \end{cases}$$

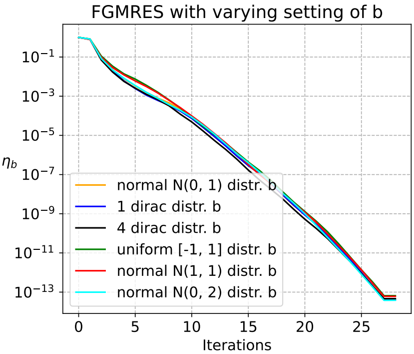
- The effectiveness of trained U-Net preconditioner is close to (could be the same as) spilu(M) with thresh= 10^{-5} (the best algebra preconditioner for this example)

Network generalizability: varying the source function b

Solve $A(\mathrm{c})\mathrm{u} = \mathrm{b}$ on 2D domain 64×64 (i.e., $A(\mathrm{c}) \in \mathbb{C}^{64^2 \times 64^2}$):



(a). Visualize the fixed $\mathrm{c} \in \mathbb{R}^{64^2}$

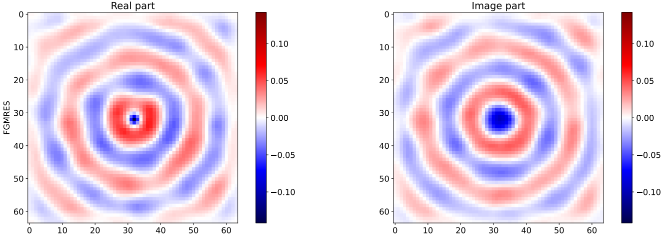


(b). Relative residual of FGMRES

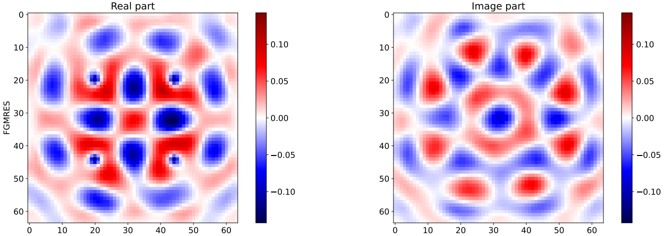
- Speed of sound $\mathrm{c} \in \mathbb{R}^{64^2}$ is fixed and satisfying uniform distribution on interval $[1, 2]$
- Performance of trained U-Net preconditioner is independent from varying the datatype of the $\mathrm{b} \in \mathbb{C}^{64^2}$ or varying the mean and median value of the normal setting of b

Network generalizability: varying the source function b

Visualize wavefiled $u \in \mathbb{C}^{64^2}$ solved by 1 dirac for $b \in \mathbb{C}^{64^2}$ (with fixed c):



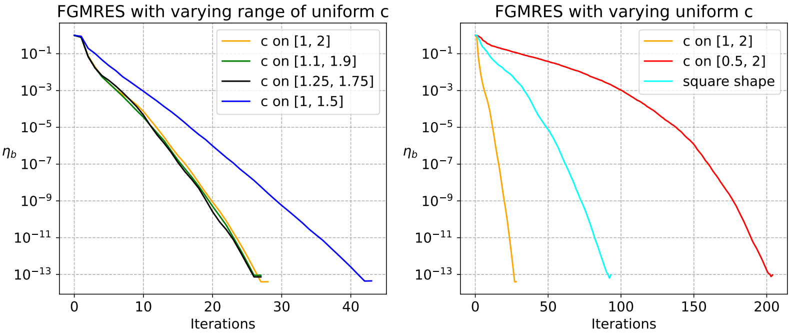
Visualize wavefiled $u \in \mathbb{C}^{64^2}$ solved by 4 dirac for $b \in \mathbb{C}^{64^2}$ (with fixed c):



Testing trained U-Net operator with $\mathcal{N}(0,1)$ source function on 2D

Network generalizability: varying the speed of sound c

Solve $A(\mathrm{c})\mathrm{u} = \mathrm{b}$ on 2D domain 64×64 (i.e., $A(\mathrm{c}) \in \mathbb{C}^{64^2 \times 64^2}$):

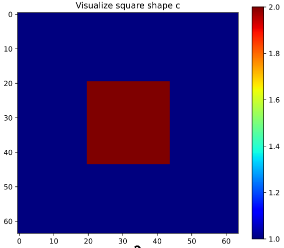


(a). shrink the interval (b). enlarge the interval & special structure

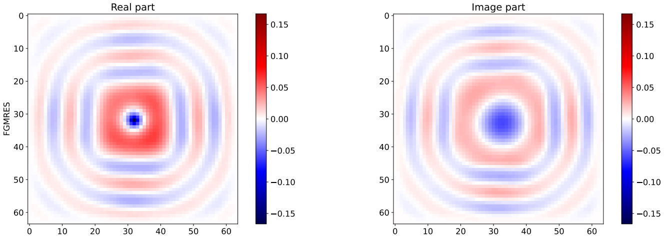
- Source function $\mathrm{b} \in \mathbb{C}^{64^2}$ is fixed with 1 dirac setting, 1 in grid position (32, 32), the center of domain 64×64, and 0 elsewhere in domain
- Square shape of $\mathrm{c} \in \mathbb{R}^{64^2}$: domain $[20:44, 20:44] = 2$ and 1 elsewhere
- Varying the range of the c satisfying uniform distribution and varying the its shape can effect the performance of the trained U-Net preconditioner

Network generalizability: varying the speed of sound c

Visualize $c \in \mathbb{R}^{64^2}$ with square shape:

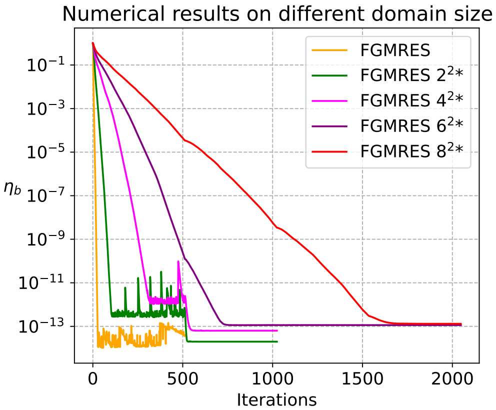


Visualize complex wavefiled $u \in \mathbb{C}^{64^2}$ solved by $c \in \mathbb{R}^{64^2}$ in square shape:



Network generalizability: varying the domain size

Solve $A(c)u = b$ from 2D domain 64×64 until 512×512 (i.e., from linear operator $A(c) \in \mathbb{C}^{64^2 \times 64^2}$ to $A(c) \in \mathbb{C}^{512^2 \times 512^2}$):



FGMRES — domain 64×64

FGMRES 2^2* — domain 128×128

FGMRES 4^2* — domain 256×256

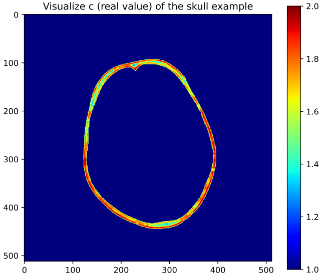
FGMRES 6^2* — domain 384×384

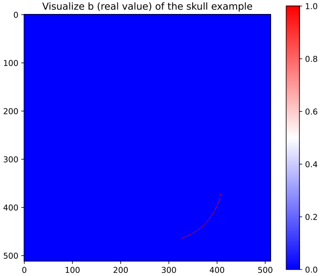
FGMRES 8^2* — domain 512×512

- U-Net trained on 2D domain 64×64 (with normal distr. $\mathcal{N}(0, 1)$ $b \in \mathbb{C}^{64^2}$ and uniform distr. $c \in \mathbb{R}^{64^2}$ in interval [1,2]) exhibits excellent network generalizability from the 4x larger domain 128×128 until the **64x larger** domain 512×512

Network generalizability: Adult human skull example

Solve $A(\mathrm{c})\mathrm{u} = \mathrm{b}$ with the **structured dataset** for both $\mathrm{c} \in \mathbb{R}^{512^2}$ and $\mathrm{b} \in \mathbb{R}^{512^2}$ on a 64x larger 2D domain 512×512 ($A(\mathrm{c}) \in \mathbb{C}^{512^2 \times 512^2}$):





This example is downloaded from the qure.ai dataset[a]

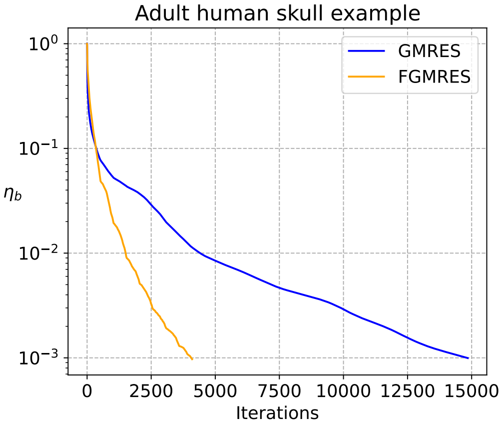
Recall part of the training settings:

- Random training datasets on domain 64×64: $\mathrm{b} \in \mathbb{C}^{64^2}$ satisfies standard Normal distr. $\mathcal{N}(0, 1)$; $\mathrm{c} \in \mathbb{R}^{64^2}$ is Uniform distr. on interval $[1, 2]$

[a] http://headctstudy.qure.ai/dataset

Network generalizability: Adult human skull example

Solve $A(c)u = b$ with the **structured dataset** for both c and b on 2D domain 512×512 (i.e., $A(c) \in \mathbb{C}^{512^2 \times 512^2}$):

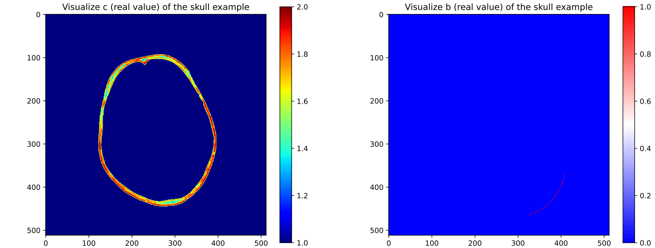


- Comparison of FGMRES (NNs trained on domain 64×64) to GMRES on solving the skull example (on 512×512 from CQ500 with 491 scans) to reaching accuracy at 10^{-3}
- Consumed its & CPU time (Training time of U-Net on 2 V100 GPUs is 49.83min): FGMRES = 4097 & 4.24h; GMRES = 14849 & 13.16h

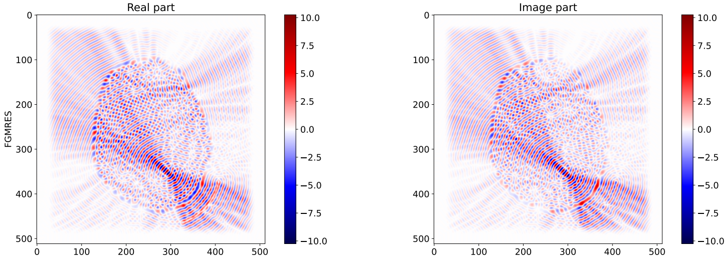
Testing trained U-Net operator with $\mathcal{N}(0,1)$ source function on 2D

Network generalizability: Adult human skull example

Visualization the structured dataset of the skull example on 2D domain 512×512:



Visualize the complex wavefiled $c \in \mathbb{R}^{512^2}$ of human skull example solved by FGMRES:



PINNs & DeepONet & FNO

Other neural networks (NNs) architectures for the parametric Helmholtz equations:

- NNs solver:
  - PINNs: Lu et al., Physics-Informed Neural Networks with Hard Constraints for Inverse Design. SISC. 2021
- NNs operators:
  - DeepONet: Lu et al., Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. 2021;
  - FNO: Kovachki et al., Neural Operator: Learning Maps Between Function Spaces With Applications to PDEs. 2023

$\Rightarrow$ Compare to above NNs architectures, **U-Net** is the optimal one that meets all our goal and exhibits the robust preconditioning behavior

Three random setting for the source function b:

- **Normal distr.** $\mathcal{N}$**(0,1)**: satisfying the standard normal distribution $\mathcal{N}(0,1)$;
- Uniform distr. $[-1, 1]$: satisfying the uniformly distribution on interval $[-1, 1]$;
- Dirac setting: with one non-zero value in the random position in the 2D domain;

Take home message of this work

Goal: To learn the optimal neural operator $\mathcal{F}_\theta$ for accelerating the solution of the parametric Helmholtz Eqs.

Training different neural networks (NNs) $\Rightarrow$ choose the optimal NNs architecture —> **U-Net is the optimal one for our case**

Training U-Net on 2D with different settings for b $\Rightarrow$ choose the optimal training dataset —> **Standard Normal distr. $\mathcal{N}$(0,1) for** b

$\Rightarrow$ The performance of trained neural operator depends on:

- the choosing of NNs architecture;
- the setting of training datasets;
- the tuning of hyper-parameters of NNs;
- the utilities of training tools like pytorch-lightning.

⌚ Research report version of this work will soon be accessible online at HAL (https://inria.hal.science/) !

$\longrightarrow$ Yanfei Xiang (yanfei.xiang@inria.fr)

My co-workers from Inria and Cerfacs

- Inria: Luc Giraud and Maksym Shpakovych
- Cerfacs: Paul Mycek and Carola Kruse

Luc Giraud

Paul Mycek

Maksym Shpakovych

Carola Kruse

*We are **Concace** joint Inria team with Airbus CR&T and Cerfacs.*

Acknowledgement

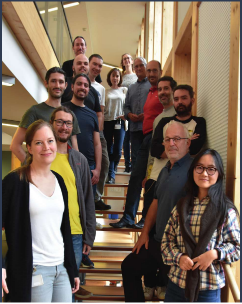
Concace

Numerical & Parallel Composability for High Performance Computing

Joint Inria-Industry Project Team with Airbus Central R&T and Cerfacs

To deal with large size and large dimension problems coming from model- and data-driven applications, Concace will take advantage of modern development tools and languages to design high-level expressions of complex parallel algorithms.

While the traditional approach to HPC is to fully exploit hardware, Concace's complementary approach will enable a richer composability of numerical methods, allowing to fully exploit existing and new numerical algorithms.

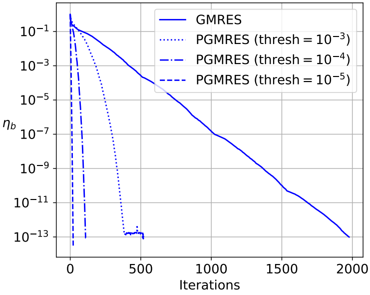


Thank you for your attention!

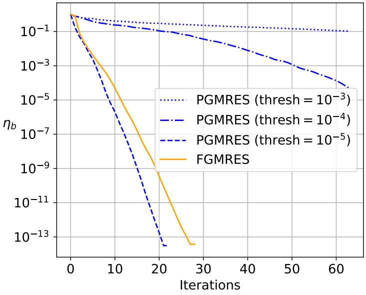
Questions ?

Consuming time

Solve $A(c)u = b$ on 2D domain 64×64 ($A(c) \in \mathbb{C}^{64^2 \times 64^2}$):



(a). PGMRES with varying `thresh`



(b). FGMRES and PGMRES

- PGMRES: GMRES precondioned by `spilu`(M), which is realized by applying sparse `ilu` to the sparse matrix M with selected elements from coefficient matrix A
- The effectiveness of trained U-Net preconditioner is close to (could be the same as) `spilu`(M) with `thresh`$= 10^{-5}$ (the best algebra preconditioner for this example)
- Iterations & **GPUs time**: GMRES: 1978 & 141.8737s;
  FGMRES: 29 & 4.3403s; PGMRES (`thresh`$= 10^{-3}$): 522 & 43.0996s;
  PGMRES (`thresh`$= 10^{-4}$): 111 & 3.2276s; PGMRES (`thresh`$= 10^{-5}$): 23 & 0.6582s