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Yanfei Xiang, Luc Giraud, Paul Mycek, Maksym Shpakovych, Carola Kruse

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

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Yanfei Xiang (✉ [yanfei.xiang@inria.fr](mailto:yanfei.xiang@inria.fr))

Concace team, Centre Inria de l'Université de Bordeaux

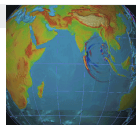
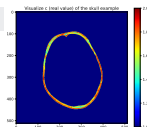
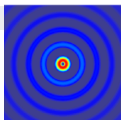
# Parametric Helmholtz equations

**Helmholtz equation:**

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

- let  $x \in \mathbb{R}^d$  be the grid points in the  $d$ -dimensional  $\Omega$  ( $d = 1, 2, 3$ );
- $u(x) : \mathbb{R}^d \rightarrow \mathbb{C}$  is the complex acoustic wavefield to be computed;
- $\rho(x) : \mathbb{R}^d \rightarrow \mathbb{C}$  is the source function (*could be fixed or not*);
- $c(x) : \mathbb{R}^d \rightarrow \mathbb{R}_+$  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:

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

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.<sup>a</sup>;
- **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).

<sup>a</sup> 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:

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

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

- are usually **costly in training<sup>b</sup>**, 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.

<sup>a</sup> Lu et al., Physics-Informed Neural Networks with Hard Constraints for Inverse Design. SISC. 2021

<sup>b</sup> 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:

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

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

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

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**  $\Omega$  but **without re-training**.

\* **Loss-function:**

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

## The generalized Arnoldi relation

Originally, the FGMRES method<sup>a</sup> have the generalized Arnoldi relation

$$AZ_m = V_{m+1}\bar{H}_m, \quad (4)$$

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

In our FGMRES case, we have

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

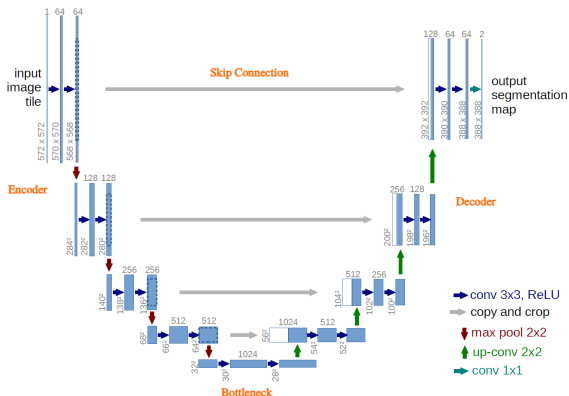
where  $\mathcal{F}_\theta$  is the trained **non-linear** neural operator satisfies  $\mathcal{F}_\theta \sim A^{-1}$ . This part is computed with **single machine precision (float 32)**, the one used in the training process, and other parts are in double precision.

⇒ 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**.

<sup>a</sup>Y. Saad, A Flexible Inner-Outer Preconditioned GMRES Algorithm. SISC. 1993

# U-Net architecture

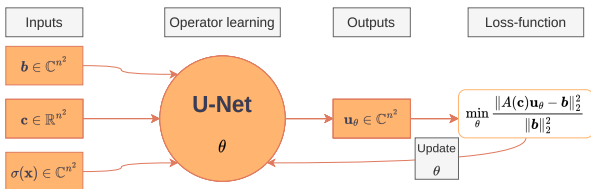
U-Net<sup>a</sup> architecture with 4 depth:



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.

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



U-Net with meshes in 2D (domain  $64 \times 64$ )

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

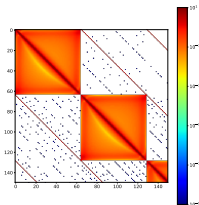
- Fixed grid point  $\mathbf{x} \in \mathbb{R}^{n^2}$  in the 2-dimensional domain ( $n = 64$  for 2D case)
- Random source term  $\mathbf{b} \in \mathbb{C}^{n^2} \sim \mathcal{N}(0, 1)$  satisfying normally distr.
- Random speed of sound  $\mathbf{c} \in \mathbb{R}^{n^2+}$  uniformly distributed on the interval  $[1, 2]$  and fixed frequency of the source  $\omega = 1 \in \mathbb{R}_+$
- Function  $\sigma(\mathbf{x}) : \mathbb{R}^{n^2} \rightarrow \mathbb{C}^{n^2}$  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  $\mathbf{b}$ ,  $\mathbf{c}$ , domain size  $\Omega$  (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:

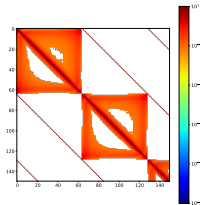


(a). Coefficient matrix  $A$  with  
 $\frac{\text{nnz}}{n^2} \times \% = 33.38\%$

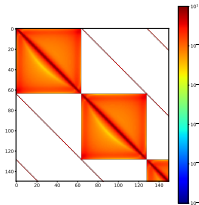
$A$  with elements  $a_{ij}$  to be placed in matrix  $M$ .

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

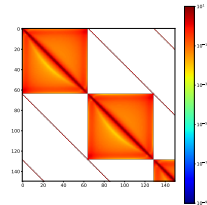
$$(2). \frac{\|A - M\|_F}{\|A\|_F} = \begin{cases} 5.41 \times 10^{-2} & \text{if thresh} = 10^{-3}, \\ 2.04 \times 10^{-3} & \text{if thresh} = 10^{-4}, \\ 1.81 \times 10^{-16} & \text{if thresh} = 10^{-5}. \end{cases}$$



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



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



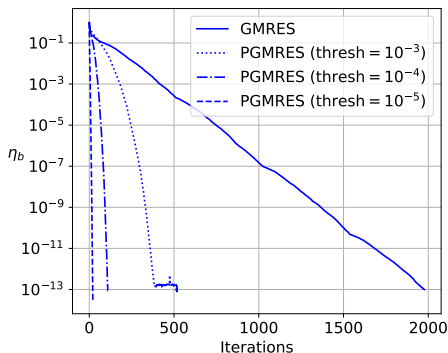
(d).  $M$  with  $\text{thresh} = 10^{-5}$ ,  
 $\frac{\text{nnz}}{n^2} \times \% = 3.10\%$

# Compare trained U-Net to algebraic preconditioner

Solve  $A(c)u = b$  on 2D domain  $64 \times 64$  (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

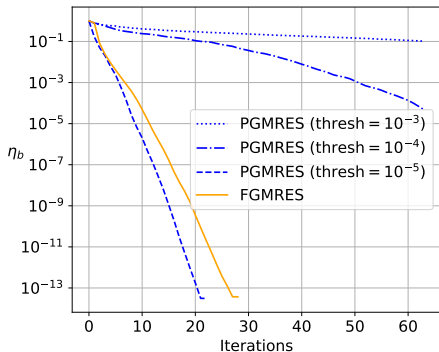
$$\frac{\|A - M\|_F}{\|A\|_F} = \begin{cases} 5.41 \times 10^{-2} & \text{if thresh} = 10^{-3}, \\ 2.04 \times 10^{-3} & \text{if thresh} = 10^{-4}, \\ 1.81 \times 10^{-16} & \text{if thresh} = 10^{-5}. \end{cases}$$

- **PGMRES: GMRES preconditioned by  $\text{spilu}(M)$** , 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  $64 \times 64$  (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**.



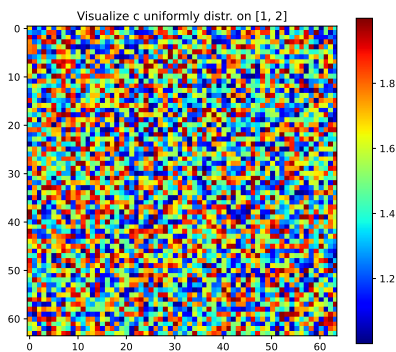
FGMRES and PGMRES

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

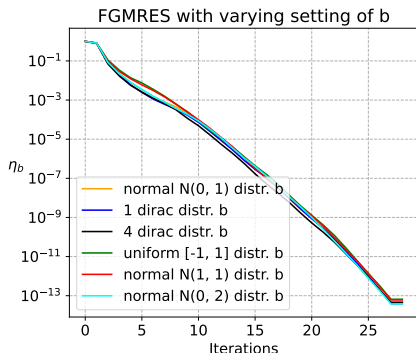
- The effectiveness of **trained U-Net preconditioner** is close to (could be the same as) **spilu(M) with thresh =  $10^{-5}$**  (the best algebra preconditioner for this example)

## Network generalizability: varying the source function $\mathbf{b}$

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



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

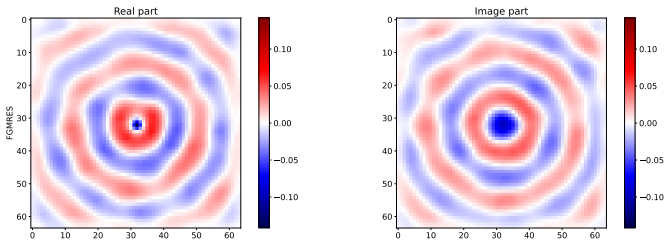


(b). Relative residual of FGMRES

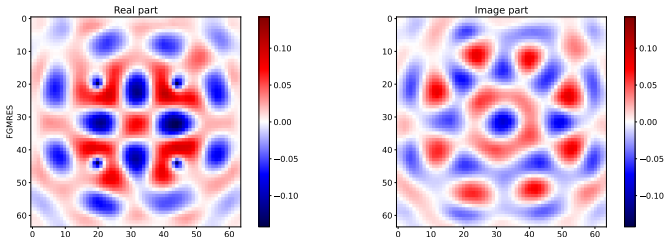
- Speed of sound  $\mathbf{c} \in \mathbb{R}^{64^2}$  is fixed and satisfying uniform distribution on interval  $[1, 2]$
- Performance of trained U-Net preconditioner is independent from varying the datatype of the  $\mathbf{b} \in \mathbb{C}^{64^2}$  or varying the mean and median value of the normal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

## 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  $c$ ):

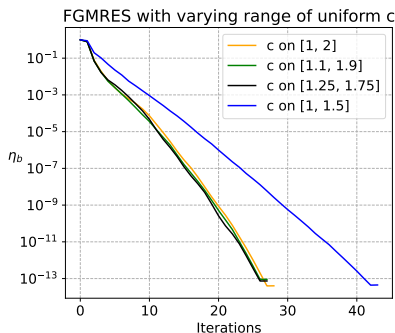


Visualize wavefiled  $u \in \mathbb{C}^{64^2}$  solved by 4 dirac for  $b \in \mathbb{C}^{64^2}$  (with fixed  $c$ ):

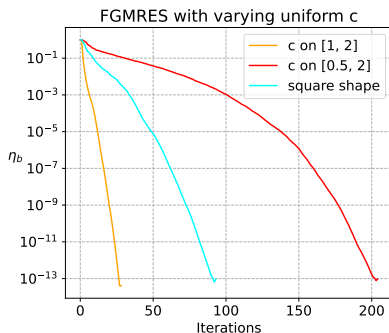


# Network generalizability: varying the speed of sound $c$

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



(a). shrink the interval

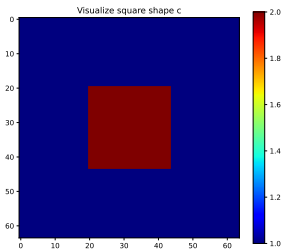


(b). enlarge the interval & special structure

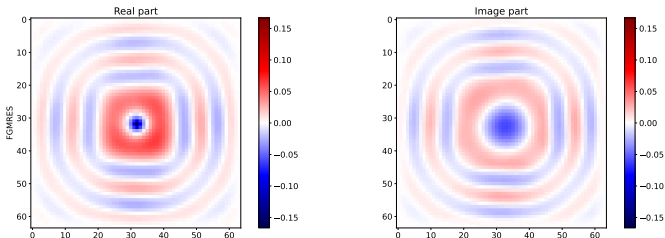
- Source function  $b \in \mathbb{C}^{64^2}$  is fixed with 1 dirac setting, 1 in grid position  $(32, 32)$ , the center of domain  $64 \times 64$ , and 0 elsewhere in domain
- Square shape of  $c \in \mathbb{R}^{64^2}$ : domain  $[20 : 44, 20 : 44] = 2$  and 1 elsewhere
- Varying the range of the  $c$  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 wavefield  $u \in \mathbb{C}^{64^2}$  solved by  $c \in \mathbb{R}^{64^2}$  in square shape:

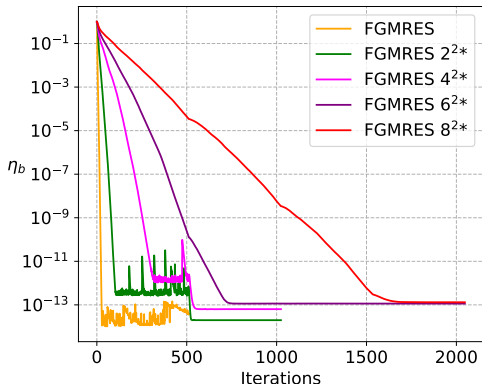




## Network generalizability: varying the domain size

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

Numerical results on different domain size



FGMRES — domain  $64 \times 64$

FGMRES  $2^{2*}$  — domain  $128 \times 128$

FGMRES  $4^{2*}$  — domain  $256 \times 256$

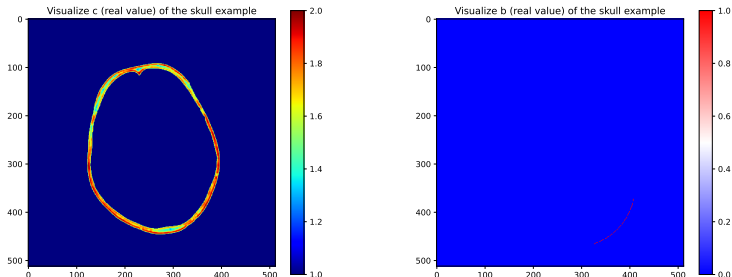
FGMRES  $6^{2*}$  — domain  $384 \times 384$

FGMRES  $8^{2*}$  — domain  $512 \times 512$

- U-Net trained on 2D domain  $64 \times 64$  (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  $128 \times 128$  until the 64x larger domain  $512 \times 512$

## Network generalizability: Adult human skull example

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



This example is downloaded from the qure.ai dataset<sup>a</sup>

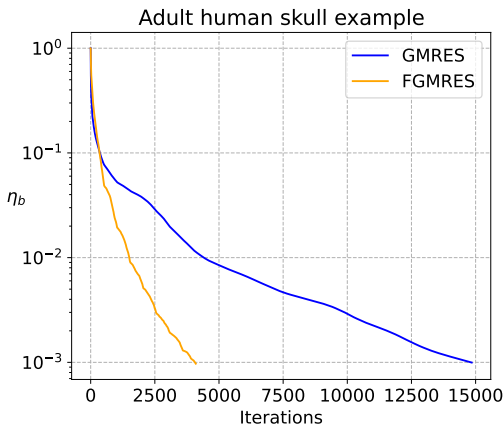
Recall part of the training settings:

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

<sup>a</sup><http://headctstudy.qure.ai/dataset>

## Network generalizability: Adult human skull example

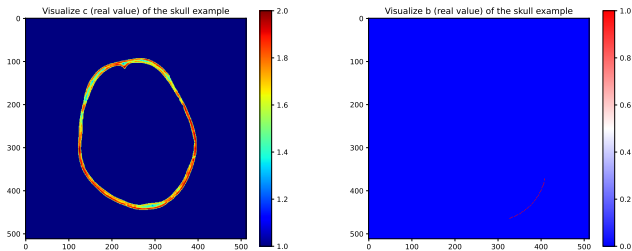
Solve  $A(c)u = b$  with the **structured dataset** for both  $c$  and  $b$  on 2D domain  $512 \times 512$  (i.e.,  $A(c) \in \mathbb{C}^{512^2 \times 512^2}$ ):



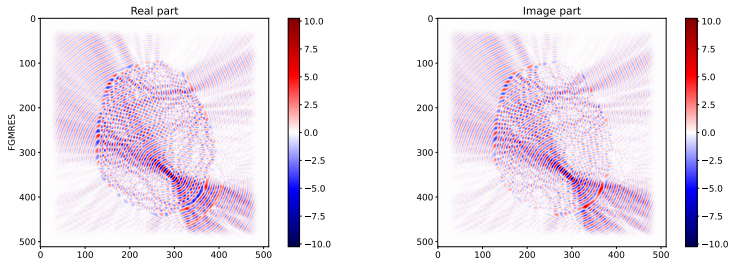
- Comparison of FGMRES (NNs trained on domain  $64 \times 64$ ) to GMRES on solving the skull example (on  $512 \times 512$  from CQ500 with 491 scans) to reaching accuracy at  $10^{-3}$
- Consumed its & CPU time (Training time of U-Net on 2 V100 GPUs is 49.83min):  
FGMRES = 4097 & 4.24h; GMRES = 14849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

## Network generalizability: Adult human skull example

Visualization the structured dataset of the skull example on 2D domain  $512 \times 512$ :



Visualize the complex wavefield  $c \in \mathbb{R}^{512^2}$  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

⇒ 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.**  $\mathcal{N}(\mathbf{0},1)$ : 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

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**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  $\rightarrow$  **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  $\rightarrow$  **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/>) !**

$\rightarrow$  **Yanfei Xiang ([yanfei.xiang@inria.fr](mailto:yanfei.xiang@inria.fr))**

## My co-workers from Inria and Cerfacs

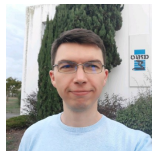
- Inria: Luc Giraud and Maksym Shpakovych
- Cerfacs: Paul Mycek and Carola Kruse



Luc Giraud



Paul Mycek



Maksym Shpakovych



Carola Kruse

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

# 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.



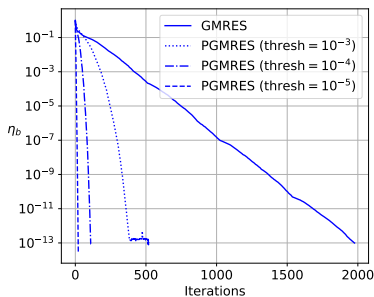
*Thank you for your attention!*

*Questions ?*

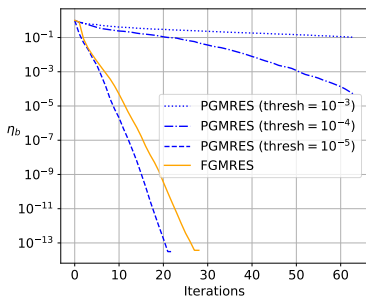


## Consuming time

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



(a). PGMRES with varying thresh



(b). FGMRES and PGMRES

- **PGMRES: GMRES preconditioned by  $\text{spilu}(M)$** , 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)  **$\text{spilu}(M)$  with  $\text{thresh} = 10^{-5}$**  (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