Physics-Embedded Machine Learning for Electromagnetic Data Imaging

Examining three types of data-driven imaging methods

Rui Guo , Tianyao Huang , Maokun Li ,
Haiyang Zhang , and Yonina C. Eldar

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Introduction

- Electromagnetic(EM) imaging:

  measured EM fields → the value distribution of EM parameters
- permittivity(介电常数), permeability(磁导率), conductivity(电导率)
- Biomedicine: microwave imaging

  detect anomalies in the permittivity distribution caused

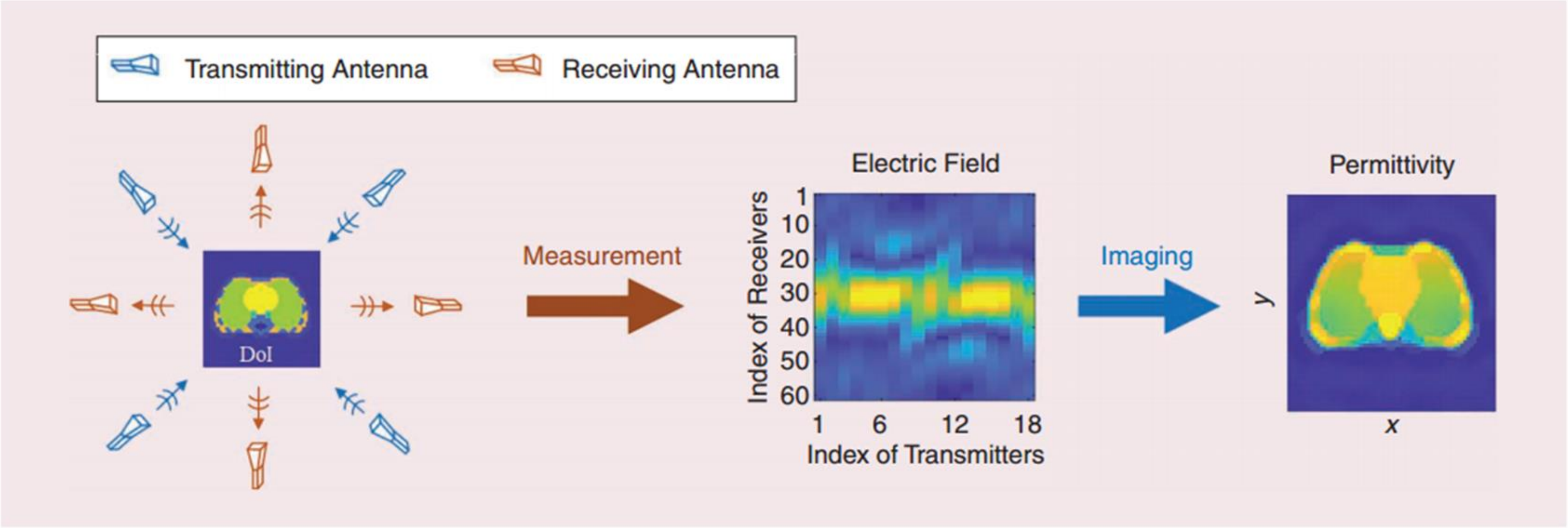


FIGURE 1. The EM-imaging setup. EM imaging converts measured data to the spatial distribution of electric parameters in the DoI.

- EM field propagates according to **Maxwell's equations**, which describe how electric and magnetic fields are generated by charges, currents, and changes of the fields.
- In the frequency domain, EM propagation can be described by the following PDE:

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - \omega^2 \mu \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = i\omega\mu \mathbf{J}(\mathbf{r})$$

E: vector electric field → **measurement**

r: spatial position → **measurement**

μ: permeability

ε: complex permittivity, σ is conductivity $\epsilon = \epsilon_R + i\sigma/\omega$ → **recover**

J: electric current source

ω: angular frequency

∇×: curl operator

Formulations of EM imaging

- EM imaging: an **inverse problem** that calculates electric parameters of the domain of investigation(DoI) from measured EM fields.
- It can be described as minimizing the “misfit” between the observed and simulated data:

$$L(\boldsymbol{\epsilon}) = \left\| \mathbf{d}_{\text{obs}} - F(\boldsymbol{\epsilon}) \right\|^2 + \lambda \phi_r(\boldsymbol{\epsilon})$$

where d_{obs} is the field observed by receivers, ε is complex permittivity, $F(\varepsilon)$ represents the EM-modeling function, Φ_r is the regularization term, and λ is a regularization factor.

- Equation is usually minimized by iterative gradient descent methods.

Challenges of EM imaging

- Each iteration requires computing the forward problem and its Fréchet derivative, which make this problem **computationally intensive**.
- The objective function is **nonconvex**.
- Gradient descent methods **lack flexibility in exploiting the prior knowledge** that is not described by simple regularization.

- Physics-embedded ML models provide potential solutions to the challenges.

1. Use conventional physical methods and ML models sequentially
2. Optimize network parameters with physics constraints
3. Unroll the physical methods with neural networks

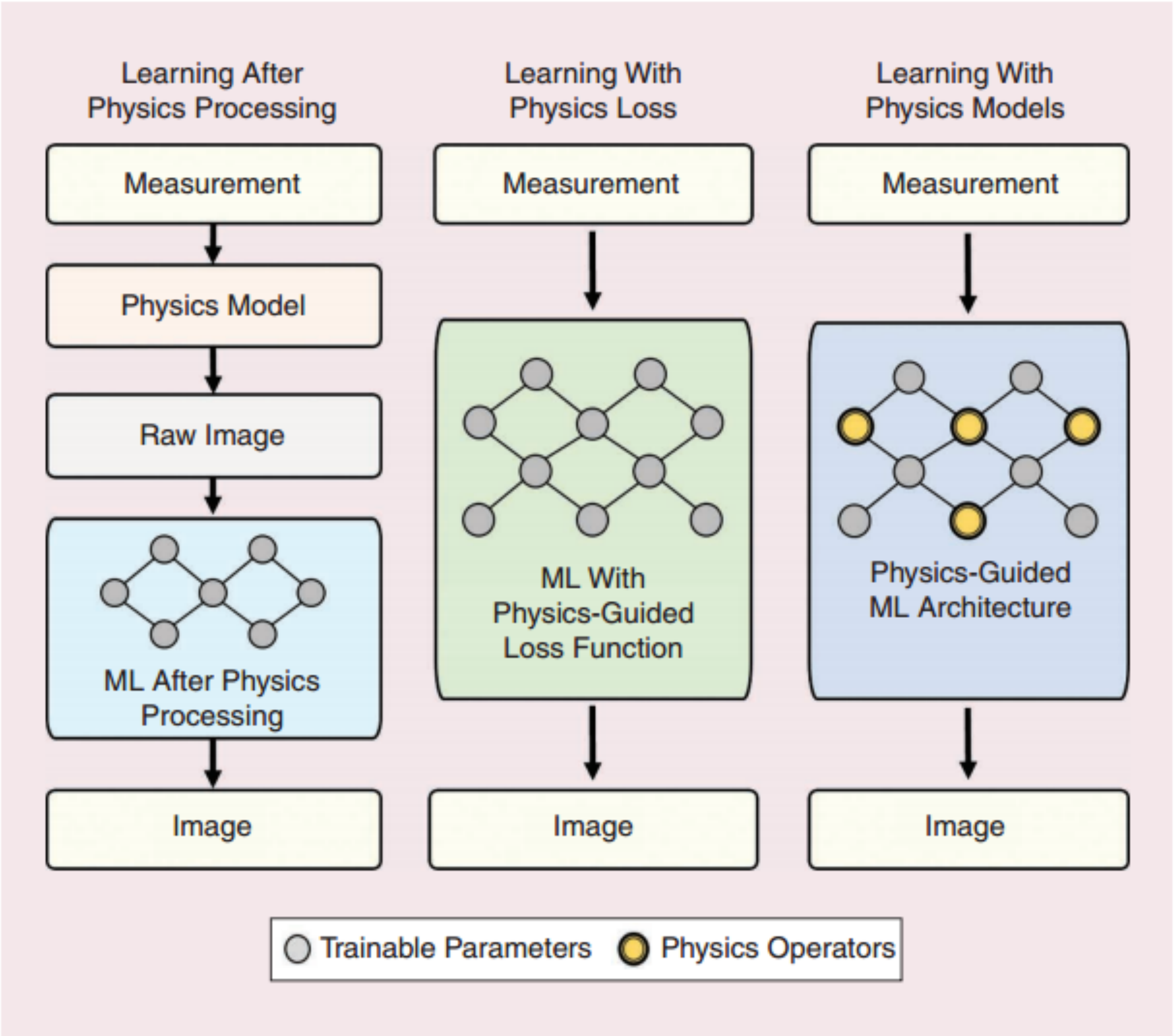


FIGURE 2. The three ways of incorporating physics into the ML model. (a) Learning after physics processing: the physics model is employed to initialize the input of ML models. (b) Learning with physics loss: physics knowledge is incorporated into the loss functions. (c) Learning with physics models: physics knowledge is used to guide design of the ML architecture.

Learning after physics processing

- Two steps:
  - A roughly estimated image is recovered using classical qualitative or quantitative methods.
  - The rudimentary image is polished using a DNN trained with the ground truth as labels. (image processing)

- In DNN, the more the input is processed by physics, the better the generalizability will be.

Learning with physics loss

- Incorporating Forward Modeling in Loss: A Mathematical Example

If the forward process has analytical solutions $m \coloneqq F(p) = p^2$, the inversion has two branches of solutions $p = \pm\sqrt{\mathrm{m}}$

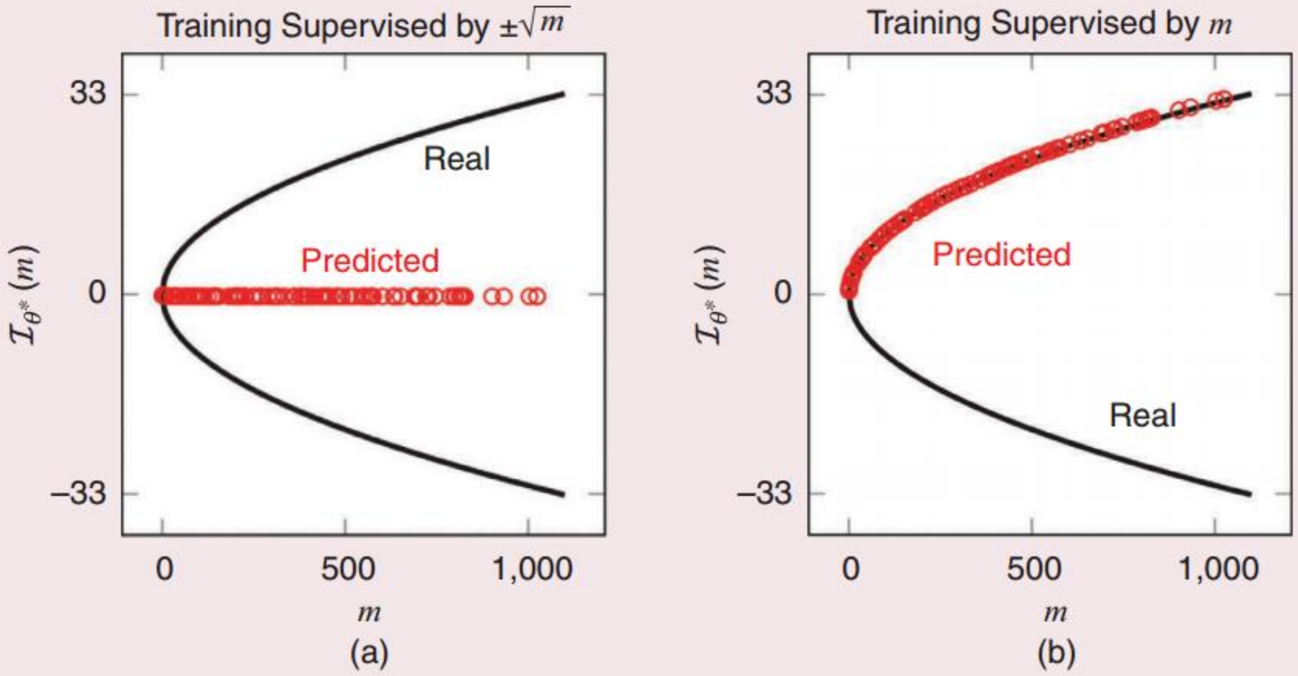


FIGURE S1. Incorporating forward modeling into training to reduce nonuniqueness of the inverse problem [19]. (a) When training is supervised by p ($\pm\sqrt{m}$), the predictions are zeros and (b) when training is supervised by labels p^2, the correct branch can be predicted by controlling the signs of solutions.

Training with a rigorous measurement loss

- Consider the inverse problem solved by a DNN with the measured data **d** as the input and the permittivity $\boldsymbol{\varepsilon}$ as the output.
- Let $\boldsymbol{\varepsilon}_T$ and $\mathbf{d}_T$ denote the labeled permittivity and EM data, respectively.
- Purely data-driven imaging use permittivity loss for training:

$$L_\epsilon = \| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_T \|^2$$

- The physics-embedded one further incorporates the measurement loss:

$$L = \alpha L_\epsilon + \beta L_\mathrm{d} = \alpha \| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_T \|^2 + \beta \| F(\boldsymbol{\epsilon}) - \mathbf{d}_T \|^2$$

Training with a learned measurement loss

- Surrogate the numerical forward solver $F(\cdot)$ with a DNN $\Theta_F(\cdot)$
- The training contains two stages: 1) training the forward solver 2) training the inverse operator

$$\Theta_F^* = \arg\min_{\Theta_F} \left\| \Theta_F(\boldsymbol{\epsilon}_T) - \mathbf{d}_T \right\|^2,$$

$$\Theta_I^* = \arg\min_{\Theta_I} \left\| \Theta_F^*(\Theta_I(\mathbf{d}_T)) - \mathbf{d}_T \right\|^2.$$

- Both stages take the measurement misfit as the loss function, which involves physical rules.

Training with a PDE-constrained loss

- The PDE-constrained loss inserts PDEs into the loss function.
- Physics-informed neural network (PINN)

Consider the 1D time-domain electromagnetic wave equation

$$\frac{\partial^2 E(x,t)}{\partial x^2} - \mu\epsilon(x)\frac{\partial^2 E(x,t)}{\partial t^2} = 0 \quad \text{(S2)}$$

where E is the electric field, ϵ is permittivity, μ is permeability, and t and x are the time and spatial coordinate, respectively. Together with some boundary conditions, the equation can be analytically or numerically solved to yield E (forward problem) or ϵ (inverse problem) given t and x.

Take the inverse problem with one-source multiple receivers as an example. A physics-informed neural network (PINN) specifies two separate deep neural networks (DNNs), namely, Θ_F and Θ_I. The input of Θ_F is x and t and its output is the electric field $\tilde{E}$, denoted by $\tilde{E} = \Theta_F(x,t)$. Similarly, the input of Θ_I is x and its output is permittivity $\tilde{\epsilon}$, denoted by $\tilde{\epsilon} = \Theta_I(x)$. The two separate DNNs are simultaneously trained with a shared loss function L, which includes a supervised measurement loss of E regarding initial and boundary conditions

$$L_{\text{data}} = \frac{1}{N_{\text{data}}}\sum_{i=1}^{N_{\text{data}}}\left(\tilde{E}(x_i,t_i) - E_T(x_i,t_i)\right)^2 \quad \text{(S3)}$$

and an unsupervised loss of partial differential equation constructed according to (S2)

$$L_{\text{PDE}} = \frac{1}{N_{\text{PDE}}}\sum_{j=1}^{N_{\text{PDE}}}\left(\frac{\partial^2 \tilde{E}(x_j,t_j)}{\partial x^2} - \mu\tilde{\epsilon}(x_j)\frac{\partial^2 \tilde{E}(x_j,t_j)}{\partial t^2}\right)^2 \quad \text{(S4)}$$

given by $L = \alpha_{\text{data}}L_{\text{data}} + \alpha_{\text{PDE}}L_{\text{PDE}}$. Here (x_i,t_i) and (x_j,t_j) are sampled at the initial/boundary position and in the domain of investigation (DoI), respectively. In addition, E_T is the labeled measurement, N_{data} is the number of labeled samples, N_{PDE} is the number of unlabeled samples in the DoI, and $\alpha_.$ are weights. The partial differentiations are achieved by the automatic differentiation in the deep learning framework. After training, one can use Θ_I to predict permittivity at arbitrary location x. Therefore, the PINN is mesh free.

Learning with physics models

- Unrolling measurement-to-image mapping(inverse)
- Unrolling image-to-measurement mapping(forward)
- Simultaneously unrolling both mappings

Unrolling measurement-to-image mapping(inverse)

- We demonstrate the unrolling of **linear** inverse problems through radar imaging. Here, the electric parameters of interest are **intensities of scatterers** in the DoI, denoted by ε. $F(\boldsymbol{\epsilon}) = \boldsymbol{\Phi}\boldsymbol{\epsilon}$
- Conventional radar imaging can be formulated as a compressed sensing problem:

$$\min_{\boldsymbol{\epsilon}} \| \mathbf{d}_{\mathrm{obs}} - \boldsymbol{\Phi}\boldsymbol{\epsilon} \|^2 + \lambda | \boldsymbol{\epsilon} |_1$$

- Iterative Shrinkage Thresholding Algorithm(ISTA):

$$\boldsymbol{\epsilon}_k = \mathcal{S}_{\frac{\lambda}{L}}\left(\frac{1}{L}\boldsymbol{\Phi}^H \mathbf{d}_{\mathrm{obs}} + \left(\boldsymbol{I} - \frac{1}{L}\boldsymbol{\Phi}^H \boldsymbol{\Phi}\right)\boldsymbol{\epsilon}_{k-1}\right)$$

- Learned ISTA(LISTA): learn $\lambda/L, (1/L)\boldsymbol{\Phi}^H$ and $(\boldsymbol{I} - (1/L)\boldsymbol{\Phi}^H\boldsymbol{\Phi})$
- Embedding physics models into the neural networks reduces the number of variables while maintaining fast convergence rate.

- Embedding physics models into the neural networks reduces the number of variables while maintaining fast convergence rate.
- The mutual inhibition matrix $\boldsymbol{I} - (1/L)\boldsymbol{\Phi}^H\boldsymbol{\Phi}$ has a Toeplitz or a doubly block Toeplitz structure due to the nature of radar-forward models.

$$A = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & \cdots & a_{-(n-1)} \\ a_1 & a_0 & a_{-1} & \ddots & & \vdots \\ a_2 & a_1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & a_{-1} & a_{-2} \\ \vdots & & \ddots & a_1 & a_0 & a_{-1} \\ a_{n-1} & \cdots & \cdots & a_2 & a_1 & a_0 \end{bmatrix}$$

- The objective function of **nonlinear** EM imaging

$$\left\| \mathbf{d}_{\text{obs}} - F(\boldsymbol{\epsilon}) \right\|^2, \text{ where } F(\boldsymbol{\epsilon}) \text{ is numerically solved from PDEs}$$

- Gauss–Newton method:

$$\boldsymbol{\epsilon}_{k+1} = \boldsymbol{\epsilon}_k + (\mathbf{S}^H \mathbf{S})^{-1} \mathbf{S}^H (\mathbf{d}_{\text{obs}} - F(\boldsymbol{\epsilon}_k))$$

where S is the Fréchet derivative of F at $\boldsymbol{\varepsilon}_0$.

- By unrolling, a set of descent directions Ks can be learned, which is called the supervised descent method(SDM)

$$\boldsymbol{\epsilon}_{k+1} = \boldsymbol{\epsilon}_k + \mathbf{K}_k (\mathbf{d}_{\text{obs}} - F(\boldsymbol{\epsilon}_k))$$

- In training, the EM response is taken as the input, while the corresponding ground truth of complex permittivity is the label.
- The SDM shows high generalizability in EM imaging.

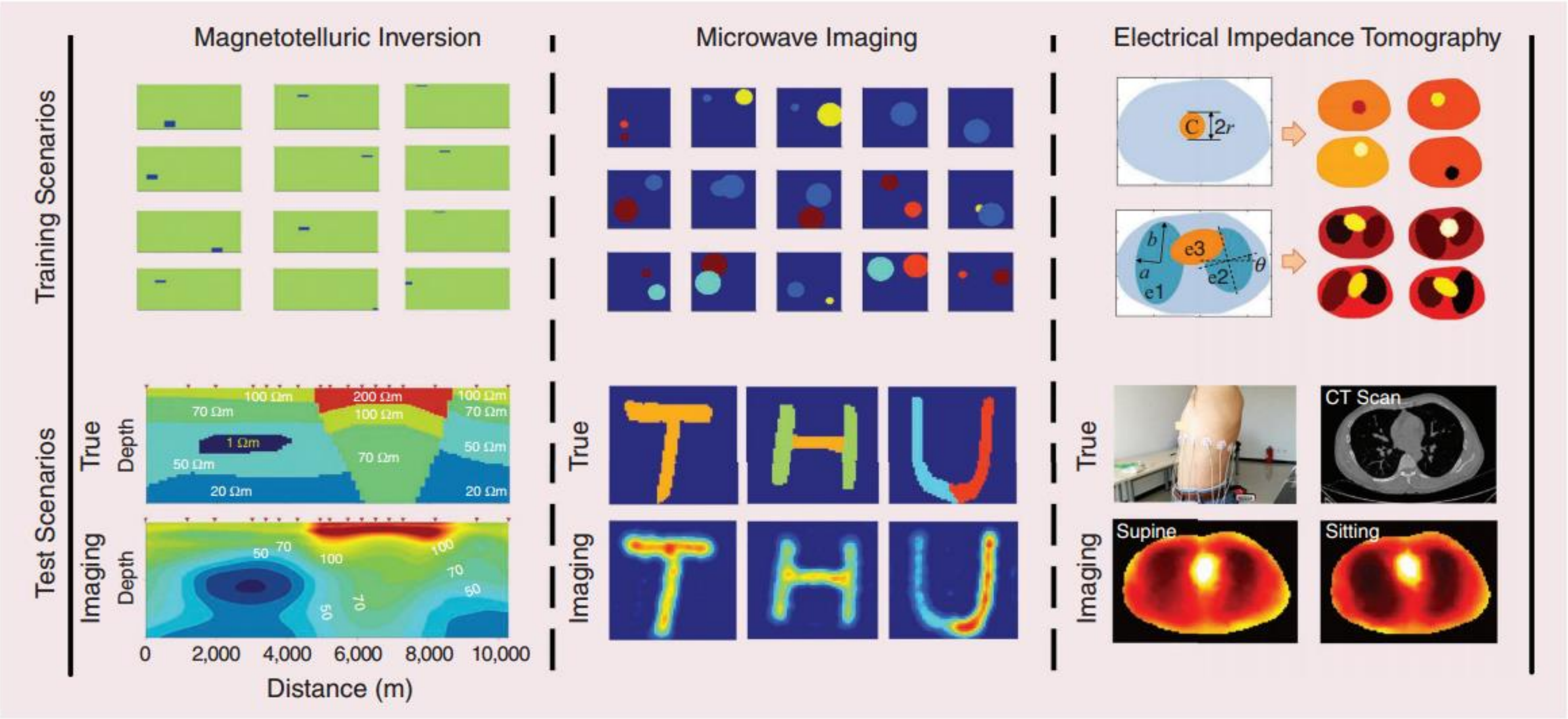


FIGURE 4. Imaging with the SDM for geophysics [55], microwave [21] and biomedical data [61]. The SDM is able to reconstruct complex inhomogeneous media while the training scenarios are simple. CT: computerized tomography.

Unrolling image-to-measurement mapping(forward)

- ***Unrolling the integral operation***

The integral form of the wave equation is

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \omega^2 \mu \int_V \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}')[\epsilon(\mathbf{r}') - \epsilon_0]\mathbf{E}(\mathbf{r}')d\mathbf{r}'$$

where E^{inc} is the incident field generated by the source, G_0 is the Green's function describing wave propagation, ε_0 is the permittivity of the background, and V is the DoI.

- Physics-embedded DNN (PE-Net)

The forward modeling $F(\varepsilon)$ involving integral operations is unrolled as a physics-embedded network Θ_F.

After the networks are trained, they are combined with generic networks Θ_I that perform inverse mappings.

- Solving the integral form is simplified as calculating **x** (representing the unknown **E**) from $\mathbf{A}(\epsilon)\mathbf{x} = \mathbf{b}$
- Conjugate Gradient Method

compute the conjugate direction **p** and update the solution in an iterative manner

- Update-learning Method

iterations in conjugate gradient approach are unrolled by N neural network blocks

Conjugate gradient method.

Input $\mathbf{x}_0$

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0, \mathbf{p}_1 = \mathbf{r}_0$

$\alpha_1 = (\mathbf{r}_0^T \mathbf{r}_0)/\mathbf{p}_1^T(\mathbf{A}\mathbf{p}_1)$

$\mathbf{x}_1 = \mathbf{x}_0 + \alpha_1 \mathbf{p}_1$

for $k = 1, 2, \ldots$ until $\|\mathbf{r}_k\| \leqq \varepsilon$

    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k(\mathbf{A}\mathbf{p}_k)$

    $\beta_{k+1} = (\mathbf{r}_k^T \mathbf{r}_k)/(\mathbf{r}_{k-1}^T \mathbf{r}_{k-1})$

    $\mathbf{p}_{k+1} = \mathbf{r}_k + \beta_{k+1}\mathbf{p}_k$

    $\alpha_{k+1} = (\mathbf{r}_k^T \mathbf{r}_k)/\mathbf{p}_{k+1}^T(\mathbf{A}\mathbf{p}_{k+1})$

    $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_{k+1}\mathbf{p}_{k+1}$

Update-learning method.

Input $\mathbf{x}_0$

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0, \mathbf{p}_1 = \mathbf{r}_0$

$\mathbf{x}_1 = \mathbf{x}_0$

for $k = 1, 2, \ldots, N,$

    $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$

    $\mathbf{p}_{k+1} = \Theta_p^k(\mathbf{p}_k, \mathbf{r}_k, \mathbf{r}_{k-1})$

    $\mathbf{x}_{k+1} = \mathbf{x}_k + \Theta_{dx}^k(\mathbf{p}_{k+1}, \mathbf{A}\mathbf{p}_{k+1}, \mathbf{r}_k)$

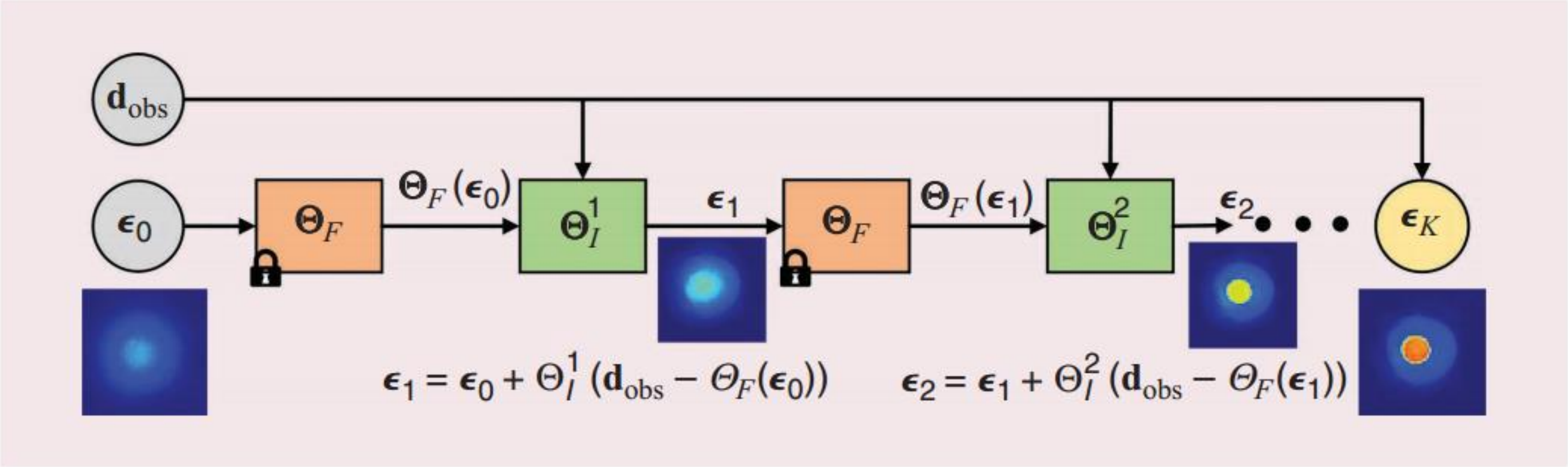


FIGURE 5. Physics-embedded DNNs for microwave imaging [22], where the forward modeling is unrolled into a neural network. The parameters of the forward solver Θ_F are fixed when training the inverse networks Θ_Is.

$$\epsilon_K = \Theta_I(\epsilon_0, \mathbf{d}_{obs}) = \epsilon_0 + \sum_{k=1}^{K} \Theta_I^k(\mathbf{d}_{obs} - \Theta_F(\epsilon_{k-1}))$$

- ***Unrolling the differential operation***

Unroll the time-domain wave equation with recurrent neural networks (RNNs)

$$\begin{cases} \epsilon_R \dfrac{\partial E_z}{\partial t} = \dfrac{\partial H_y}{\partial x} - \dfrac{\partial H_x}{\partial y} - \sigma E_z, \\ \mu \dfrac{\partial H_x}{\partial t} = -\dfrac{\partial E_z}{\partial y}, \\ \mu \dfrac{\partial H_y}{\partial t} = \dfrac{\partial E_z}{\partial x} \end{cases}$$

where **E** and **H** are the electric and magnetic fields, respectively, that are coupled with each other; the subscripts represent spatial components of the vector field. After discretization, for instance,

$$\mu \frac{H_x^{n+1/2}\left(i, j+\frac{1}{2}\right) - H_x^{n-1/2}\left(i, j+\frac{1}{2}\right)}{\Delta t} = -\frac{E_z^n(i, j+1) - E_z^n(i, j)}{\Delta y}$$

$$H_x^{n+1/2} = H_x^{n-1/2} + \Theta_F(E_z^n)$$

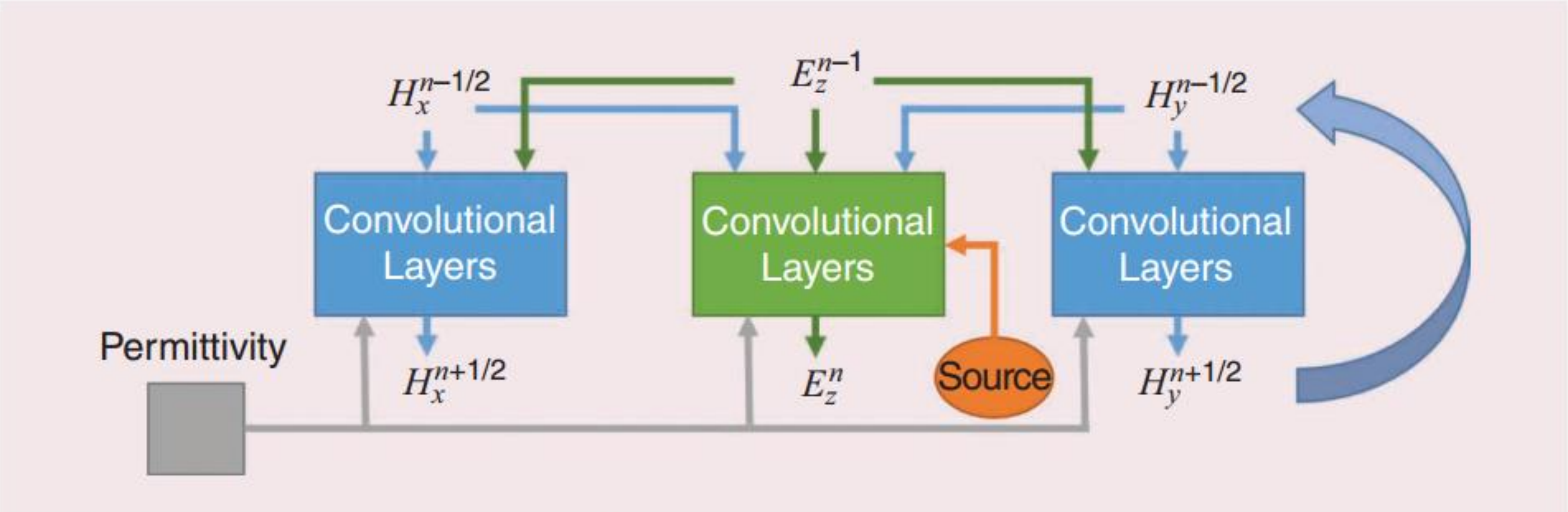


FIGURE 6. The cell architecture of an RNN for simulating wave propagation [20]. At each time step, the RNN outputs the E-field E_z and H-fields H_x, H_y in the entire DoI, which are computed from their values in the previous time step, according to Maxwell's equations. The partial derivatives are approximated with finite differences. Taking the permittivity as a trainable layer, training this network and updating its weights is equivalent to gradient-based EM imaging.

Simultaneously unrolling both mappings

- They first reconstruct permittivity from a linear process by approximating the electric field **E** in the integration of (9) to the incident field $\boldsymbol{E^{inc}}$.
- Intermediate parameters, e.g., total field and contrast source, can be estimated with this permittivity.
- A more accurate permittivity model is computed from the intermediate parameters and measurements.

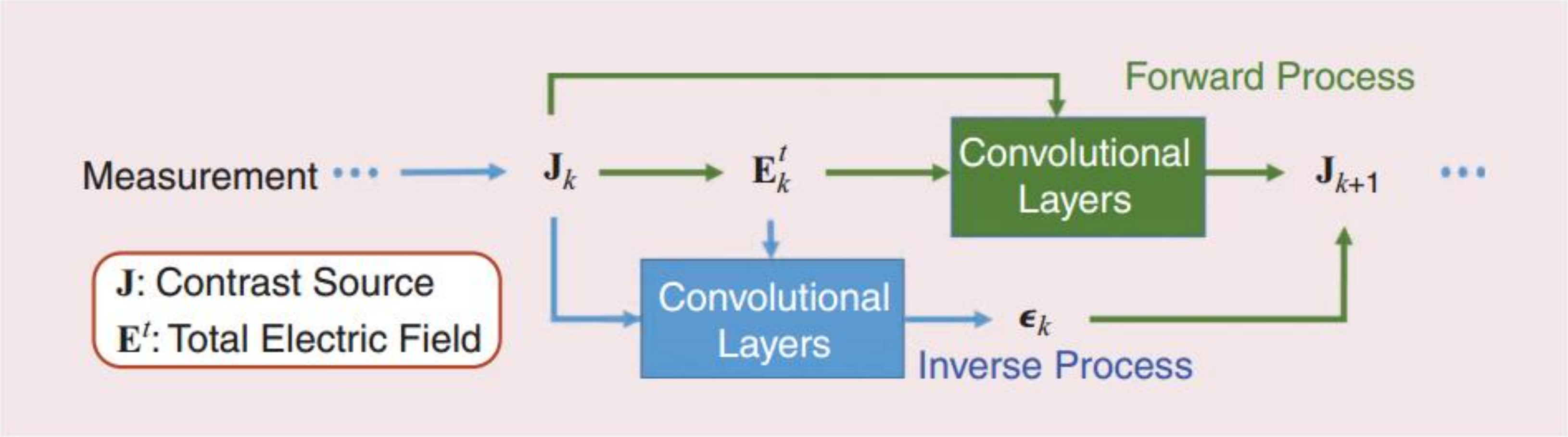
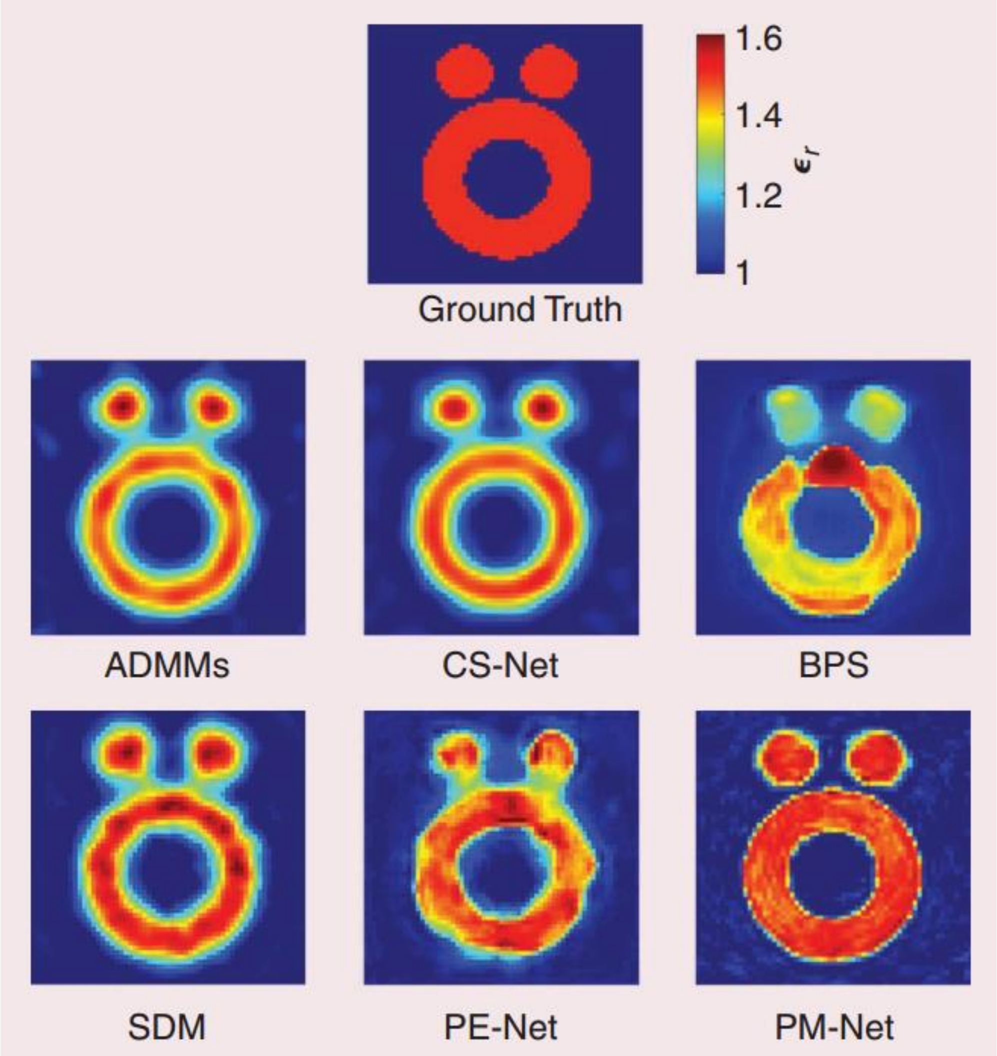


FIGURE 7. Simultaneously unrolling forward and inverse processes into neural networks [16]. The forward process (in green) computes the contrast source $\mathbf{J}$ and total field $\mathbf{E}^t$ given permittivity, while the inverse process (in blue) infers permittivity from measurements $\mathbf{J}$ and $\mathbf{E}^t$.

Comparisons



- **Contrast source network(CS-Net):**

gradient-based optimization, whose initial guess is provided by a DNN

- **Back Projection Scheme (BPS):**

learning after physics processing

- **Supervised descent method(SDM):**

unroll the inverse mapping

- **Physics-embedded DNN (PE-Net):**

unroll the forward mapping

- **Physical model-inspired neural network (PM-Net):**

unroll both mappings

Challenges and opportunities

- **Data**

Obtain the exact electric properties of targets.

- **Physics**

Incorporate physics theory into data-driven methods. The DoI is partitioned into triangle (2D) or tetrahedral (3D) elements.

- **Algorithm**

The credibility of predictions needs to be improved.

THANKS