Solving Inverse Scattering Problem Efficiently Using Reciprocity Theorem

Yifeng Shao / 03-Nov-2022

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LINX (Lensless Imaging of 3D Nanostructures with Soft X-Rays)

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Linx

ASML

activefiber systems

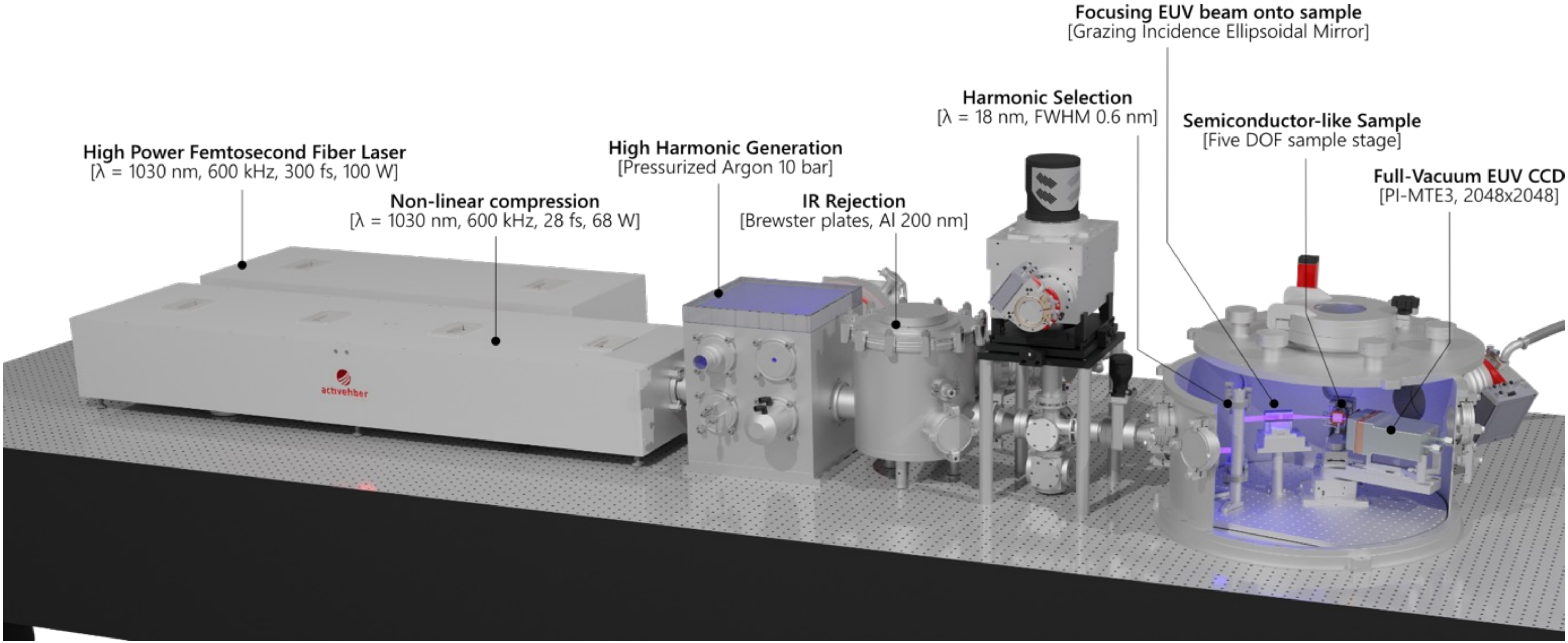
TNO

COHERENT®

VSL

Malvern Panalytical
a spectris company

LINX (Lensless Imaging of 3D Nanostructures with Soft X-Rays)



LINX (Lensless Imaging of 3D Nanostructures with Soft X-Rays)

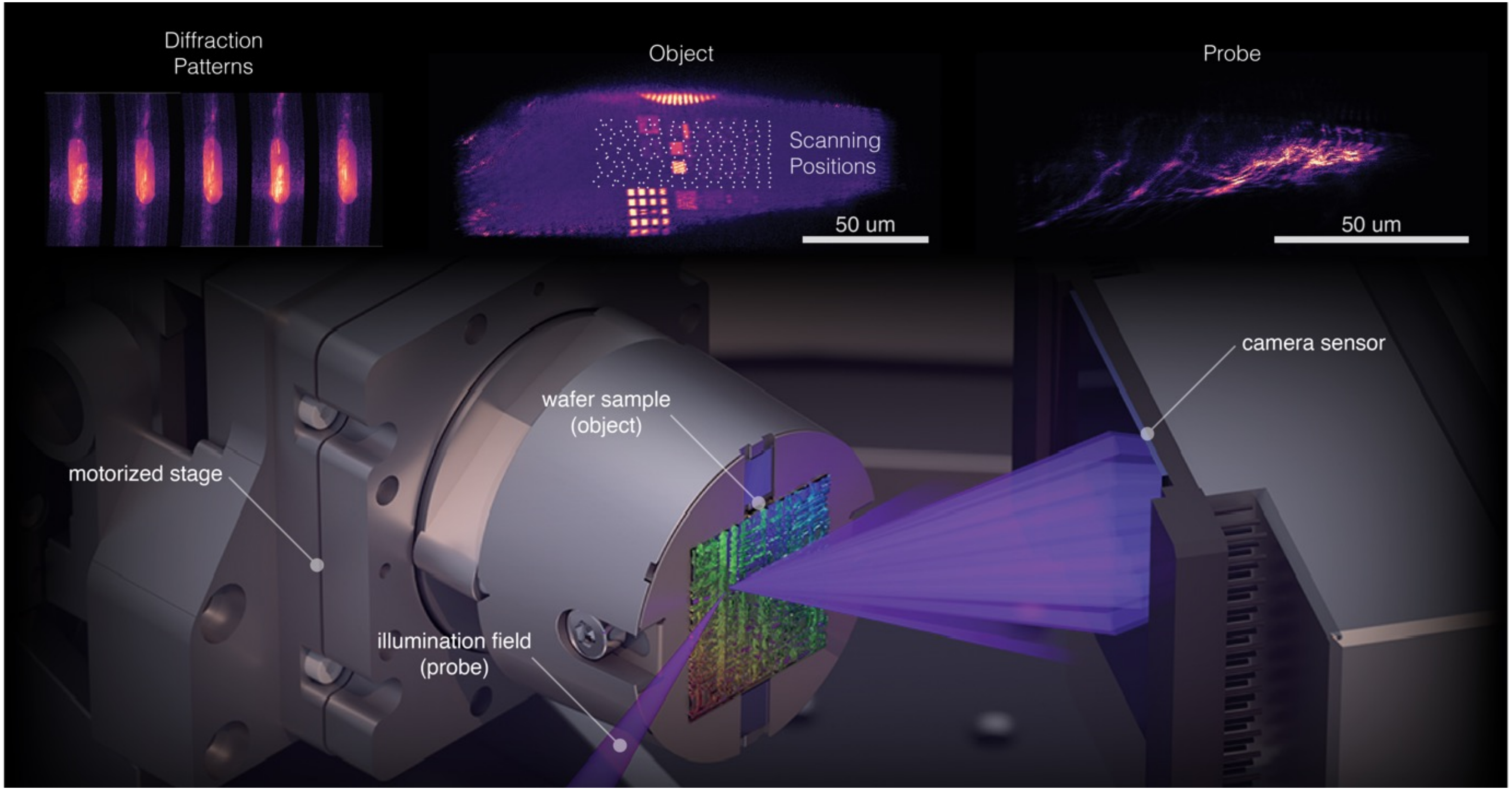


Table of Content

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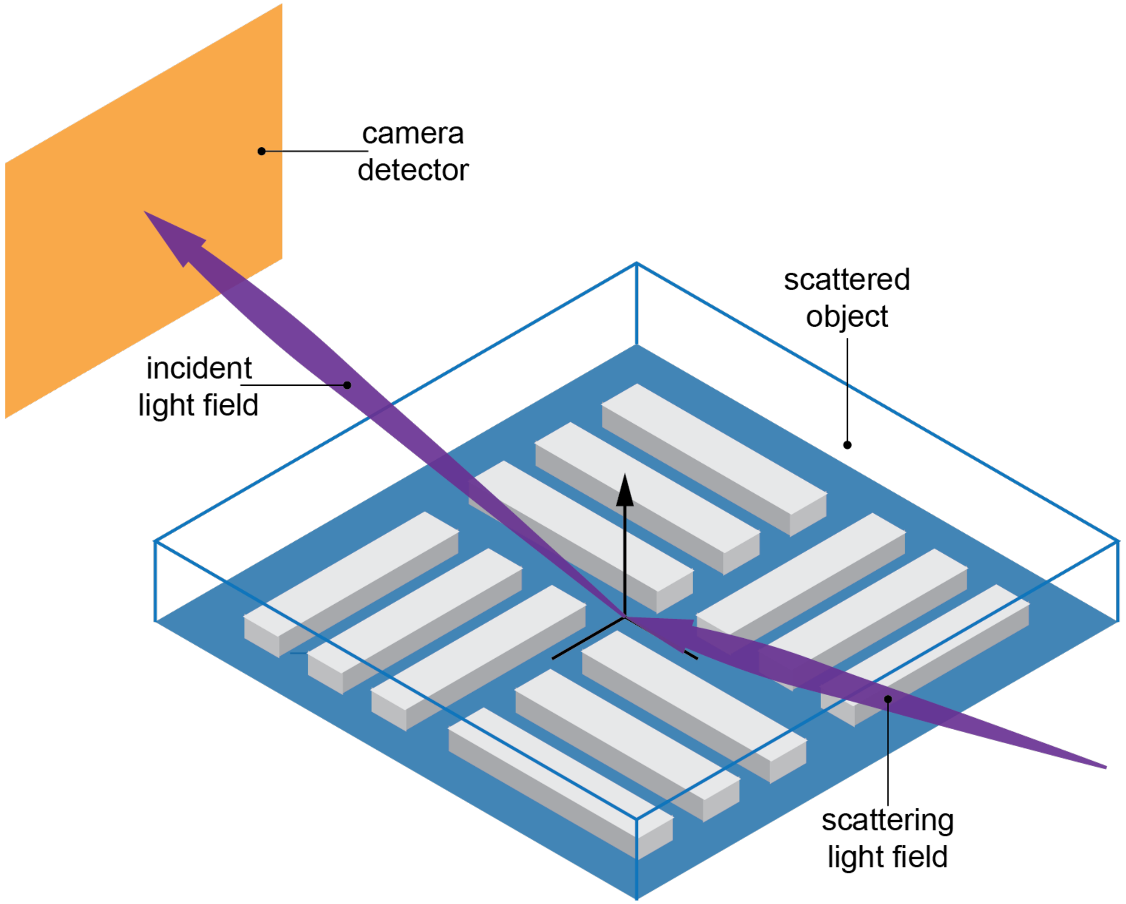
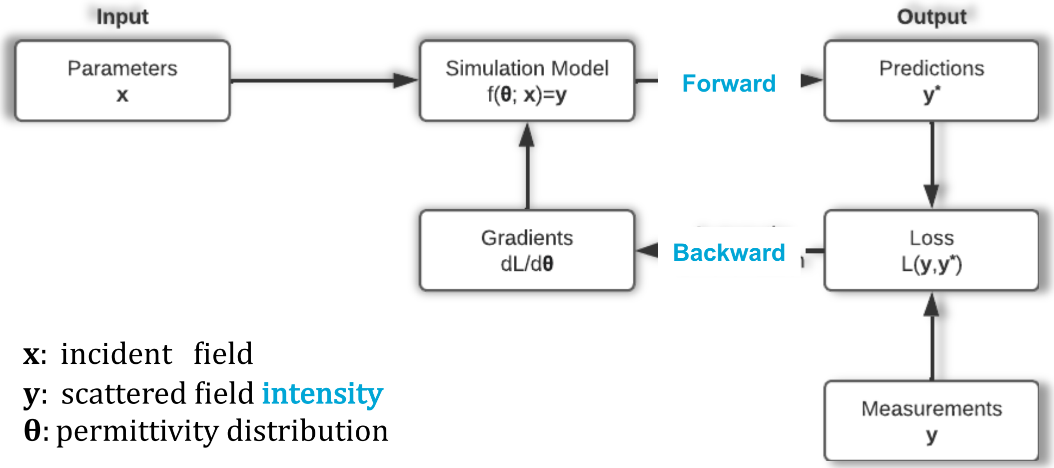
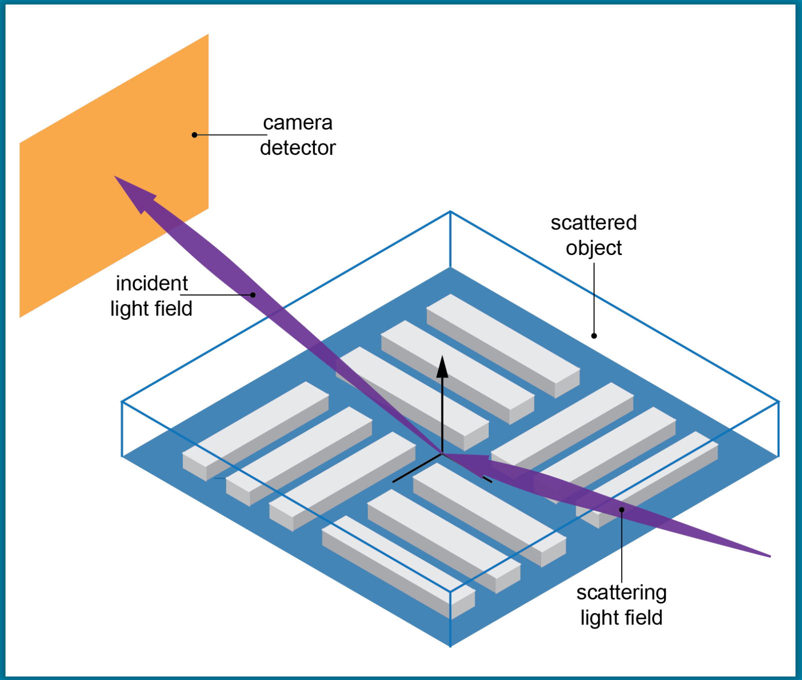


The Inverse (Optical) Scattering Problem



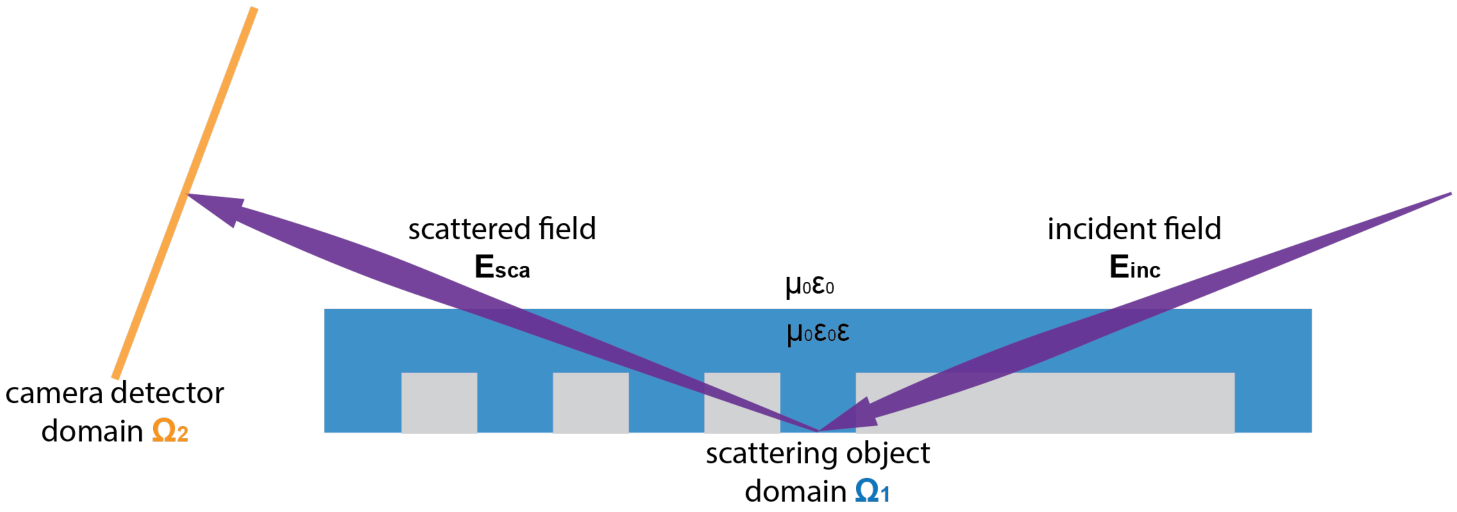
x: incident field
y: scattered field **intensity**
θ: permittivity distribution



Forward Computation

Light-Structure Interaction

- Incident Field satisfies Maxwell Equations in homogeneous medium
- Total Field satisfies Maxwell Equations in inhomogeneous medium



$$\nabla\times\mathbf{E}_{\mathrm{inc}} = -i\omega\mu_0\mathbf{H}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{E}_{\mathrm{tot}} = -i\omega\mu_0\mathbf{H}_{\mathrm{tot}}$$

$$\nabla\times\mathbf{H}_{\mathrm{tot}} = i\omega\epsilon_0\boldsymbol{\epsilon}\mathbf{E}_{\mathrm{tot}}$$

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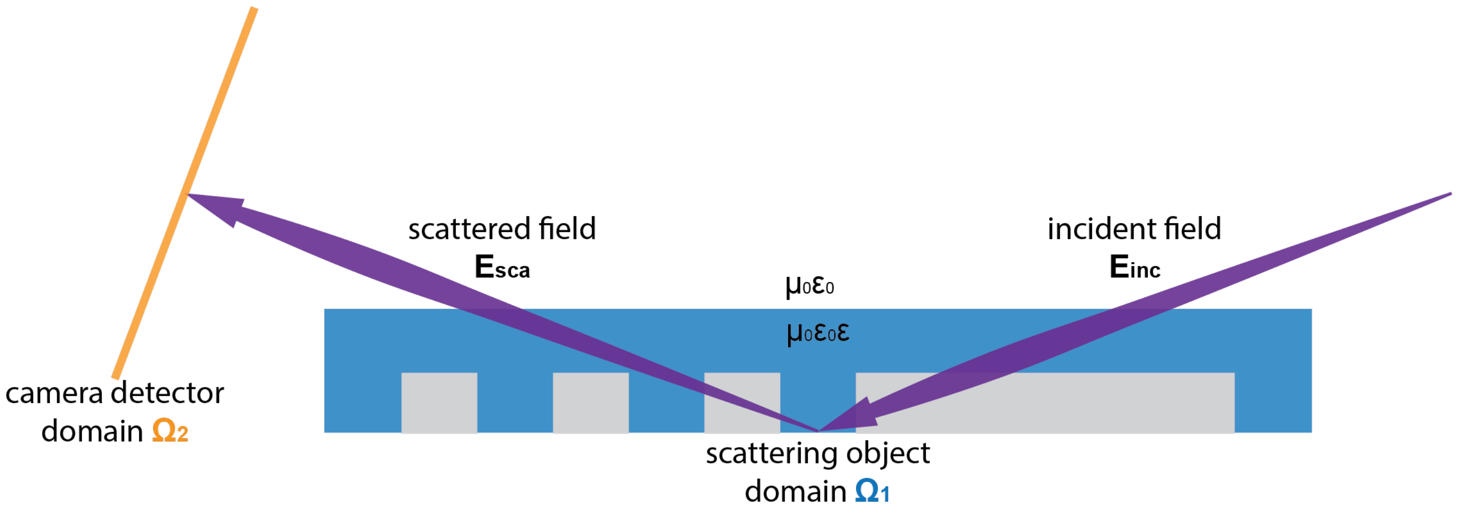
Forward Computation

Light-Structure Interaction

- Incident Field satisfies Maxwell Equations in homogeneous medium
- Total Field satisfies Maxwell Equations in inhomogeneous medium



$$\nabla\times\mathbf{E}_{\mathrm{inc}} = -i\omega\mu_0\mathbf{H}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{inc}}$$

$$\nabla\times[\mathbf{E}_{\mathrm{inc}}+\mathbf{E}_{\mathrm{sca}}] = -i\omega\mu_0[\mathbf{H}_{\mathrm{inc}}+\mathbf{H}_{\mathrm{sca}}]$$

$$\nabla\times[\mathbf{H}_{\mathrm{inc}}+\mathbf{H}_{\mathrm{sca}}] = i\omega\epsilon_0\epsilon[\mathbf{E}_{\mathrm{inc}}+\mathbf{E}_{\mathrm{sca}}]$$

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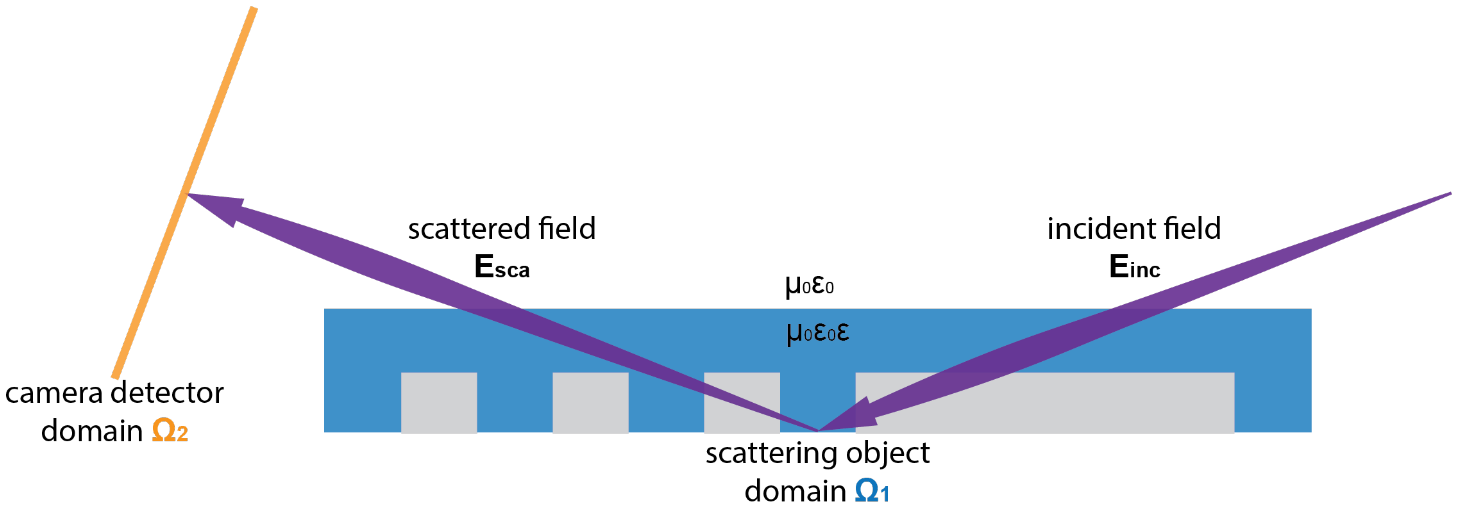
Forward Computation

Light-Structure Interaction

- Incident Field satisfies Maxwell Equations in homogeneous medium
- Total Field satisfies Maxwell Equations in inhomogeneous medium



$$\nabla\times\mathbf{E}_{\mathrm{inc}} = -i\omega\mu_0\mathbf{H}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{inc}}$$

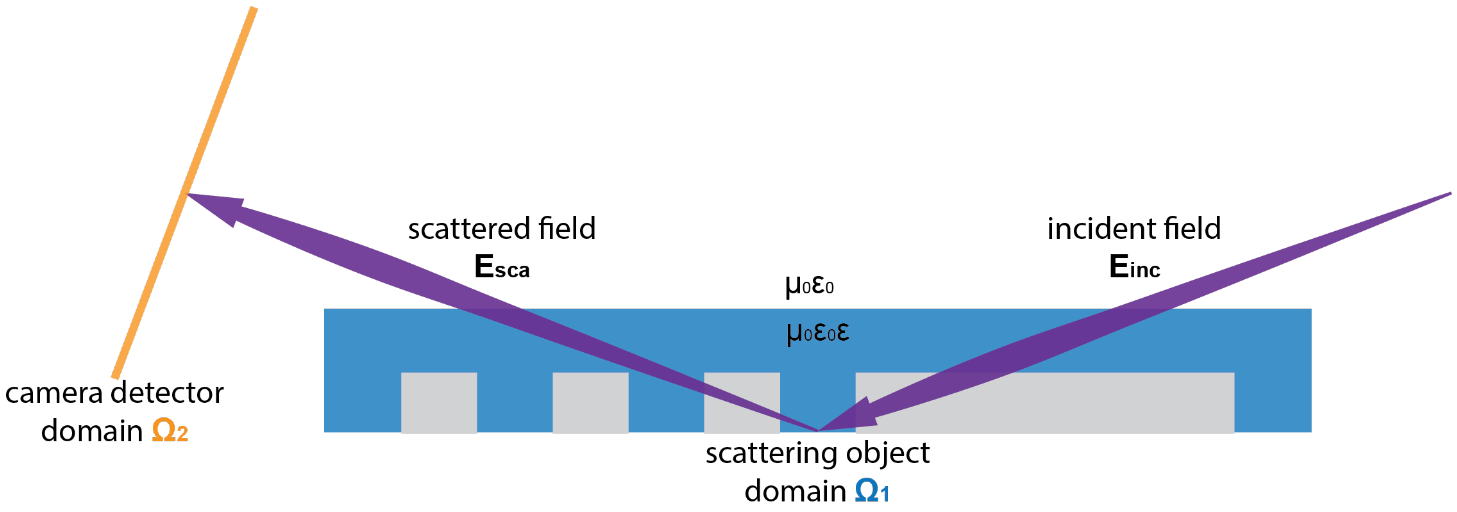
$$\nabla\times[\mathbf{E}_{\mathrm{inc}}+\mathbf{E}_{\mathrm{sca}}] = -i\omega\mu_0[\mathbf{H}_{\mathrm{inc}}+\mathbf{H}_{\mathrm{sca}}]$$

$$\nabla\times[\mathbf{H}_{\mathrm{inc}}+\mathbf{H}_{\mathrm{sca}}] = i\omega\epsilon_0[\mathbf{E}_{\mathrm{inc}}+\mathbf{E}_{\mathrm{sca}}] + i\omega\epsilon_0(\epsilon-1)[\mathbf{E}_{\mathrm{inc}}+\mathbf{E}_{\mathrm{sca}}]$$

Forward Computation

Light-Structure Interaction

- Incident Field satisfies Maxwell Equations in homogeneous medium
- Total Field satisfies Maxwell Equations in inhomogeneous medium



$$\nabla\times\mathbf{E}_{\mathrm{inc}} = -i\omega\mu_0\mathbf{H}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{inc}}$$

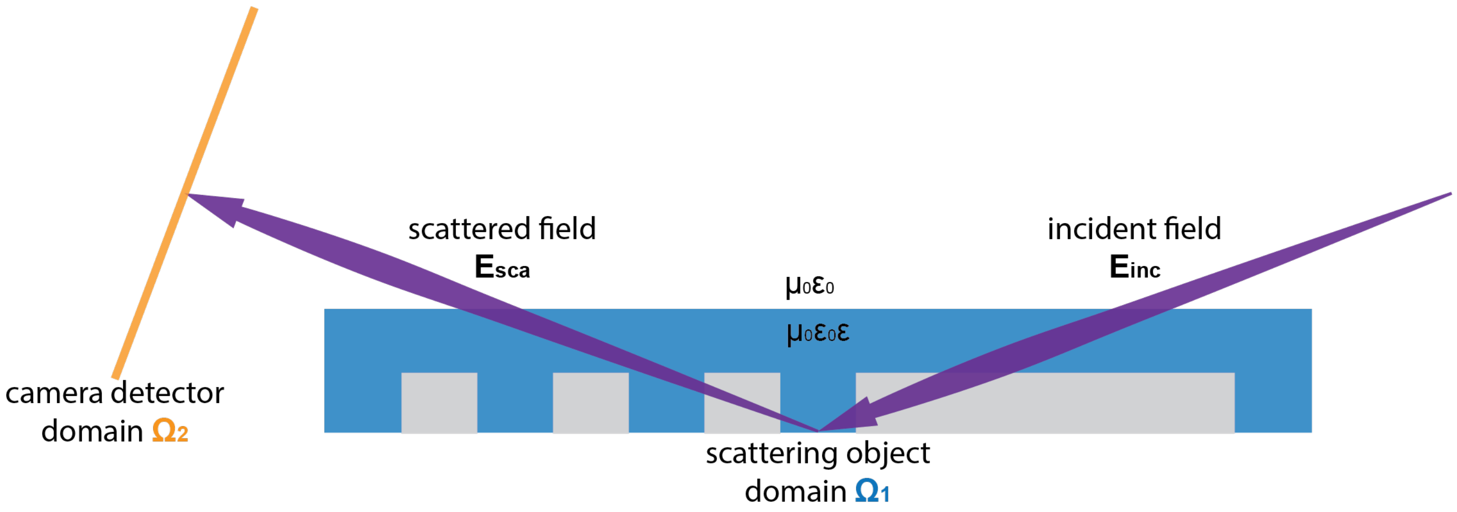
$$\nabla\times[\cancel{\mathbf{E}_{\mathrm{inc}}} + \mathbf{E}_{\mathrm{sca}}] = -i\omega\mu_0[\cancel{\mathbf{H}_{\mathrm{inc}}} + \mathbf{H}_{\mathrm{sca}}]$$

$$\nabla\times[\cancel{\mathbf{H}_{\mathrm{inc}}} + \mathbf{H}_{\mathrm{sca}}] = i\omega\epsilon_0[\cancel{\mathbf{E}_{\mathrm{inc}}} + \mathbf{E}_{\mathrm{sca}}] + i\omega\epsilon_0(\epsilon - 1)[\mathbf{E}_{\mathrm{inc}} + \mathbf{E}_{\mathrm{sca}}]$$

Forward Computation

Light-Structure Interaction

- Incident Field satisfies Maxwell Equations in homogeneous medium
- Total Field satisfies Maxwell Equations in inhomogeneous medium
- Scattered Field satisfies Maxwell Equations in homogeneous medium but driven by effective source



$$\nabla\times\mathbf{E}_{\mathrm{inc}} = -i\omega\mu_0\mathbf{H}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{inc}}$$

$$\nabla\times\mathbf{E}_{\mathrm{sca}} = -i\omega\mu_0\mathbf{H}_{\mathrm{sca}}$$

$$\nabla\times\mathbf{H}_{\mathrm{sca}} = i\omega\epsilon_0\mathbf{E}_{\mathrm{sca}} + \mathbf{J}$$

$$\mathbf{J} = i\omega\epsilon_0(\epsilon - 1)[\mathbf{E}_{\mathrm{inc}} + \mathbf{E}_{\mathrm{sca}}]$$

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Forward Computation

Light-Structure Interaction

- Scattered Field satisfies Maxwell Equations in homogeneous medium but driven by effective source
- Scattered Field computed using Green's Function

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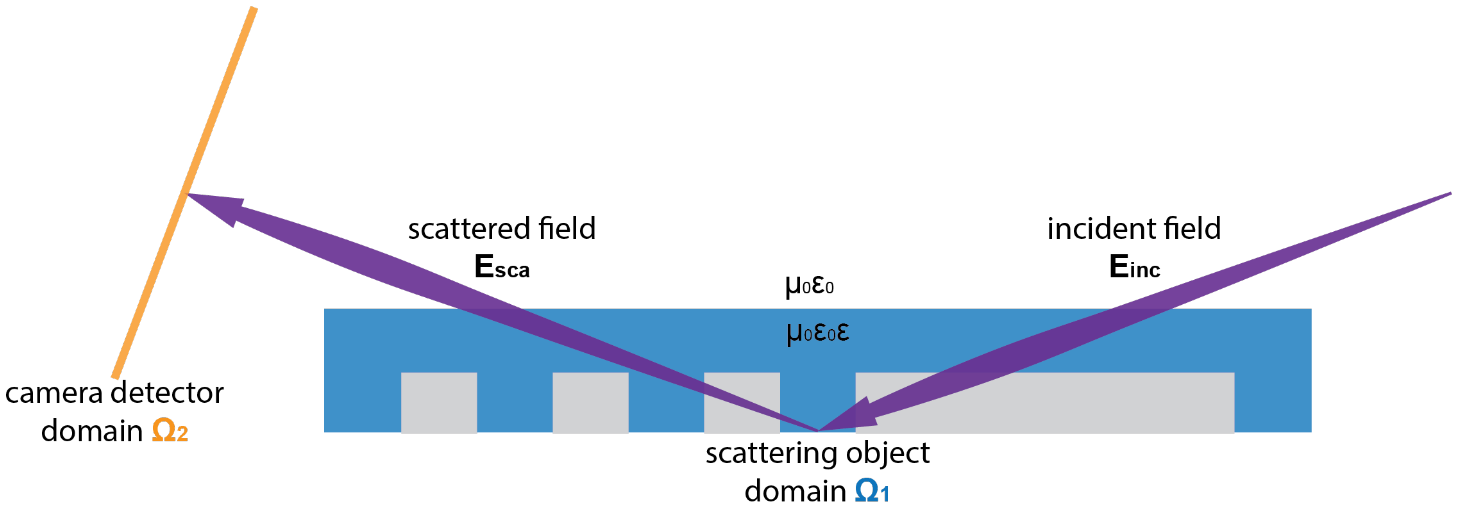
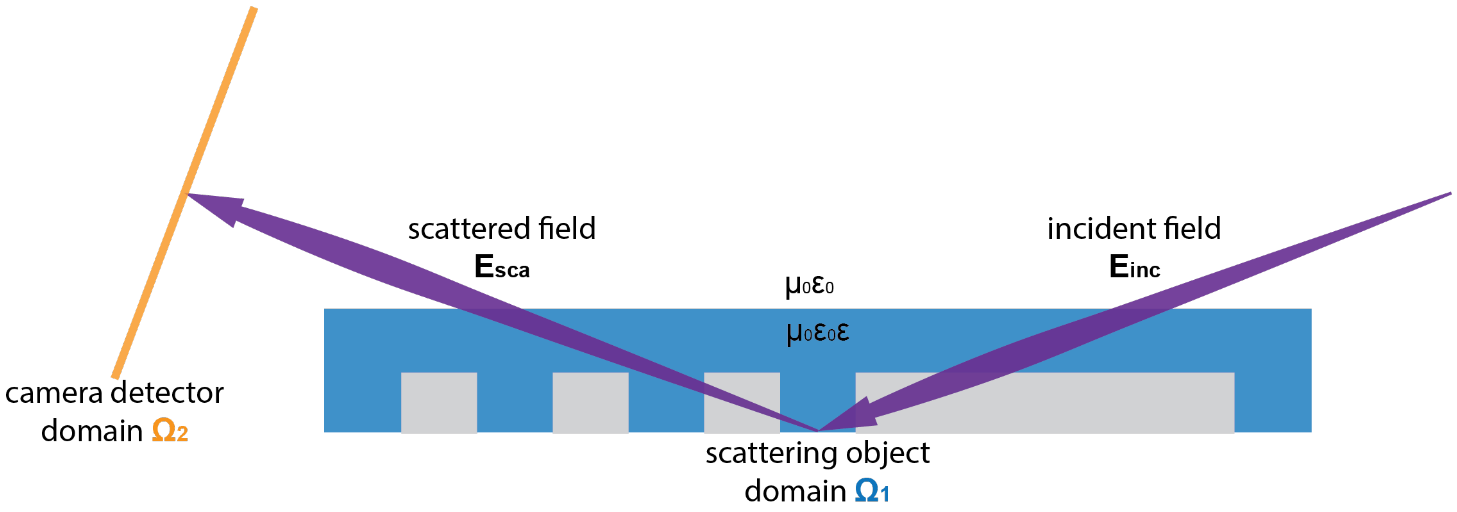


$$\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2) = \iiint_{\Omega_1} \underbrace{\mathrm{G}(\mathbf{r}_1 - \mathbf{r}_2)}_{\text{Green's Function}} \underbrace{\frac{\mathbf{J}(\mathbf{r}_1)}{i\omega}}_{\text{Effective Source}} \mathrm{d}^3\mathbf{r}_1$$

Forward Computation

Light-Structure Interaction

- Scattered Field satisfies Maxwell Equations in homogeneous medium but driven by effective source
- Scattered Field computed using Green's Function:
- Lippmann-Schwinger Equation
  $\chi(\mathbf{r}) = \epsilon_0[\epsilon(\mathbf{r}) - 1]$
- Other methods:
  RCWA, FEM, etc…



$$\underbrace{\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)}_{\text{unknown}} = \iiint_{\Omega_1} \mathrm{G}(\mathbf{r}_1 - \mathbf{r}_2)\chi(\mathbf{r}_1)[\underbrace{\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_1)}_{\text{unknown}} + \mathbf{E}_{\mathrm{inc}}(\mathbf{r}_1)]\mathrm{d}^3\mathbf{r}_1$$

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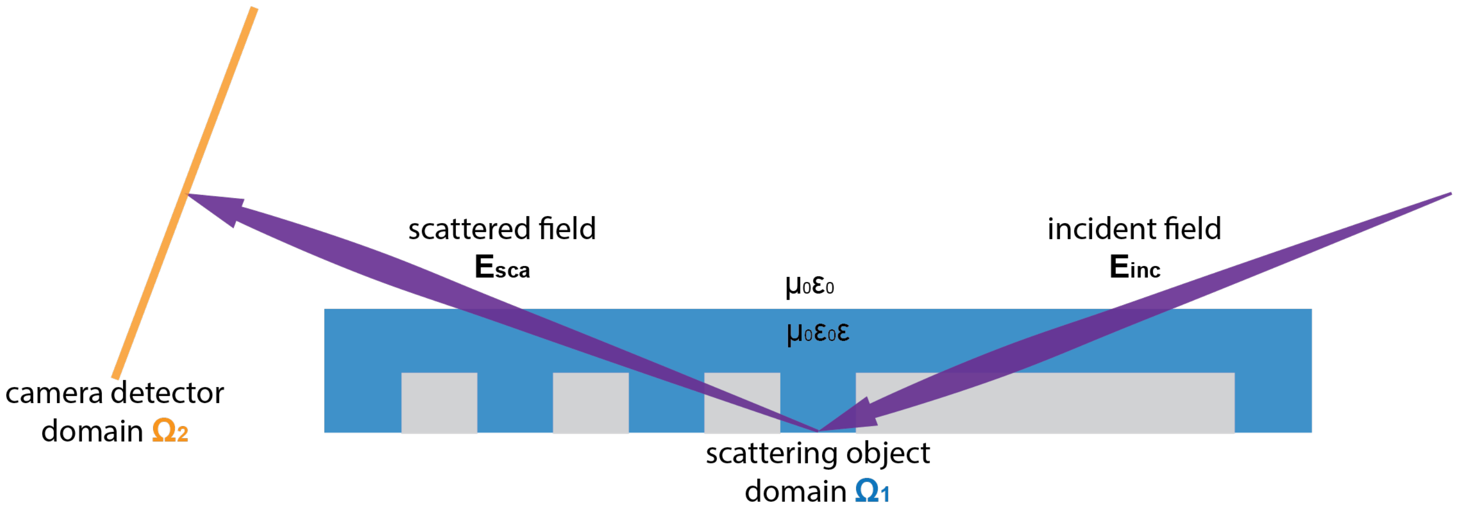
Backward Computation

Solving Inverse Problem

- Lippmann-Schwinger Equation
  $\chi(\mathbf{r}) = \epsilon_0[\epsilon(\mathbf{r}) - \mathbf{1}]$
- Compare the difference between meas and pred on the camera detector



$$\mathcal{L} = \iint_{\Omega_2} [|\bar{\mathbf{E}}_{\mathrm{sca}}(\mathbf{r}_2)| - |\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)|]^2 \mathrm{d}^2\mathbf{r}_2$$

meas pred

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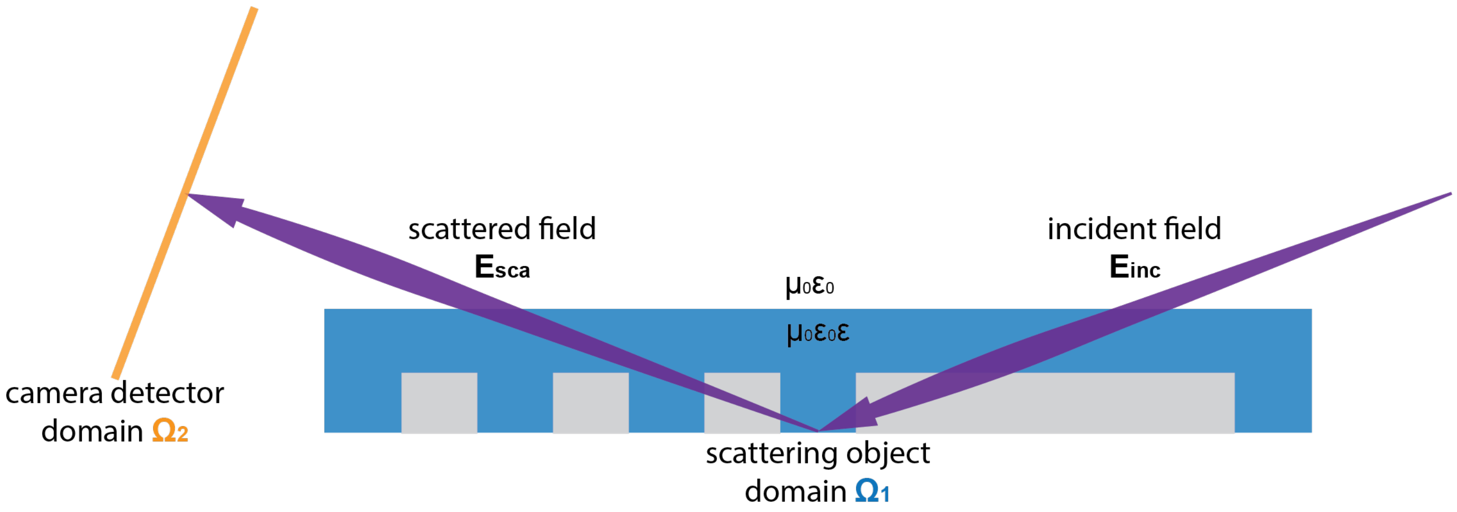
Backward Computation

Solving Inverse Problem

- Lippmann-Schwinger Equation
  $\chi(\mathbf{r}) = \epsilon_0[\epsilon(\mathbf{r}) - \mathbf{1}]$
- Compare the difference between meas and pred on the camera detector
- The chain of gradient derivation cannot be completed.
- Cannot derive the derivative of $\mathrm{E}_{\mathrm{sca}}$ with respect to χ



$$\delta\mathcal{L} = \iint_{\Omega_2} \frac{\partial\mathcal{L}}{\partial\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)} \cdot \delta\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)\mathrm{d}^2\mathbf{r}_2$$

$$\delta\mathcal{L} = \iint_{\Omega_2} \frac{\partial\mathcal{L}}{\partial\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)} \cdot \boxed{\frac{\partial\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)}{\partial\chi(\mathbf{r}_1)}} \cdot \delta\chi(\mathbf{r}_1)\ \mathrm{d}^2\mathbf{r}_2$$

~~analytical expression~~

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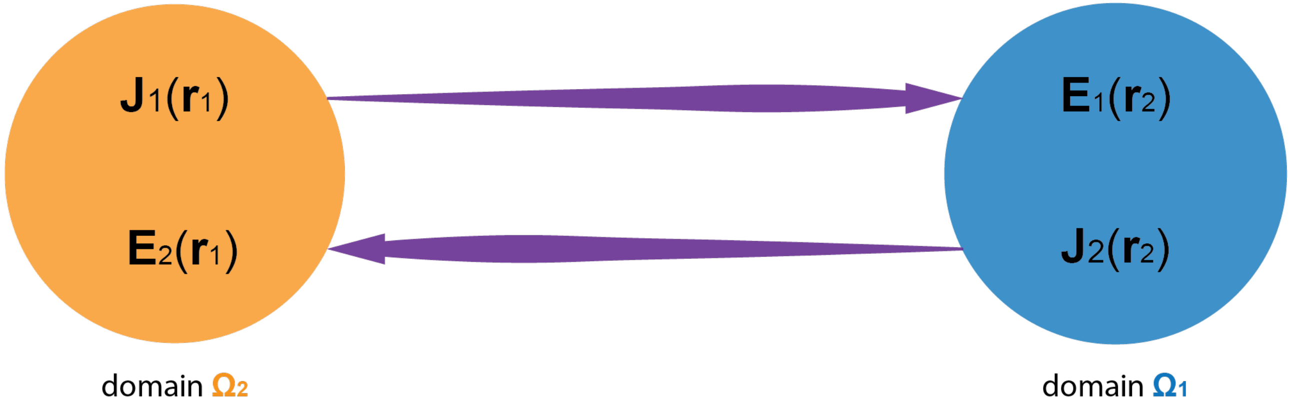
Reciprocity Theorem

- Derived from the Maxwell Equations
- Applies to linear, isotropic materials, and time-harmoic sources and fields



$$\iiint_{\Omega_2} \mathbf{J}_2\,(\mathbf{r}_2)\cdot\mathbf{E}_1(\mathbf{r}_2)\mathrm{d}^3\mathbf{r}_2 = \iiint_{\Omega_1} \mathbf{J}_1(\mathbf{r}_1)\cdot\mathbf{E}_2(\mathbf{r}_1)\mathrm{d}^3\mathbf{r}_1$$

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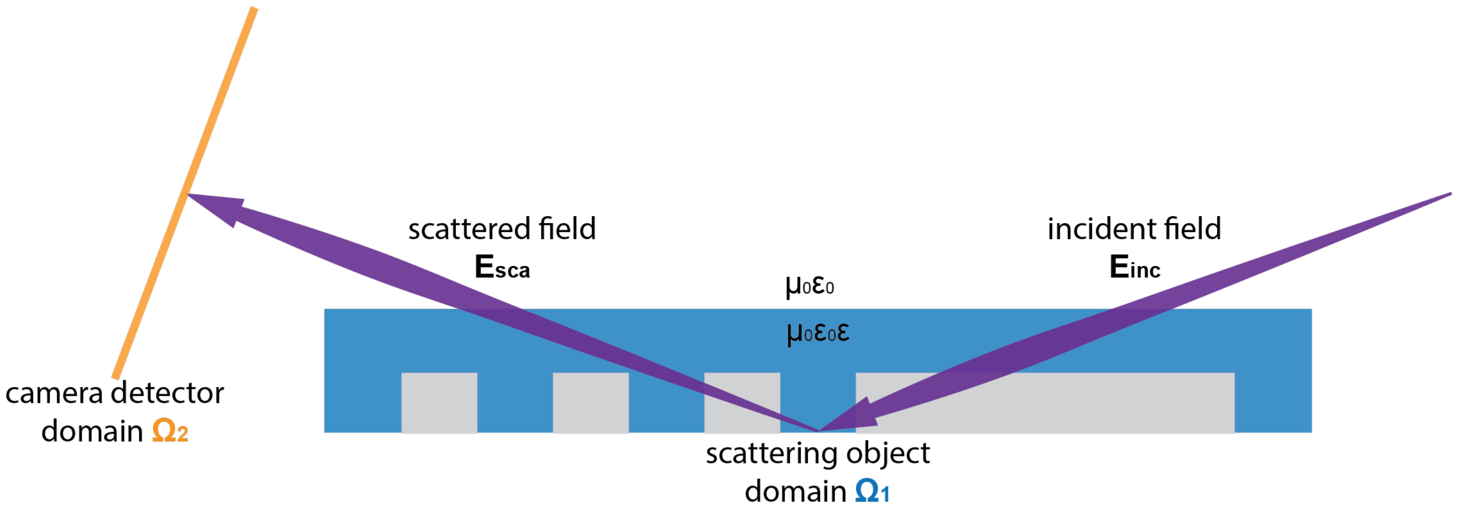
Backward Computation

Solving Inverse Problem using Reciprocity Theorem

- Identify the source and the field in the expression of $\delta\mathcal{L}$
- Find the source that generates the field $\delta\mathbf{E}_{sca}$
- Find the field that is generated by the source $\partial\mathcal{L}/\partial\mathbf{E}_{sca}$



$$\delta\mathcal{L} = \iint_{\Omega_2} \underbrace{\boxed{\frac{\partial\mathcal{L}}{\partial\mathbf{E}_{sca}(\mathbf{r}_2)}}}_{\text{Source}} \cdot \underbrace{\boxed{\delta\mathbf{E}_{sca}(\mathbf{r}_2)}}_{\text{Field}} \mathrm{d}^2\mathbf{r}_2$$

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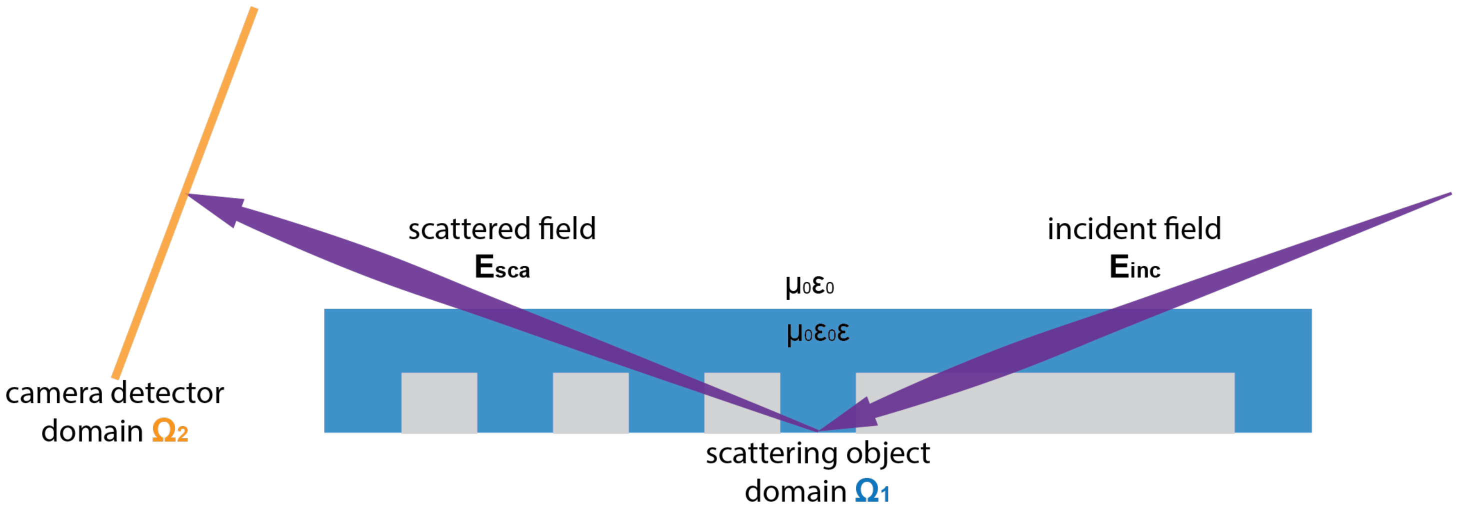
Backward Computation

Find the source that generates the field $\delta\mathbf{E}_{\text{sca}}$

- The total field $\mathbf{E}_{\text{tot}}$ satisfies the Maxwell Equation with permittivity $\epsilon_0\epsilon$
- The new total field $\mathbf{E}'_{\text{tot}}$ satisfies the Maxwell Equation with new permittivity $\epsilon_0\epsilon'$



$$\nabla\times\mathbf{E}_{\text{tot}} = -i\omega\mu_0\mathbf{H}_{\text{tot}}$$

$$\nabla\times\mathbf{H}_{\text{tot}} = i\omega\epsilon_0\epsilon\mathbf{E}_{\text{tot}}$$

$$\nabla\times\mathbf{E}'_{\text{tot}} = -i\omega\mu_0\mathbf{H}'_{\text{tot}}$$

$$\nabla\times\mathbf{H}'_{\text{tot}} = i\omega\epsilon_0\epsilon'\mathbf{E}'_{\text{tot}}$$

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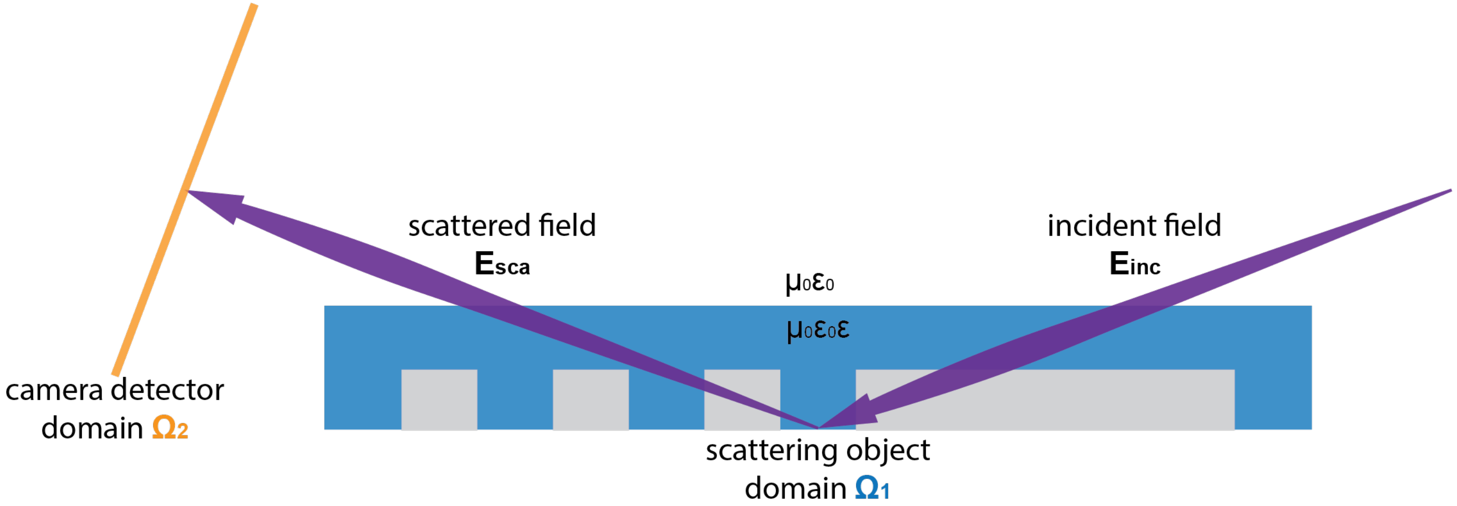
Backward Computation

Find the source that generates the field $\delta\mathbf{E}_{\mathrm{sca}}$

- The total field $\mathbf{E}_{\mathrm{tot}}$ satisfies the Maxwell Equation with permittivity $\epsilon_0\epsilon$
- The new total field $\mathbf{E'}_{\mathrm{tot}}$ satisfies the Maxwell Equation with new permittivity $\epsilon_0\epsilon'$
- $\delta\epsilon \leftrightarrow \delta\mathrm{E}_{\mathrm{sca}}$



$$\nabla\times\mathbf{E}_{\mathrm{tot}} = -i\omega\mu_0\mathbf{H}_{\mathrm{tot}}$$

$$\nabla\times\mathbf{H}_{\mathrm{tot}} = i\omega\epsilon_0\boldsymbol{\epsilon}\mathbf{E}_{\mathrm{tot}}$$

$$\nabla\times(\mathbf{E}_{\mathrm{tot}} + \delta\mathbf{E}_{\mathrm{sca}}) = -i\omega\mu_0(\mathbf{H}_{\mathrm{tot}} + \delta\mathbf{H}_{\mathrm{sca}})$$

$$\nabla\times(\mathbf{H}_{\mathrm{tot}} + \delta\mathbf{H}_{\mathrm{sca}}) = i\omega\epsilon_0(\boldsymbol{\epsilon} + \delta\boldsymbol{\epsilon})(\mathbf{E}_{\mathrm{tot}} + \delta\mathbf{E}_{\mathrm{sca}})$$

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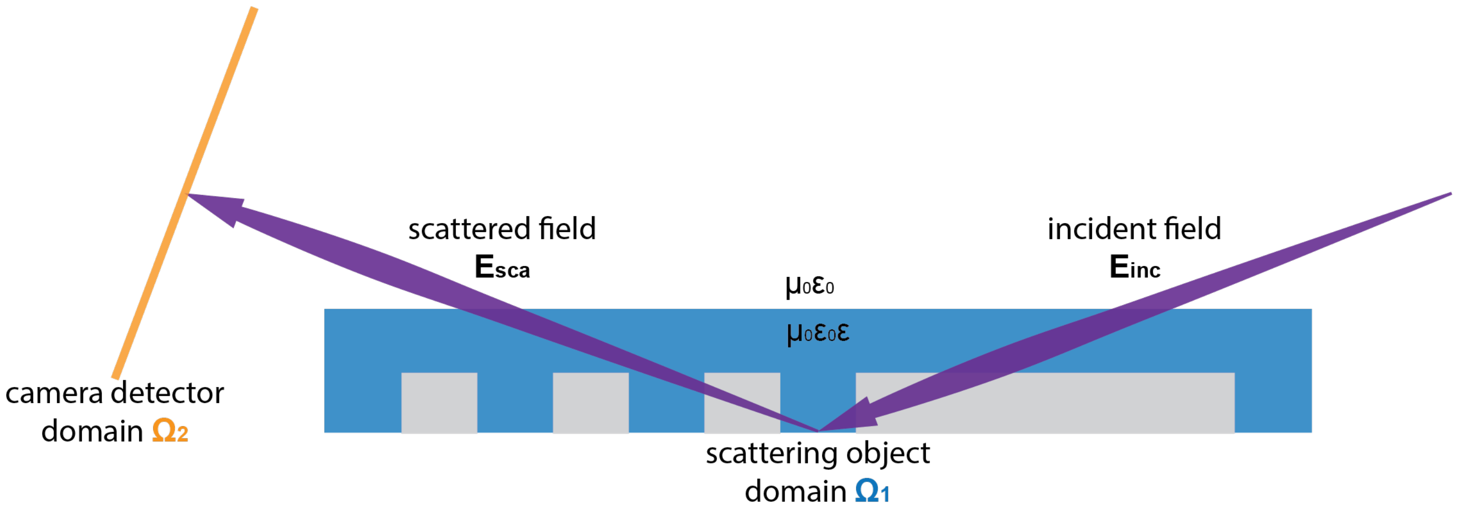
Backward Computation

Find the source that generates the field $\delta\mathbf{E}_{sca}$

- The total field $\mathbf{E}_{tot}$ satisfies the Maxwell Equation with permittivity $\epsilon_0\epsilon$
- The new total field $\mathbf{E'}_{tot}$ satisfies the Maxwell Equation with new permittivity $\epsilon_0\epsilon'$
- $\delta\epsilon \leftrightarrow \delta\mathrm{E}_{sca}$



$$\nabla\times\mathbf{E}_{tot} = -i\omega\mu_0\mathbf{H}_{tot}$$

$$\nabla\times\mathbf{H}_{tot} = i\omega\epsilon_0\epsilon\mathbf{E}_{tot}$$

$$\nabla\times(\cancel{\mathbf{E}_{tot}} + \delta\mathbf{E}_{sca}) = -i\omega\mu_0(\cancel{\mathbf{H}_{tot}} + \delta\mathbf{H}_{sca})$$

$$\nabla\times(\cancel{\mathbf{H}_{tot}} + \delta\mathbf{H}_{sca}) = i\omega\epsilon_0\epsilon(\cancel{\mathbf{E}_{tot}} + \delta\mathbf{E}_{sca}) + i\omega\epsilon_0\delta\epsilon(\mathbf{E}_{tot} + \cancel{\delta\mathbf{E}_{sca}})$$

negligible

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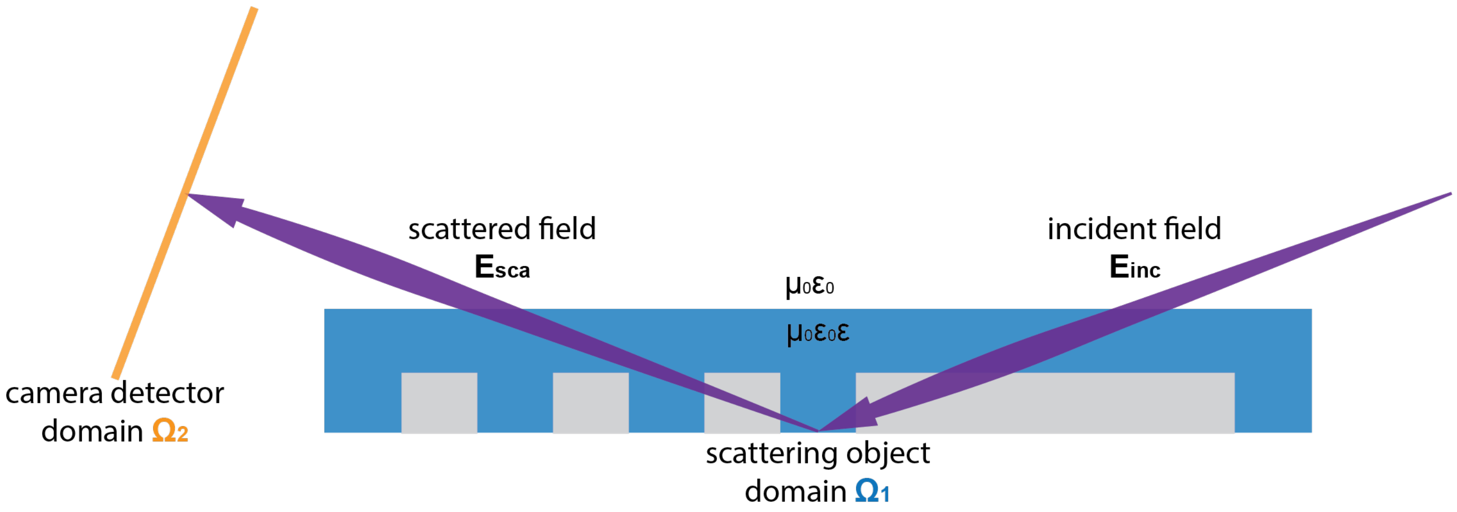
Backward Computation

Find the source that generates the field $\delta\mathbf{E}_{\mathrm{sca}}$

- The total field $\mathbf{E}_{\mathrm{tot}}$ satisfies the Maxwell Equation with permittivity $\epsilon_0\epsilon$
- The new total field $\mathbf{E}'_{\mathrm{tot}}$ satisfies the Maxwell Equation with new permittivity $\epsilon_0\epsilon'$
- $\delta\epsilon \leftrightarrow \delta\mathbf{J} \leftrightarrow \delta\mathrm{E}_{\mathrm{sca}}$



$$\nabla\times\mathbf{E}_{\mathrm{tot}} = -i\omega\mu_0\mathbf{H}_{\mathrm{tot}}$$

$$\nabla\times\mathbf{H}_{\mathrm{tot}} = i\omega\epsilon_0\boldsymbol{\epsilon}\mathbf{E}_{\mathrm{tot}}$$

$$\nabla\times\delta\mathbf{E}_{\mathrm{sca}} = -i\omega\mu_0\delta\mathbf{H}_{\mathrm{sca}}$$

$$\nabla\times\delta\mathbf{H}_{\mathrm{sca}} = i\omega\epsilon_0\boldsymbol{\epsilon}\delta\mathbf{E}_{\mathrm{sca}} + \delta\mathbf{J}$$

$$\delta\mathbf{J} = i\omega\epsilon_0\delta\boldsymbol{\epsilon}\mathbf{E}_{\mathrm{tot}}$$

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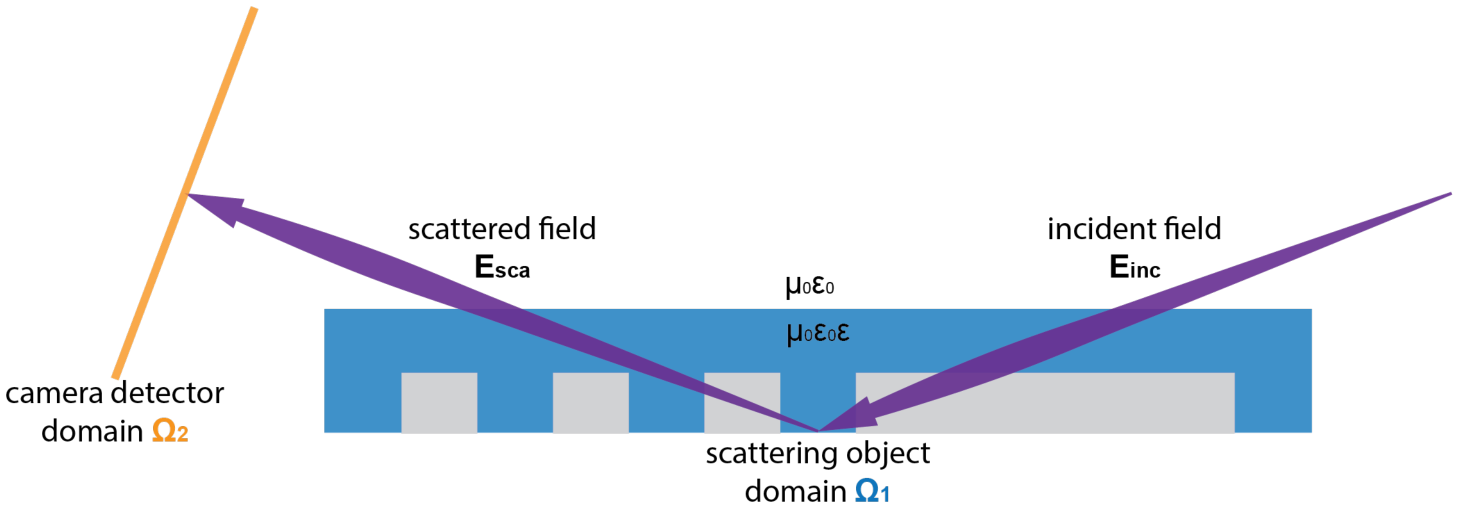
Backward Computation

Solving Inverse Problem using Reciprocity Theorem

- Identify the source and the field in the expression of $\delta\mathcal{L}$
- Find the source that generates the field $\delta\mathbf{E}_{\mathrm{sca}}$
- Find the field that is generated by the source $\partial\mathcal{L}/\partial\mathbf{E}_{\mathrm{sca}}$



source field

$$\delta\mathcal{L} = \iint_{\Omega_2} \frac{\partial\mathcal{L}}{\partial\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)} \cdot \delta\mathbf{E}_{\mathrm{sca}}(\mathbf{r}_2)\mathrm{d}^2\mathbf{r}_2$$

$$\delta\mathcal{L} = \iiint_{\Omega_1} \mathbf{E}_{\mathrm{src}}(\mathbf{r}_1) \cdot \delta\mathbf{J}(\mathbf{r}_1)\ \mathrm{d}^2\mathbf{r}_1$$

field source

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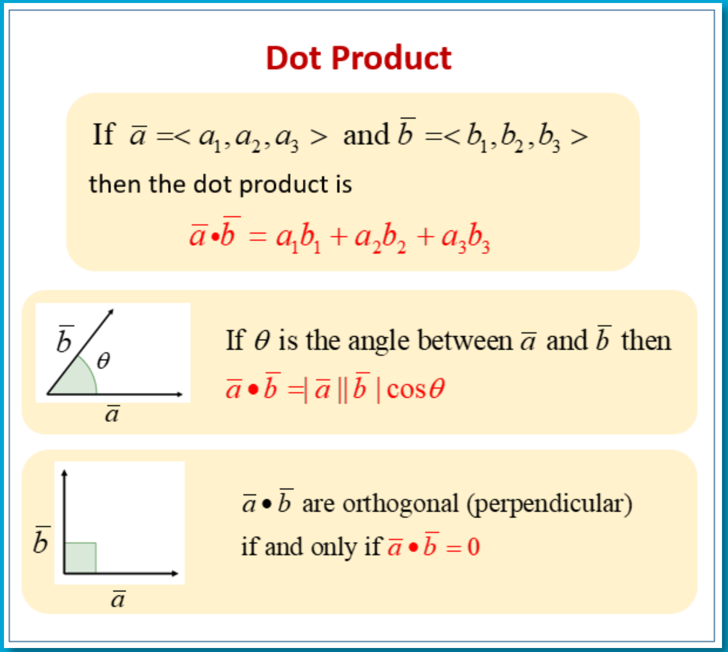
Backward Computation

Solving Inverse Problem using Reciprocity Theorem

- The variation $\delta\mathcal{L}$ proportional to the variation $\delta\epsilon$.


Dot Product

If $\bar{a} =< a_1, a_2, a_3 >$ and $\bar{b} =< b_1, b_2, b_3 >$

then the dot product is

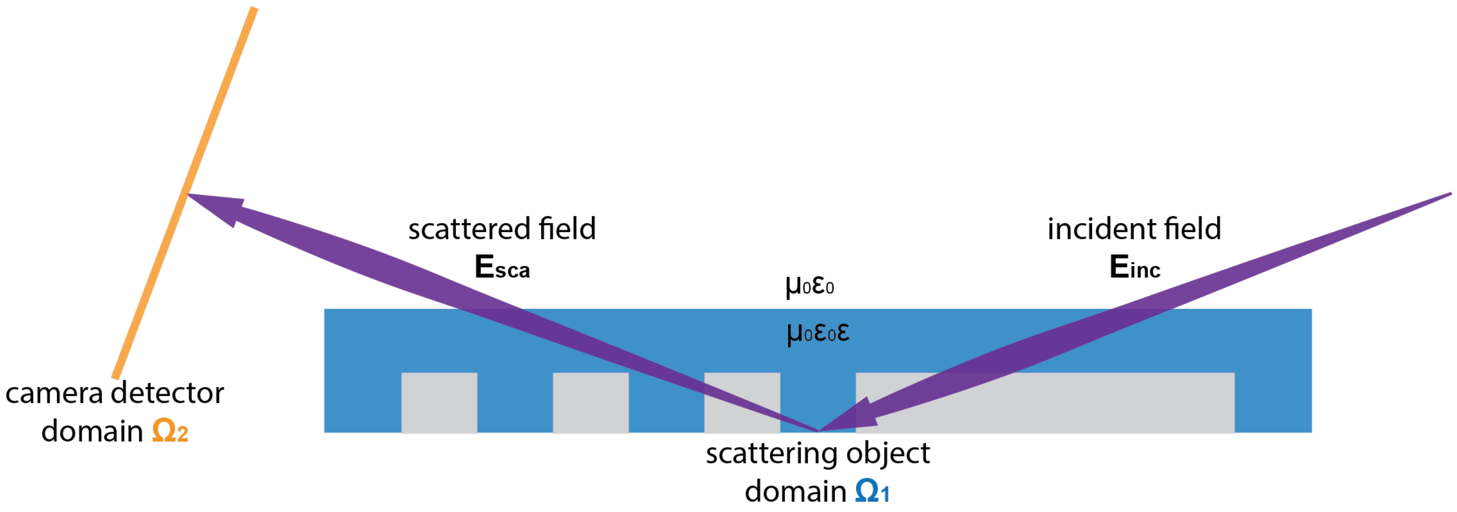
$\bar{a} \bullet \bar{b} = a_1 b_1 + a_2 b_2 + a_3 b_3$

If θ is the angle between $\bar{a}$ and $\bar{b}$ then

$\bar{a} \bullet \bar{b} = |\bar{a}||\bar{b}|\cos\theta$

$\bar{a} \bullet \bar{b}$ are orthogonal (perpendicular)

if and only if $\bar{a} \bullet \bar{b} = 0$

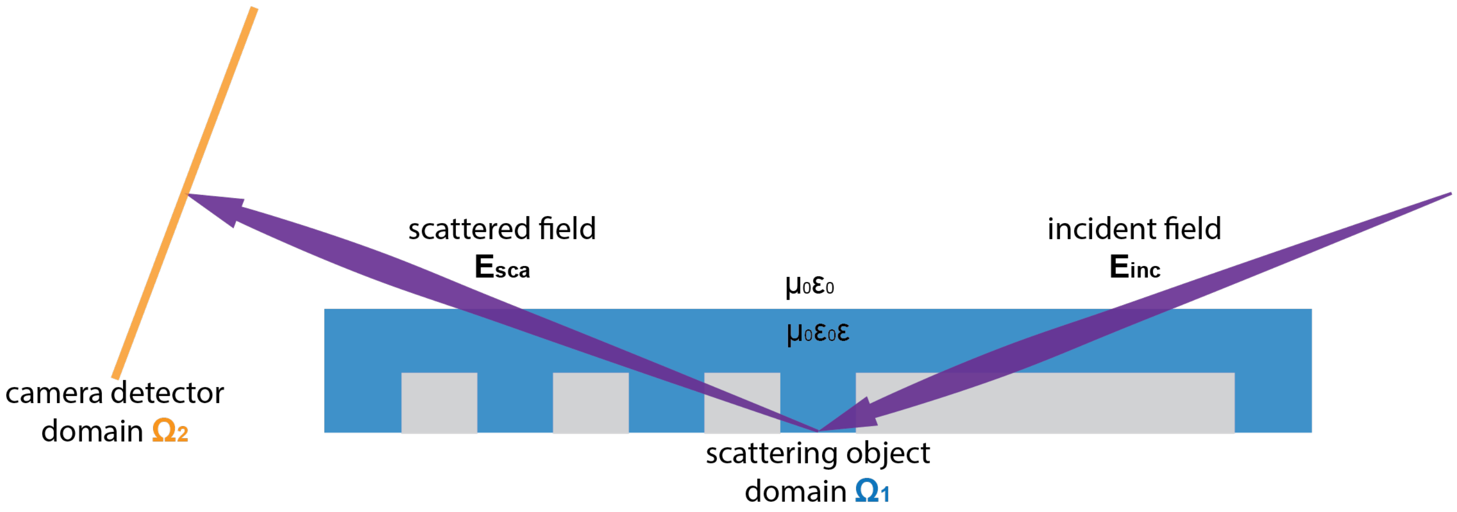


$$\delta\mathcal{L} = \iiint_{\Omega_1} \mathbf{E}_{\mathrm{src}}(\mathbf{r}_1) \cdot \delta\mathbf{J}(\mathbf{r}_1) \mathrm{d}^2\mathbf{r}_1 \geq -\iiint_{\Omega_1} |\mathbf{E}_{\mathrm{src}}(\mathbf{r}_1)|^2 \mathrm{d}^2\mathbf{r}_1$$

Backward Computation

Solving Inverse Problem using Reciprocity Theorem

- The variation $\delta\mathcal{L}$ proportional to the variation $\delta\epsilon$ through $\delta\mathbf{J}$.
- The minimum value of $\delta\mathcal{L}$ attained when $\mathbf{E}_{\mathrm{src}}$ and $\delta\mathbf{J}$ are parallel but in opposite directions.
- The steepest descent direction of $\mathcal{L}$ with respect to ϵ is derived.



$$\delta\mathbf{J}(\mathbf{r}_1) = i\omega\epsilon_0\delta\epsilon(\mathbf{r}_1)\mathbf{E}_{\mathrm{tot}}(\mathbf{r}_1) = -\mathbf{E}^*_{\mathrm{src}}(\mathbf{r}_1)$$

$$\delta\epsilon(\mathbf{r}_1) = -\frac{\mathbf{E}^*_{\mathrm{src}}(\mathbf{r}_1)}{i\omega\epsilon_0\mathbf{E}_{\mathrm{tot}}(\mathbf{r}_1)}$$

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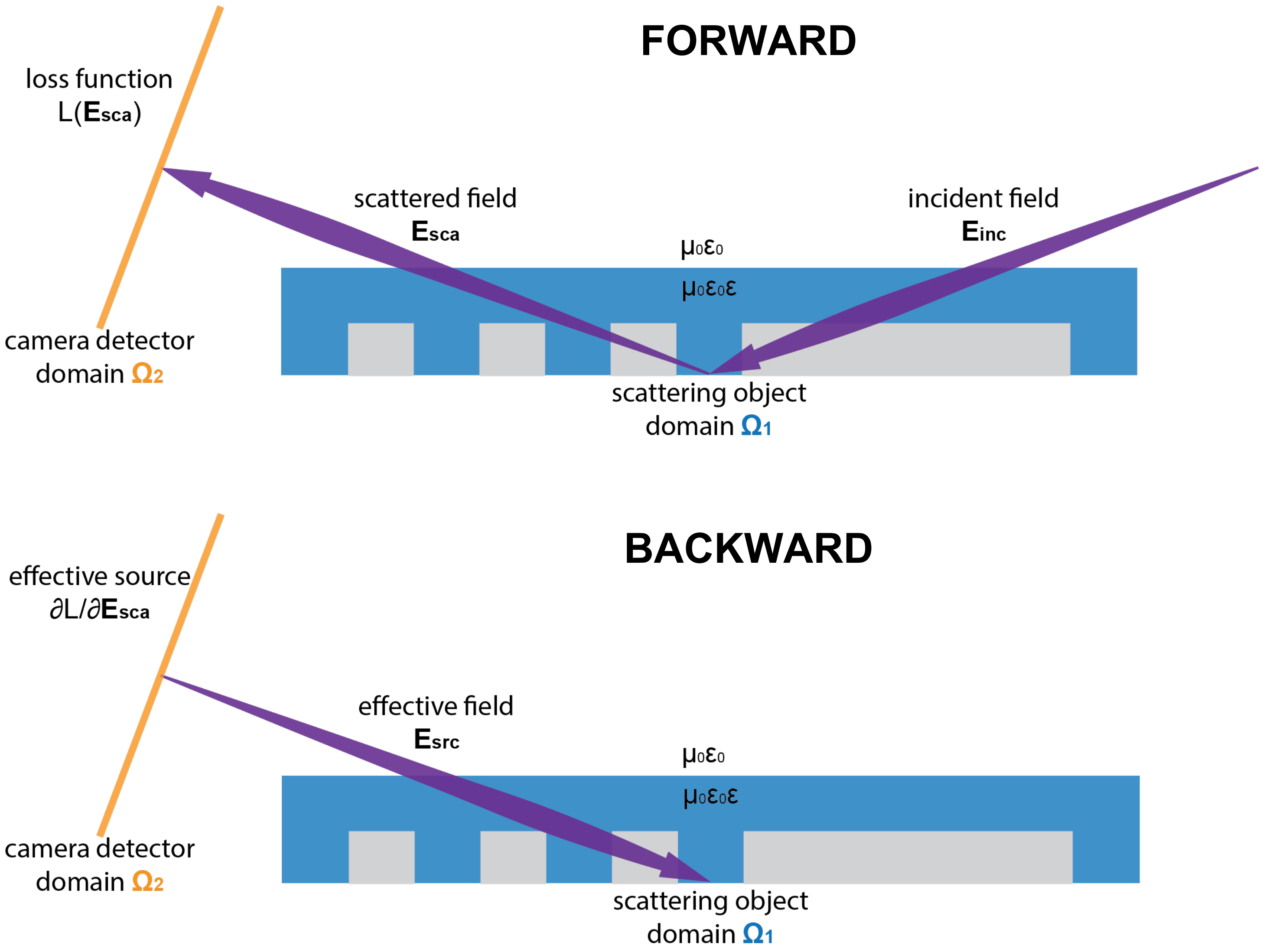
Summary

Solving Inverse Problem using Reciprocity Theorem

- Perform 2-times computation of Light-Structure Interaction.
- Update permittivity distribution ϵ at all locations together.

Compute:

1. Scattered field: $\mathbf{E}_{\mathrm{sca}}$
2. Loss function: $\mathcal{L}(\mathbf{E}_{\mathrm{sca}})$
3. Effective source: $\partial\mathcal{L}/\partial\mathbf{E}_{\mathrm{sca}}$
4. Effective field: $\mathbf{E}_{\mathrm{src}}$
5. Update function of ϵ: $\delta\epsilon$



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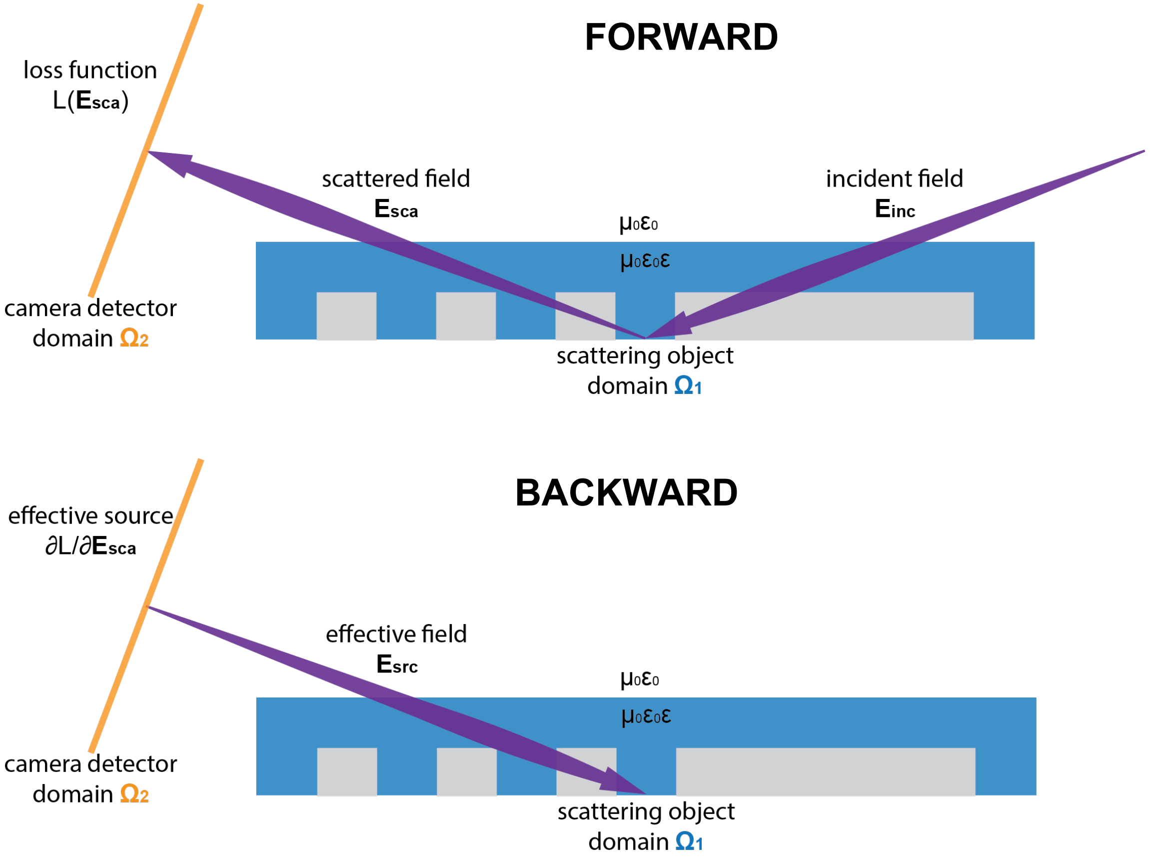
Concolusion



- Avoid gradient computation in inverse (optical) scattering problem using Reciprocity Theorem
- Requires ONLY two propagations to be able to update permittivity distribution at all locations simultaneously.

Thank you for your attention

Name