Inverse elastic scattering with adaptive FE meshes

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Aim

- Numerically model the forming of images in a Transmission Electronic Microscope (TEM)

➡forward problem

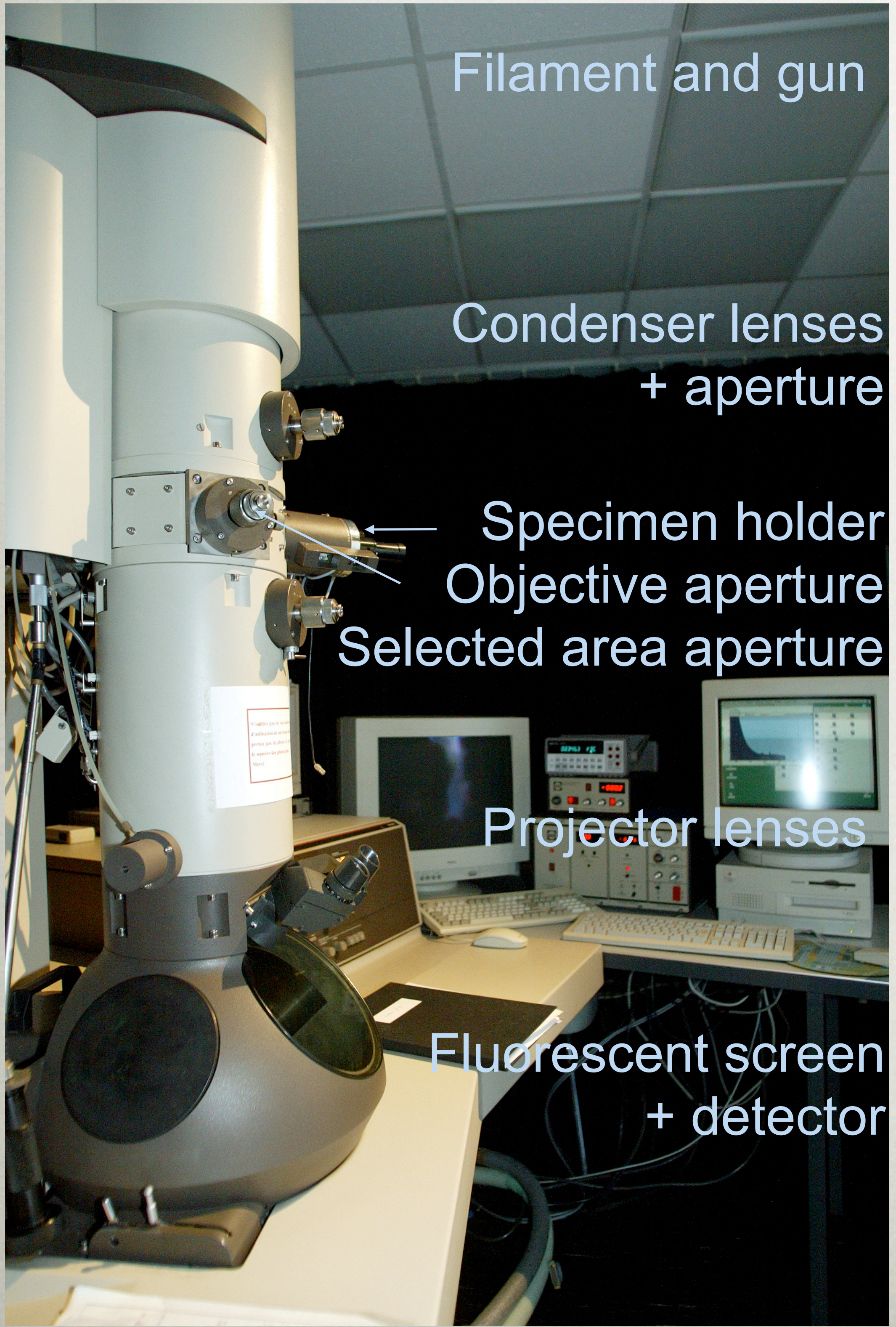
- From given images, identify defects within the studied sample

➡inverse problem

Outline

- TEM forward scattering
  - TEM principles
  - TEM forward scattering
- Inverse scattering
- Results

TEM PRINCIPLES



Philips CM20-UT

E_c = 200 keV

v = 0.70 c

λ = 2.51 10^{-12} m

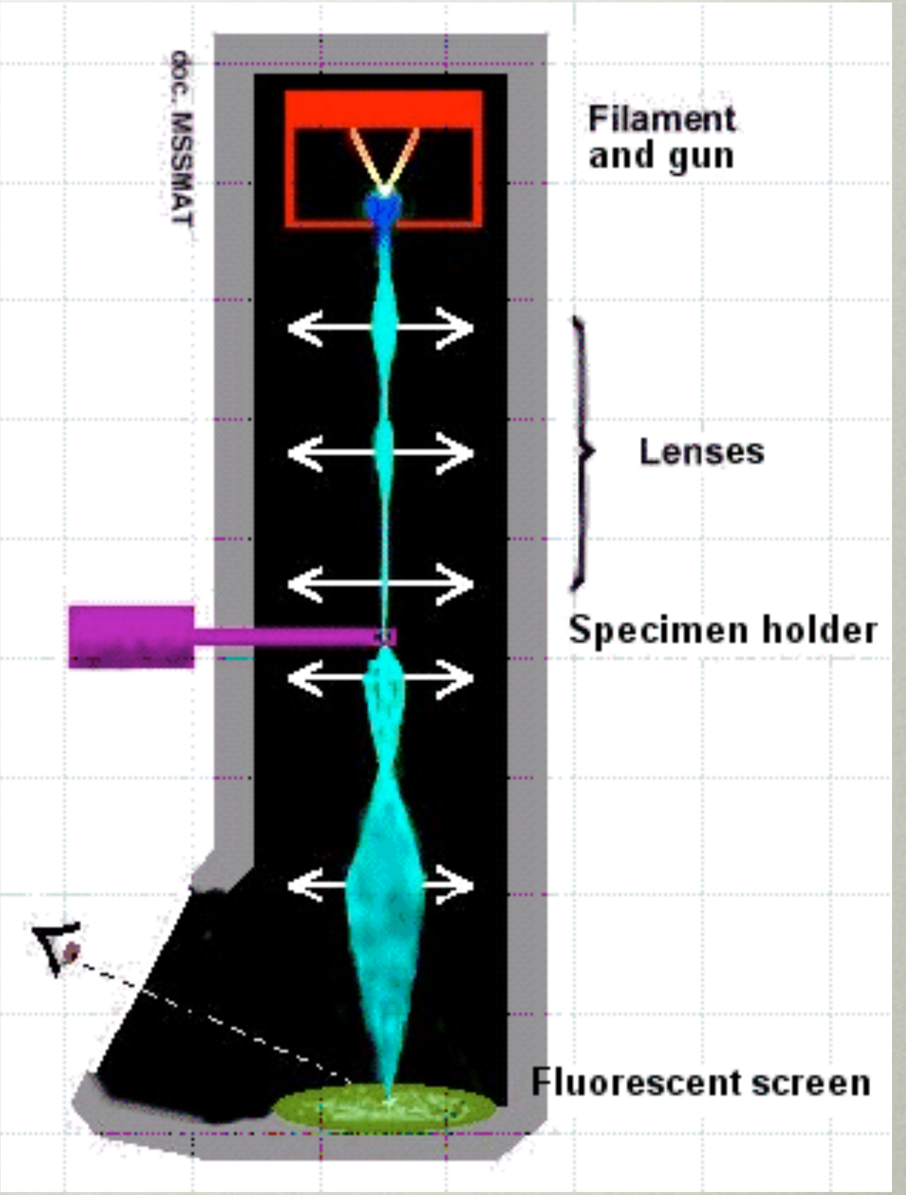
k_i = 2.51 10^{12} rad.m^{-1}

β = 13 mrad

C_s = 0.5 mm

δ = 0.19 10^{-9} m

θ_{max} ~ ±0.25 rad



TEM principles

- Incident electron:
  - plane wave

$$\psi_i(\mathbf{x}) = \tilde{\psi}_i \exp(\mathrm{i}\mathbf{k}_i \cdot \mathbf{x})$$

- Schrödinger equation:

$$-\frac{1}{2}\Delta\psi_i = E_i\psi_i$$

$$E_i = ||\mathbf{k}_i||^2/2$$

Parallel illumination

$\theta = 0$

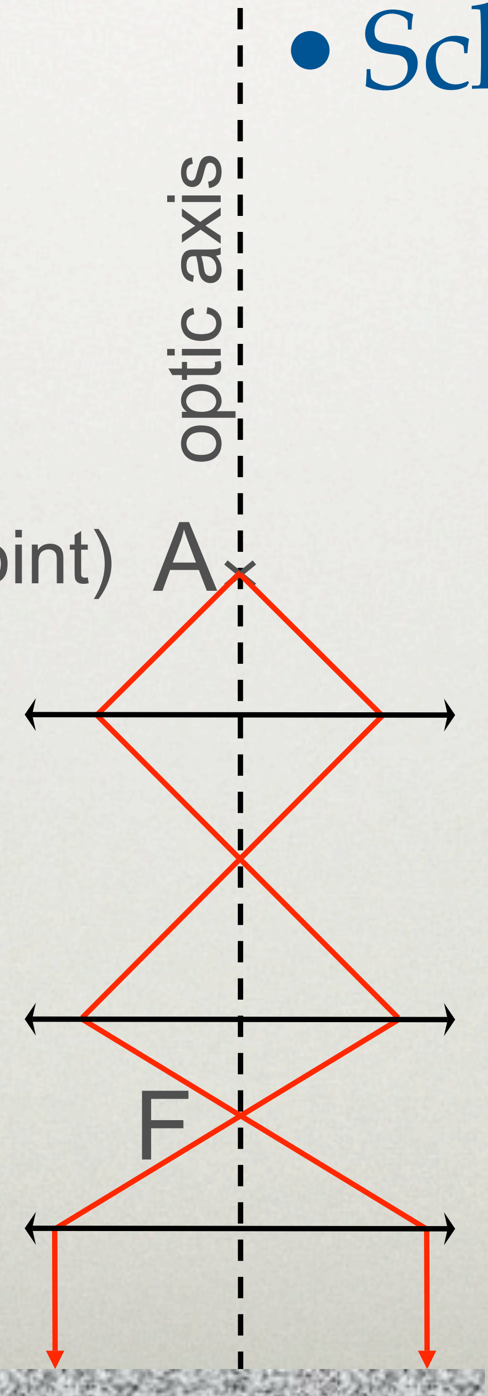
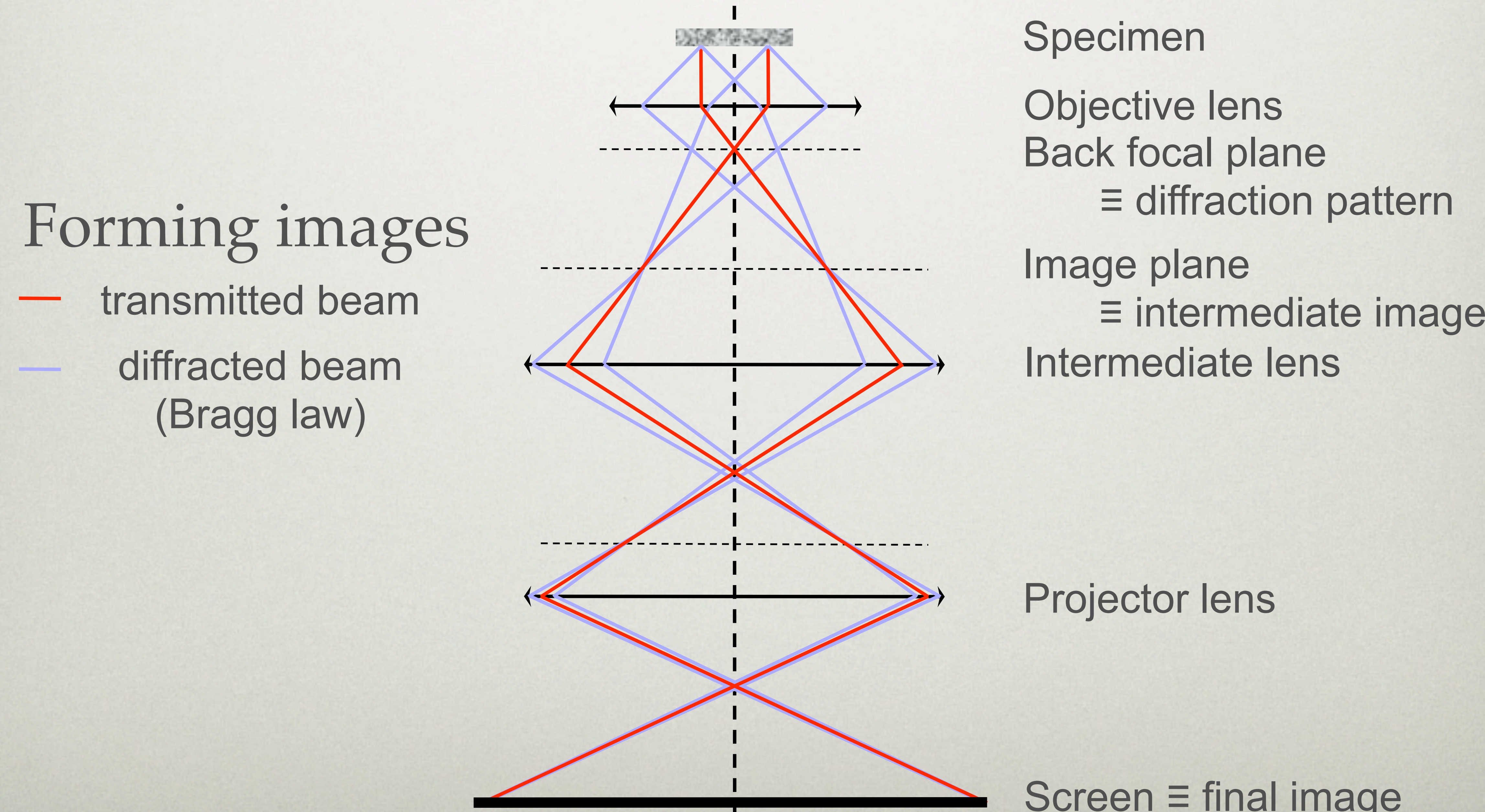


Image of A through C1 and C2
= focal point of objective lens

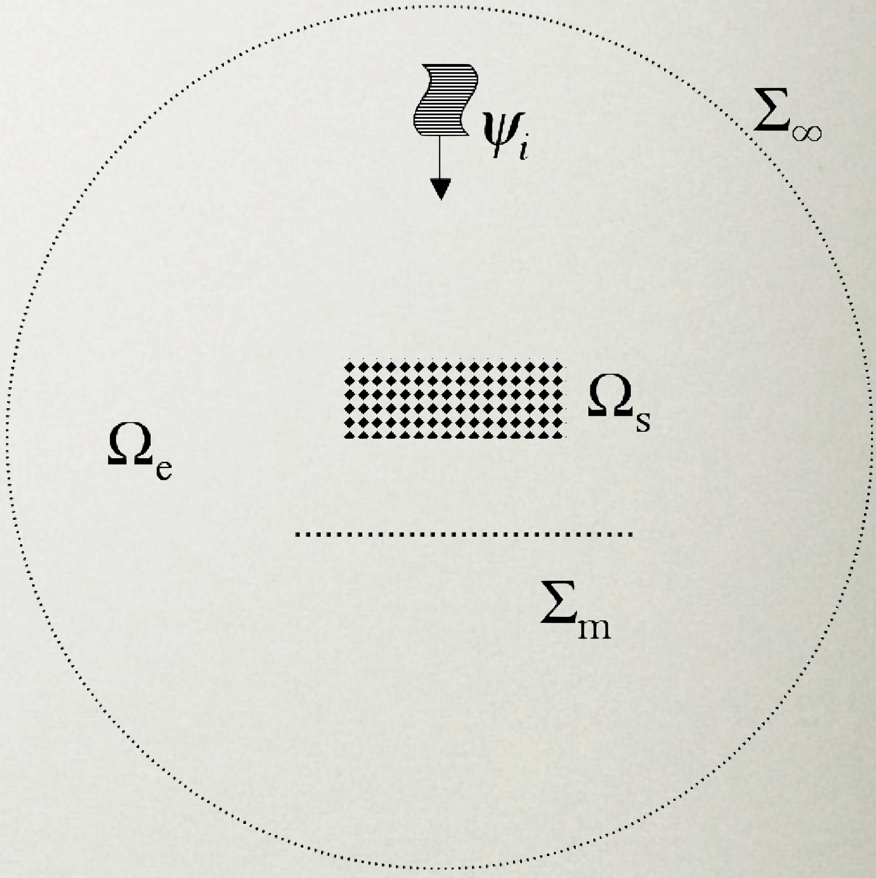
TEM principles

- Outgoing wave



TEM forward scattering

- Schrödinger equation:
  - for incident electron only [Wang 1995]
  - assumptions + decompositions
    $\psi = \psi_i + \psi_d$ ⟵ diffracted field
  - paraxial approximation
    $\psi_d(\mathbf{x}) = \tilde{\psi}_d(\mathbf{x}) \exp(\mathrm{i}\mathbf{k}_i \cdot \mathbf{x})$



$$\frac{1}{2}\Delta\tilde{\psi}_d + \mathrm{i}\mathbf{k}_i \cdot \nabla\tilde{\psi}_d = V\tilde{\psi}_i \text{ in } \Omega_e$$

$$\frac{\partial\tilde{\psi}_d}{\partial\mathbf{n}} = \mathrm{i}(||\mathbf{k}_i|| - \mathbf{k}_i \cdot \mathbf{n})\tilde{\psi}_d \text{ on } \Sigma_\infty$$

[Popov 2006]

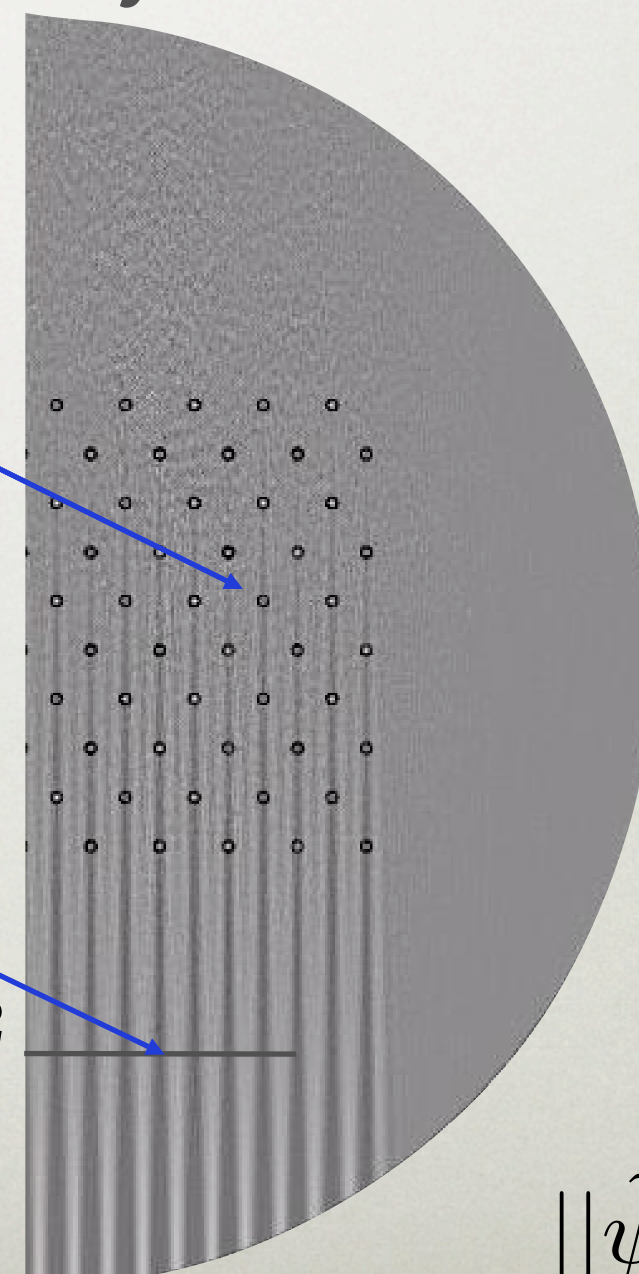
Example on α-iron [011] axis

- FE simulation on a 2D very thin sample
  - Yukawa potential for the sample

$$V_0(\mathbf{x}) = \sum_{k=1}^{N_a} K \frac{\mathrm{e}^{-a||\mathbf{x}-\mathbf{x}_k||}}{||\mathbf{x}-\mathbf{x}_k||}$$

  - Wave intensity measured on Σ_m
  - ~ 600,000 DOFs

$||\psi_m||^2$



$||\tilde{\psi}_i + \tilde{\psi}_d||^2$

Outline

- TEM forward scattering
- Inverse scattering
  - Inverse problem and misfit functional
  - Adjoint state
  - Two meshes formulation
- First results

Inverse problem

- Experimental data:
  - Simulated forward scattering of a sample with defects
  - Intensity on a specific virtual plane Σ_m
- Inverse problem:
  - Search for the unknown potential associated with the measured intensity
  - Find the corresponding defects

Misfit functional

- Misfit function [Beilina *et al* 2005] [Beilina *et al* 2006]

with an additional regularization term

$$J(V) = \frac{1}{4}\int_{\Sigma_m} \left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2 \right)^2 + \frac{\alpha}{2}\int_{\Omega_v} (V - V_0)^2$$

V_0: potential of the crystal with no defects

Adjoint state

- Similar to the forward problem

$$\frac{1}{2}\Delta z + \mathrm{i}\mathbf{k}_i^* \cdot \nabla z = 0 \text{ in } \Omega_e$$

$$\frac{\partial z}{\partial \mathbf{n}} = -\mathrm{i}(||\mathbf{k}_i|| + \mathbf{k}_i^* \cdot \mathbf{n})z \text{ on } \Sigma_\infty$$

- [[dz/dn]] discontinuity on Σ_m

$$\frac{1}{2}\left[\left[\frac{\partial z}{\partial \mathbf{n}}\right]\right] = \left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2\right)(\tilde{\psi}_i + \tilde{\psi}_d) \text{ on } \Sigma_m$$

Compatibility condition

- Derivative of the misfit function

$$\delta J = \int_{\Sigma_m} \left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2 \right) \mathrm{Re} \left((\tilde{\psi}_i + \tilde{\psi}_d) \delta \tilde{\psi}_d^* \right)$$

$$+ \alpha \int_{\Omega_v} (V - V_0) \delta V$$

$$= \int_{\Omega_v} - \mathrm{Re}(\tilde{\psi}_i z^*) \delta V + \alpha \int_{\Omega_v} (V - V_0) \delta V$$

$$\boxed{\mathrm{Re}(\tilde{\psi}_i z^*) = \alpha (V - V_0) \text{ in } \Omega_e}$$

V_0: potential of the crystal with no defects

Numerical resolution

Forward pb.

$$\frac{1}{2}\Delta\tilde{\psi}_d + \mathrm{i}\mathbf{k}_i \cdot \nabla\tilde{\psi}_d = V\tilde{\psi}_i \text{ in } \Omega_e$$

$$\frac{\partial\tilde{\psi}_d}{\partial\mathbf{n}} = \mathrm{i}(||\mathbf{k}_i|| - \mathbf{k}_i \cdot \mathbf{n})\tilde{\psi}_d \text{ on } \Sigma_\infty$$

Adjoint pb.

$$\frac{1}{2}\Delta z + \mathrm{i}\mathbf{k}_i^* \cdot \nabla z = 0 \text{ in } \Omega_e$$

$$\frac{\partial z}{\partial\mathbf{n}} = -\mathrm{i}(||\mathbf{k}_i|| + \mathbf{k}_i^* \cdot \mathbf{n})z \text{ on } \Sigma_\infty$$

$$\frac{1}{2}\left[\left[\frac{\partial z}{\partial\mathbf{n}}\right]\right] = \left(||\tilde{\psi}_i + \tilde{\psi}_d||^2 - ||\psi_m||^2\right)(\tilde{\psi}_i + \tilde{\psi}_d) \text{ on } \Sigma_m$$

Compatibility

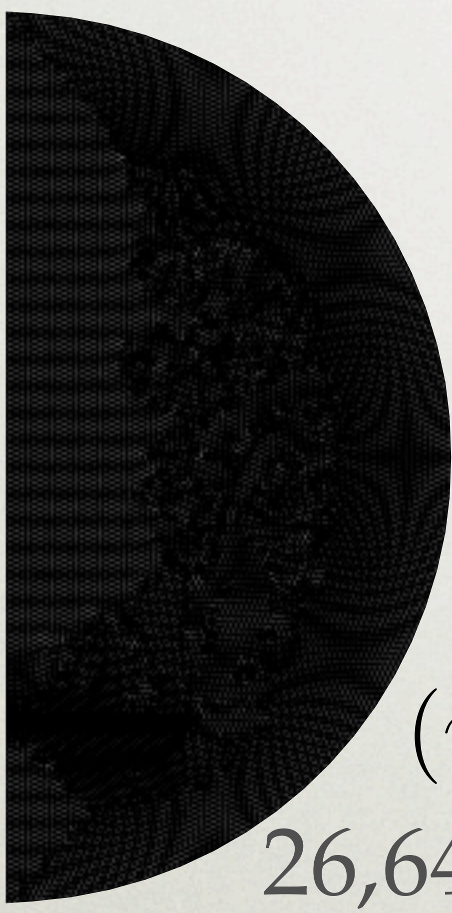
$$\mathrm{Re}(\tilde{\psi}_i z^*) = \alpha(V - V_0) \text{ in } \Omega_e$$

Numerical resolution

- Problems of convergence:
  - the sought potential is discretized (FE mesh)
  - n FE nodes ⟷ n scalar values to identify
- Possible solutions:
  - restrict the area where the potential is sought
  - use a coarser mesh

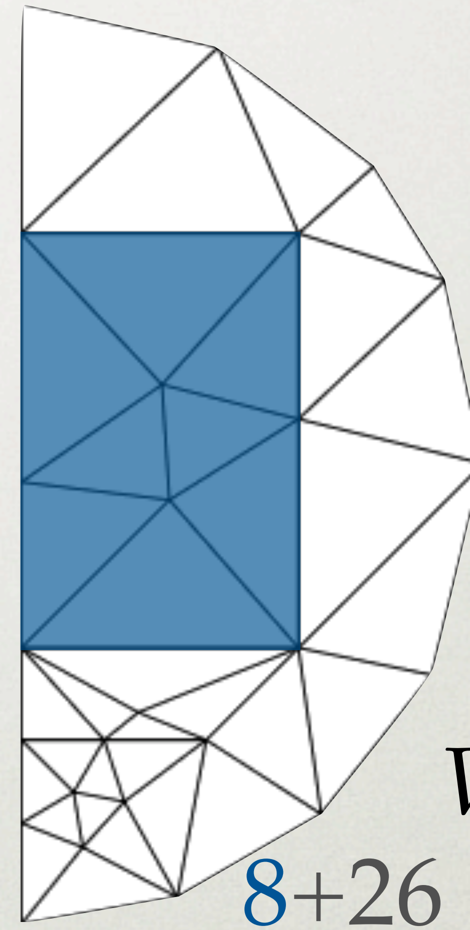
Adaptive strategy

- Introduction of two different meshes



$(\tilde{\psi}_d, z)$

26,645 elements



$V - V_0$

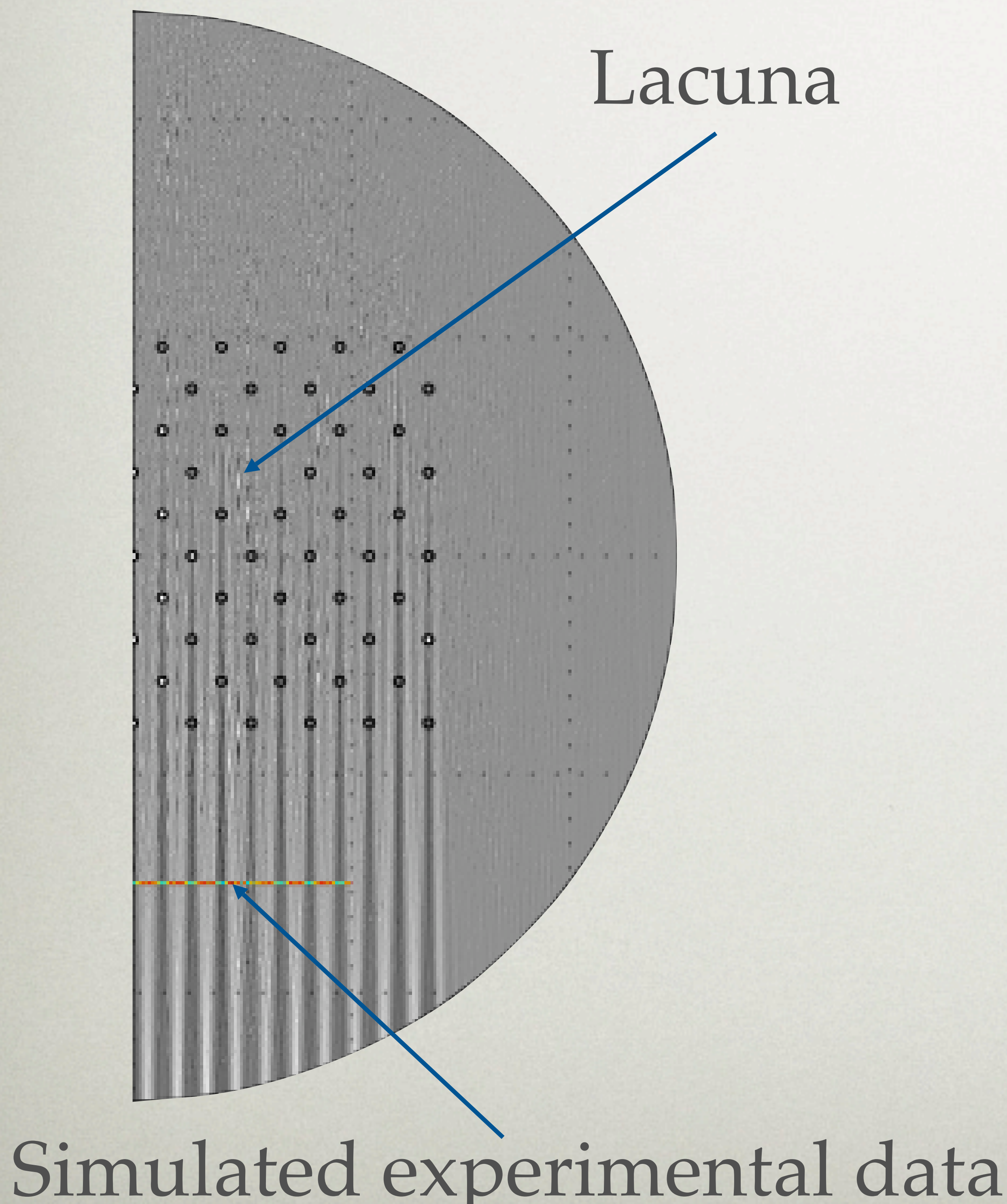
8+26 elements

- Adaption of the mesh associated with V-V_0
  - local estimators of the misfit function J [Bangerth 2003]

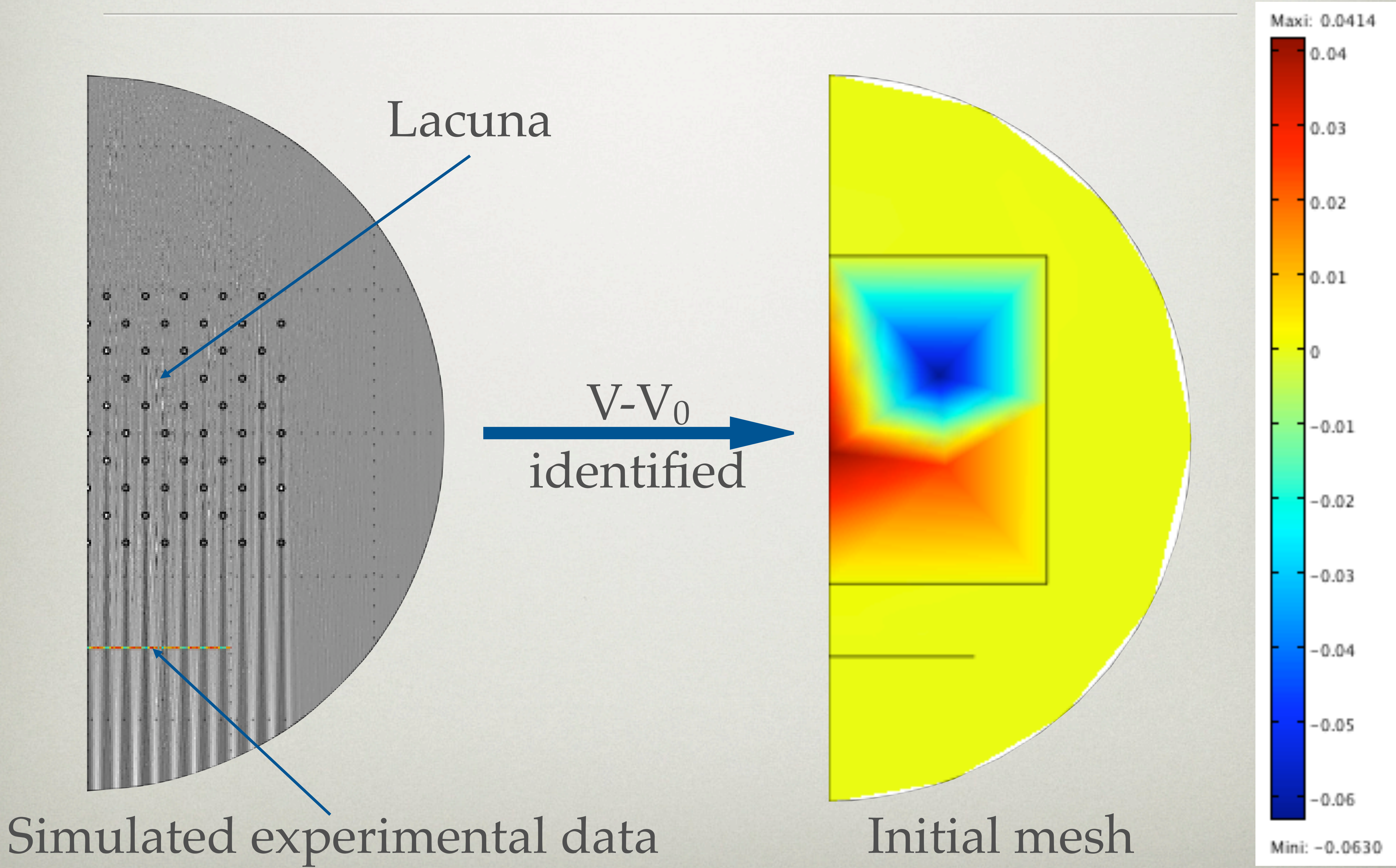
Outline

- TEM forward scattering
- Inverse scattering
- First results
  - specimen with a lacuna
  - specimen with a slit

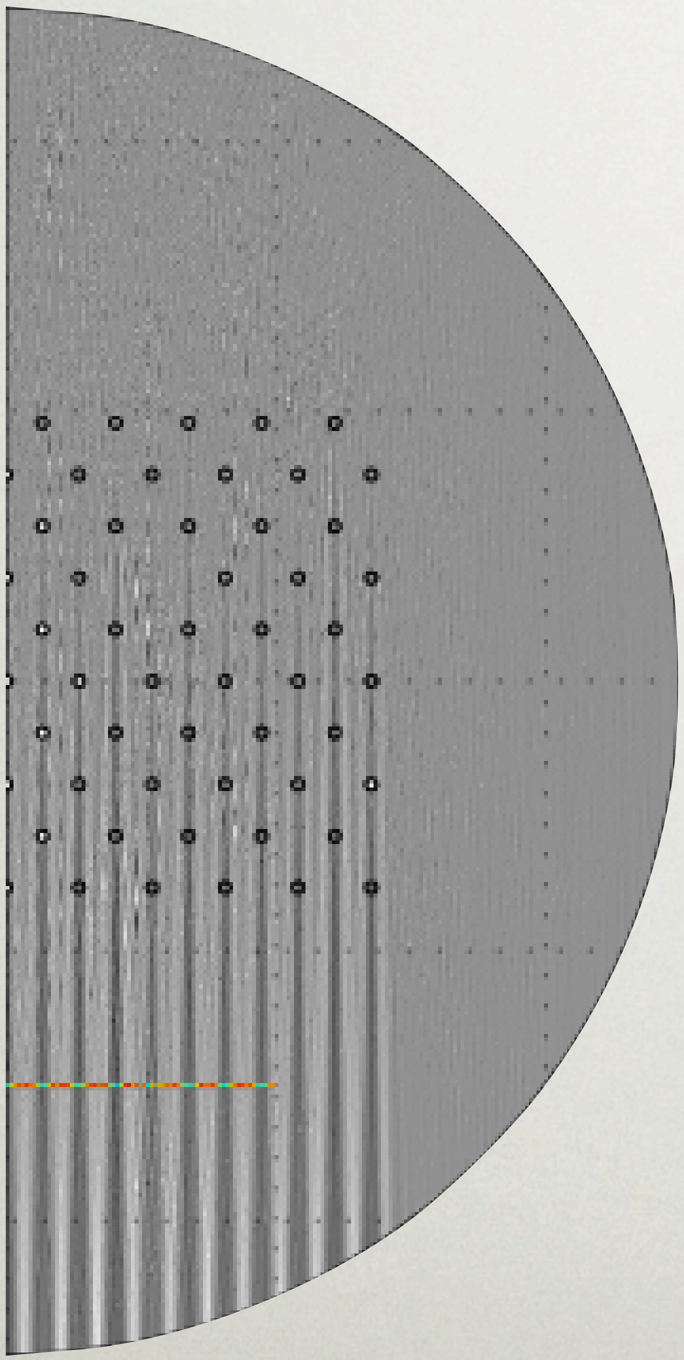
Example 1 on α-iron: sample with a lacuna



Example 1 on α-iron: sample with a lacuna

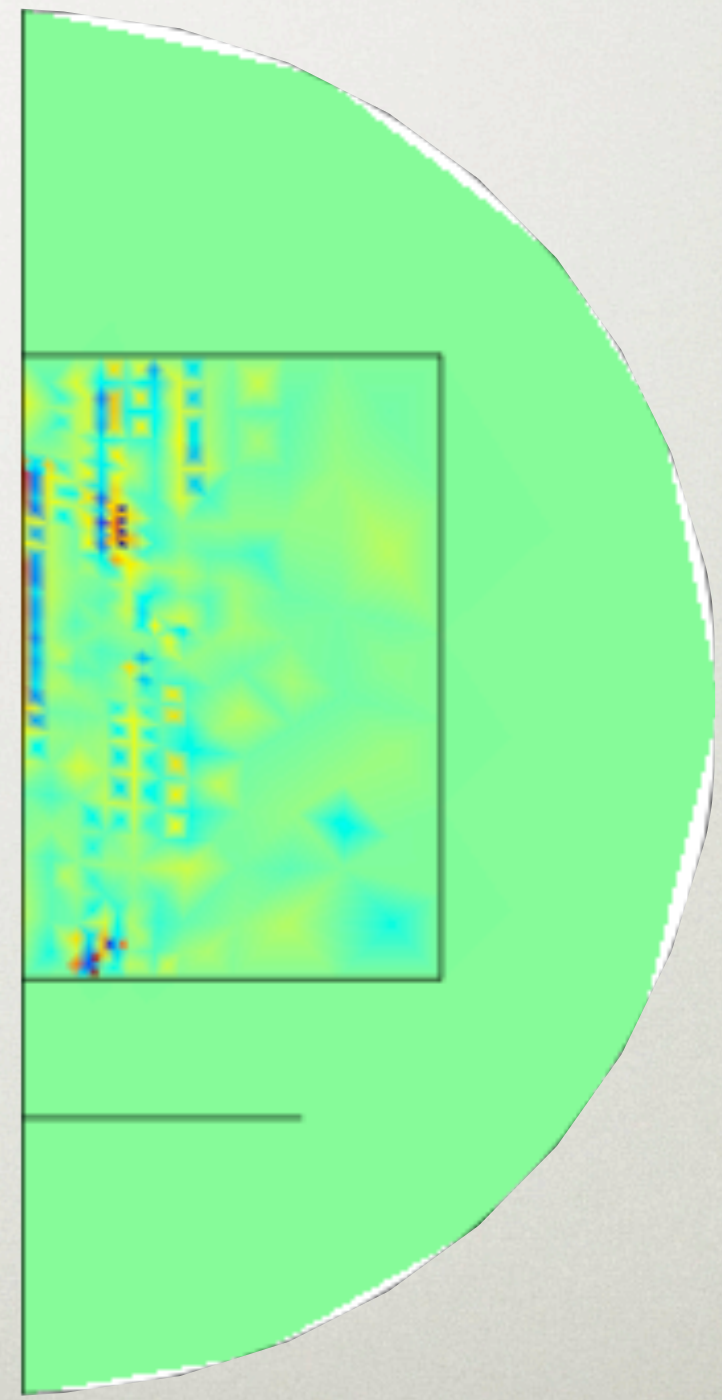


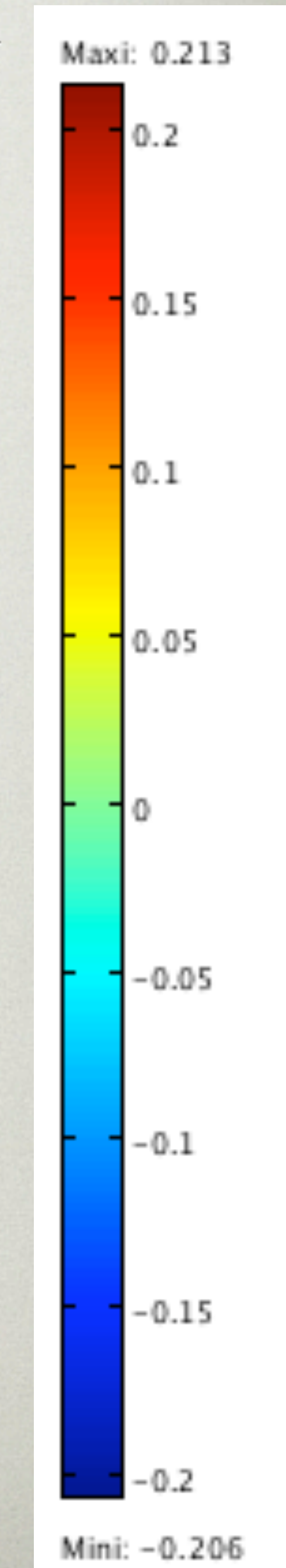
Example 1 on α-iron: sample with a lacuna



$V\text{-}V_0$

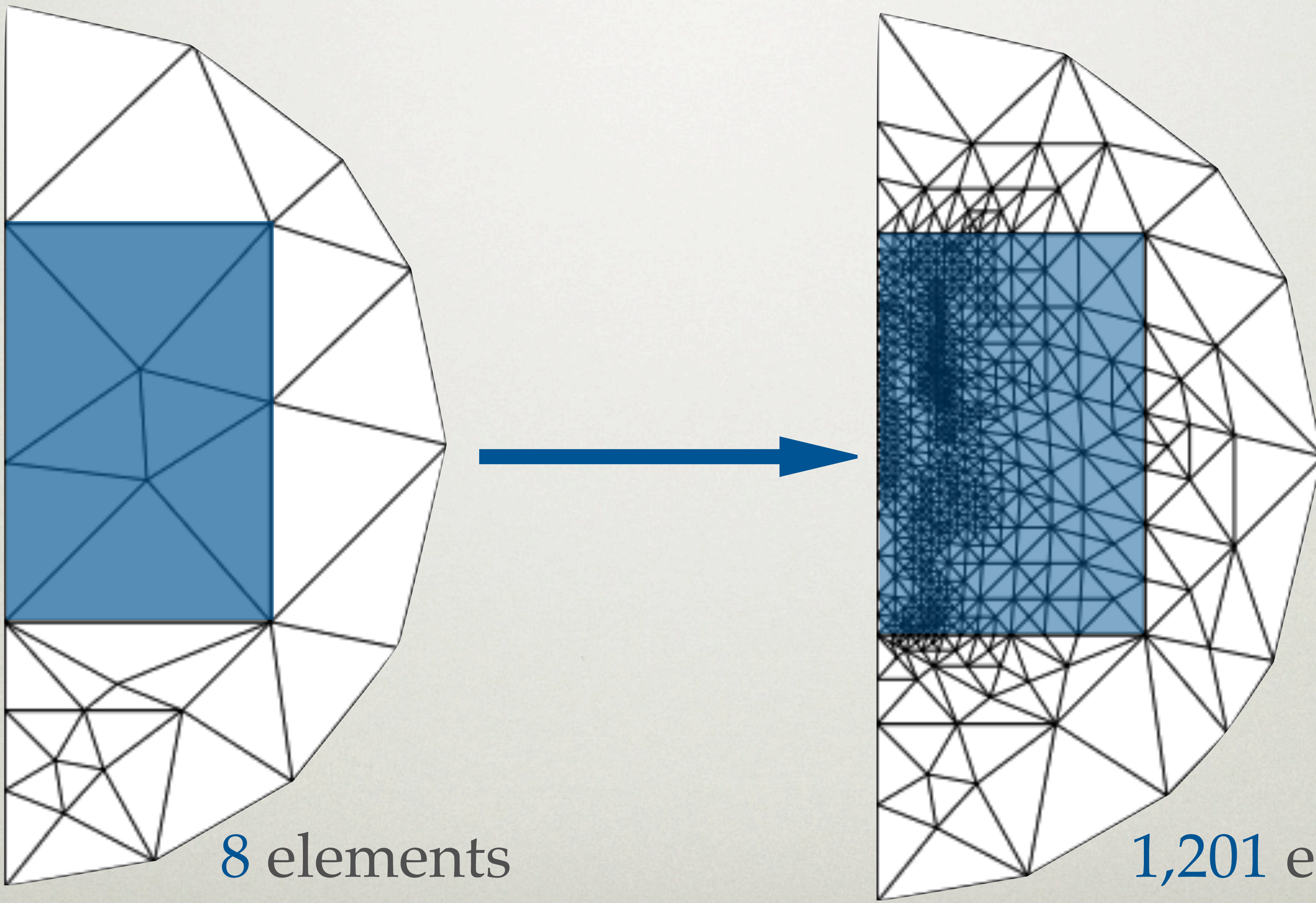
identified





Mesh after 5 iterations

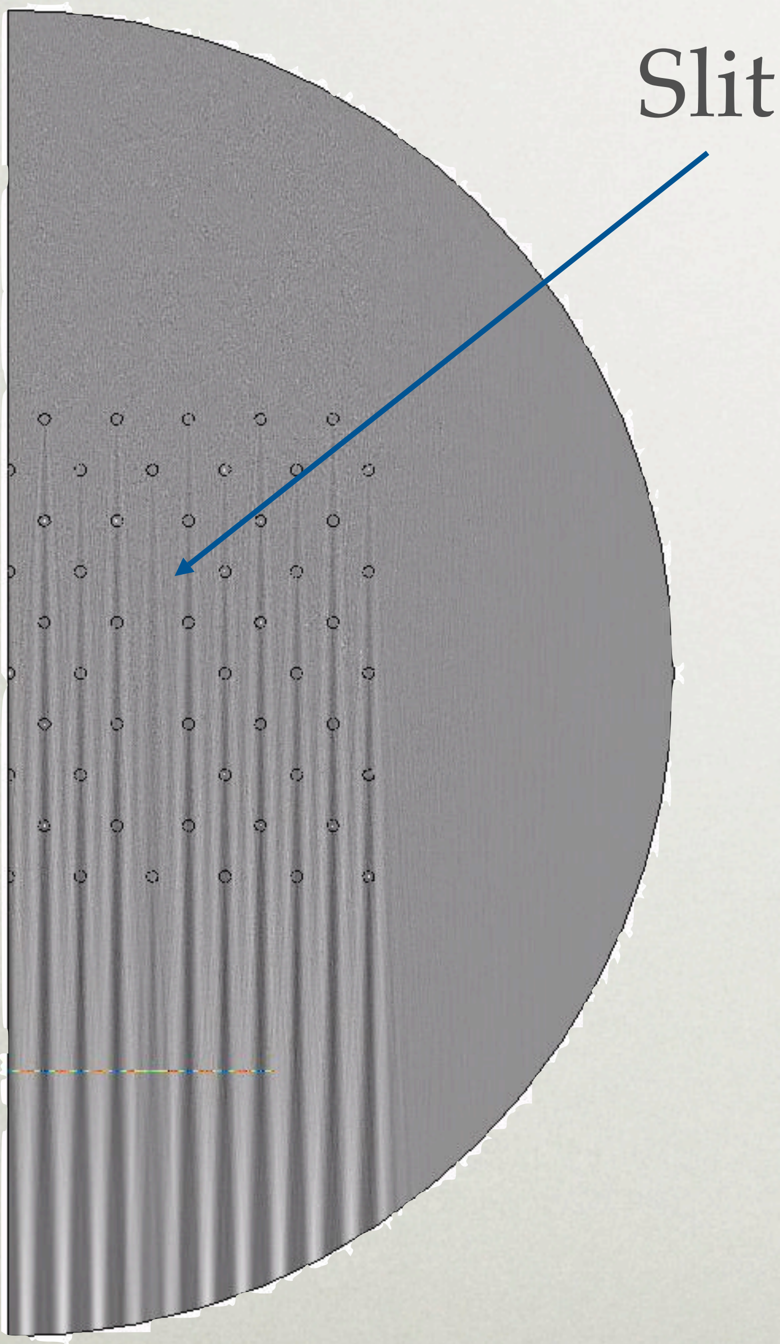
Example 1 on α-iron: sample with a lacuna



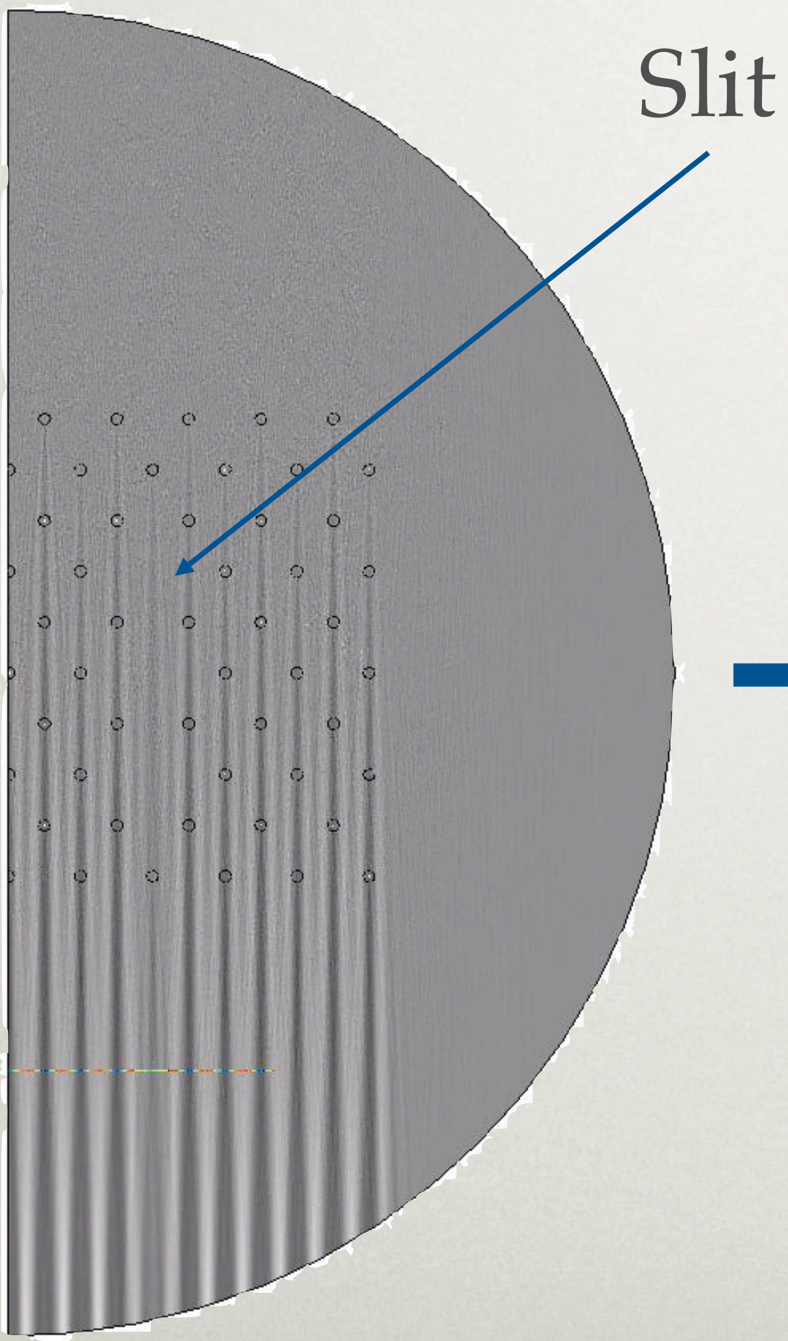
Initial mesh

Mesh after 5 iterations

Example 2 on α-iron: sample with a slit

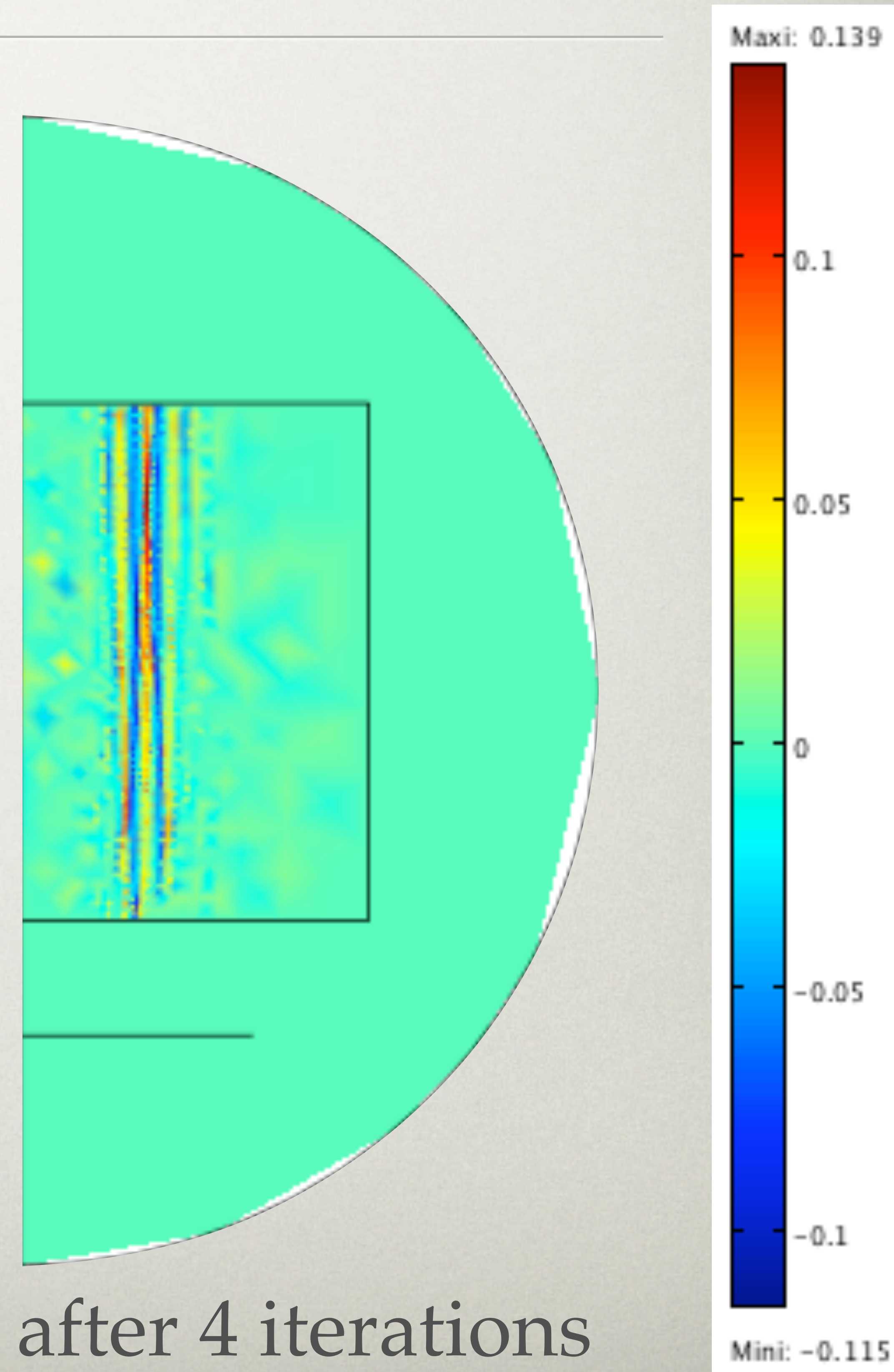


EXAMPLE 2 ON α-IRON: SAMPLE WITH A SLIT



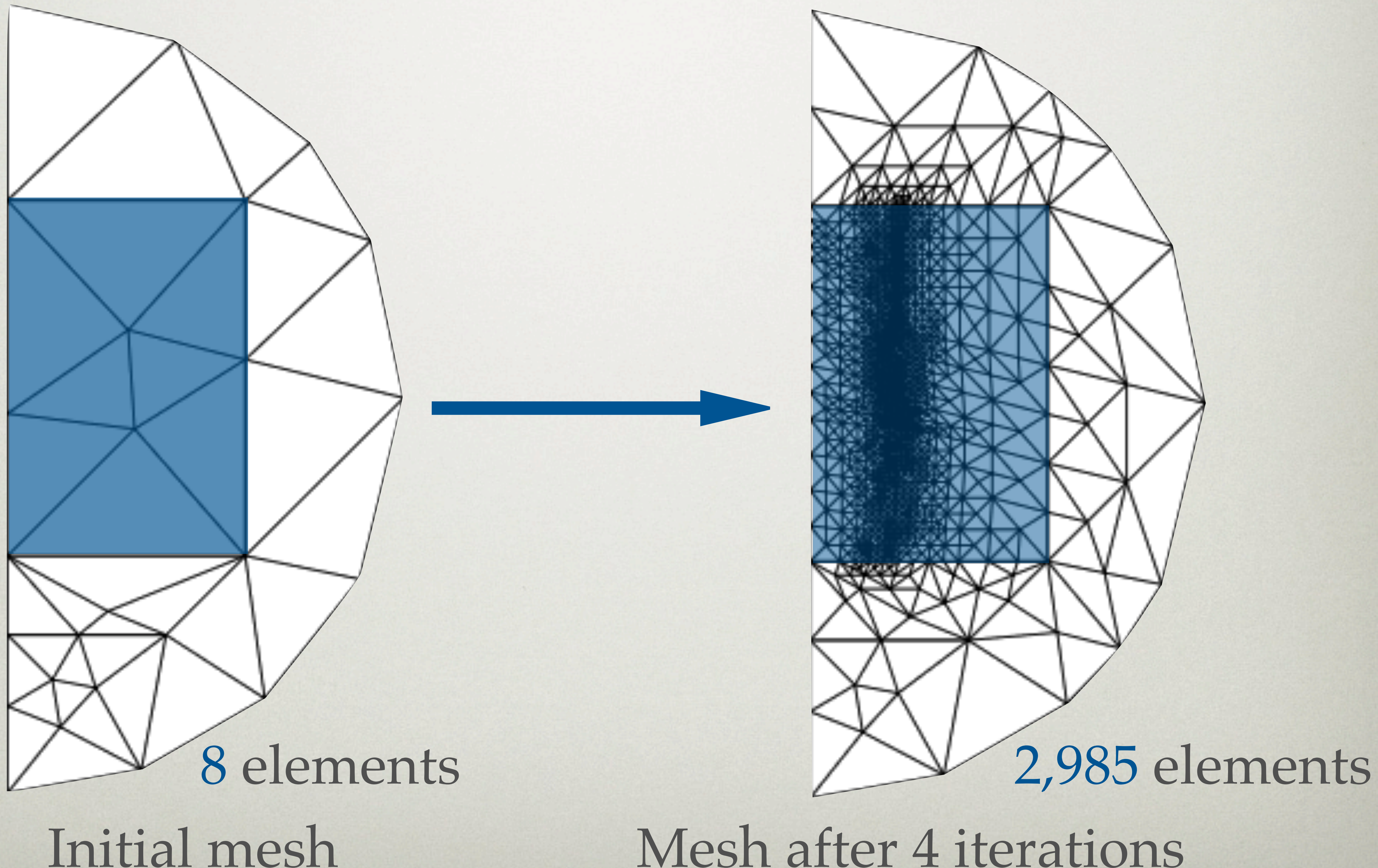
$V\text{-}V_0$

identified



Mesh after 4 iterations

Example 2 on α-iron: sample with a slit



Conclusion

- Summary :
  - iterative resolution of the inverse problem with adaptive regularization
  - first encouraging results
- Prospects :
  - effect of the sample size
  - use of alternative regularization terms

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CENTRALE
P A R I S

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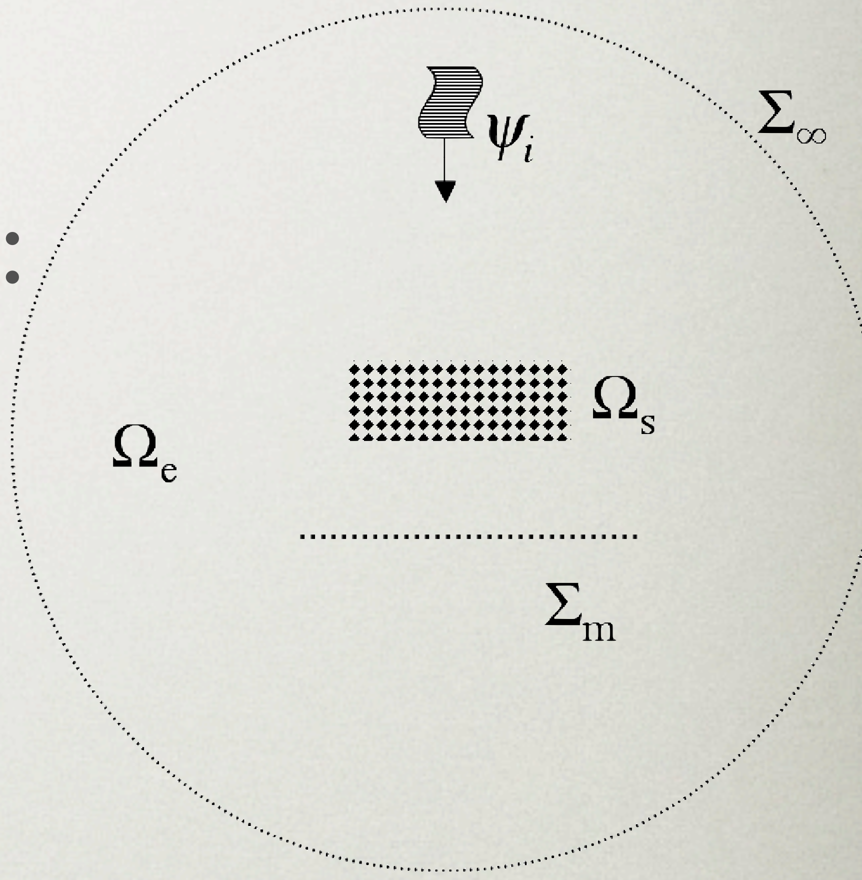
TEM forward scattering

- Schrödinger equation
  for incident electron and sample:
  - Ω_e with boundary Σ_∞
  - Sample Ω_s
  - Virtual plane Σ_m



$$
\begin{aligned}
-\frac{1}{2}(\Delta_{\mathbf{x}} + \Delta_{\mathbf{x}_s})\psi_{es}(\mathbf{x}, \mathbf{x}_s) & \\
+(V_{es}(\mathbf{x}, \mathbf{x}_s) + V_s(\mathbf{x}_s))\psi_{es}(\mathbf{x}, \mathbf{x}_s) &= E\psi_{es}(\mathbf{x}, \mathbf{x}_s)
\end{aligned}
$$

TEM forward scattering

- Further assumptions:
  - Product of wave functions $\psi_{es} = \psi_e \psi_s$

$$-\frac{1}{2}\Delta_{\mathbf{x}}\psi_{(e)}(\mathbf{x}) + V(\mathbf{x})\psi_{(e)}(\mathbf{x}) = (E - E_s)\psi_{(e)}(\mathbf{x})$$

  - Approximation (elastic scattering)

$$-\frac{1}{2}\Delta\psi + V\psi = E_i\psi$$

  - Decomposition (incident/diffracted waves)

$$-\frac{1}{2}\Delta\psi_i = E_i\psi_i \qquad \psi = \psi_i + \psi_d$$

$$\frac{1}{2}\Delta\psi_d + E_i\psi_d = V\psi_i$$

FE computational cost

- Helmholtz type equation

$$\frac{1}{2}\Delta\psi_d + E_i\psi_d = V\psi_i$$

- Far field radiation boundary condition

$$\frac{\partial \psi_d}{\partial \mathbf{n}} = \mathrm{i}||\mathbf{k}_i||\psi_d \ \text{ on } \Sigma_\infty$$

- Estimation of required DOFs
  - 10 elements/wavelength->10^9 DOFs

Paraxial approximation

- Paraxial approx: $\psi_d(\mathbf{x}) = \tilde{\psi}_d(\mathbf{x}) \exp(\mathrm{i}\mathbf{k}_i \cdot \mathbf{x})$

$$\frac{1}{2}\Delta\psi_d + E_i\psi_d = V\psi_i$$

- Helmholtz equation:

$$\frac{1}{2}\Delta\tilde{\psi}_d + \mathrm{i}\mathbf{k}_i \cdot \nabla\tilde{\psi}_d = V\tilde{\psi}_i \text{ in } \Omega_e$$

$$\frac{\partial\psi_d}{\partial\mathbf{n}} = \mathrm{i}||\mathbf{k}_i||\psi_d$$

- Far field boundary condition:

$$\frac{\partial\tilde{\psi}_d}{\partial\mathbf{n}} = \mathrm{i}(||\mathbf{k}_i|| - \mathbf{k}_i \cdot \mathbf{n})\tilde{\psi}_d \text{ on } \Sigma_\infty$$