Simulation of X-ray in-line phase contrast


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Background

• **Aim:** Monte Carlo simulation of X-ray in-line phase contrast
  – Infrastructure for grid computing exist (VIP, Gatelab, …)
  – Focus is for the moment on the physics problems
  – Master thesis Zhenjie Cen
  – PhD Loriane Weber

• **Outline**
  – What is X-ray phase contrast?
  – My focus: Image reconstruction – phase tomography
  – Application – bone imaging
  – Problems – motivation for simulation
  – Developments – Deterministic -> Probabilistic
  – Future work
X-ray phase contrast imaging

- **Acquisition:** Propagation-based imaging, using several distances [2, 3]

- High degree of coherence
- Parallel-beam set-up
- Micrometric resolution

Phase contrast increases with the propagation distance

X-ray phase contrast imaging

- Refractive index
  \[ n(x, y, z) = 1 - \delta_n(x, y, z) + i\beta(x, y, z) \]
  - \( \delta_n \) related to the phase shift
  - \( \beta \) related to the absorption

- For hard X-rays, \( \delta_n/\beta > 10^3 \) [2]

\[ \rightarrow \] PCI offers higher sensitivity than attenuation-based imaging.

Phase Retrieval

- Quantitative, non-linear relationship between phase shift and contrast

\[ I_D(x) = \left| \text{Fr}_{D,\lambda}[T_{A,\phi}(x)] \right|^2 \]

- Phase retrieval: inverse problem of calculating phase shift from phase contrast images at different distances

\[ \phi(x) = \arg \min_{\phi} \left\| \text{Fr}_{D,\lambda}[T_{A,\phi}(x)]^2 - I_D(x) \right\|^2 \]
Phase Tomography

• Phase shift is projection through refractive index
• Refractive index can be reconstructed by tomography
• Phase tomography usually divided into a two-step process
  • Phase retrieval (2D)
  • Repeated for each projection angle, tomography (3D)
• Refractive index proportional to electron density
  • I.e. mass density for most materials
X-ray phase contrast imaging

- Synchrotron Radiation [1]:
  - Intense
  - Stable
  - Coherent

- Coherence
  - Spatial → point-likeness of the source
  - Temporal → monochromaticity

ID19: micro-CT
ID16A: nano-CT
**X-ray Phase Nano-Tomography**

- **Zoom** non-destructively into a region of interest of a tissue, cell, ...
- Ideal for **multi-scale approaches**
- Magnified phase contrast imaging
  - **Quantitative** reconstruction of the **electron density**
  - Very **high sensitivity**
  - High resolution (X-ray wavelength limited)

R Mokso, P Cloetens, E Maire, W Ludwig, JY Buffière, APL, 2007, 90, 144104
Nano-Imaging end-station ID16B

Resolution >40 nm
Nano-imaging end-station ID16A

- Imaging in vacuum @ 17 & 33 keV
- Cryo-cooling capability
- Target resolution <20 nm
Projection Microscopy

Magnified in-line holograms of Au Xradia test pattern
$E = 17.3$ keV
Magnified in-line holograms of Au Xradia test pattern
$E = 17.3 \text{ keV}$
Projection Microscopy

**Magnified in-line holograms**

of Au Xradia test pattern

$E = 17.3 \text{ keV}$
Magnified in-line holograms of Au Xradia test pattern

$E = 17.3$ keV
X-radia gold test pattern
Innermost line width: 50 nm
Energy = 17.3 keV
Field of view: 80 µm
Pixel size: 53 nm

Au Fluorescence; 25 nm

Phase map

9 µm

10 µm

rad

-0.50

0.15
Phase nanotomography of bone

3D reconstruction
3D volume rendering
Analysis of the Lacuno-Canalicular network

- Can easily be segmented
- 10-20 cells/volume
Phase nano-CT: application on bone

- Example on human femoral bone data

Healthy

Osteoporotic

Osteoarthritic
Motivation: Low frequency noise
X-ray phase contrast imaging: image formation

• Fresnel model:

\[ I_D(x) = |P_D(x) * u_0(x)|^2 \]

• First order terms [8]:

Linearized with respect to the object

\[ \tilde{I}_D(f) = \delta_{Dirac}(f) - 2 \cos(\pi \lambda D |f|^2) \tilde{B}(f) + 2\sin(\pi \lambda D |f|^2) \tilde{\phi}(f) \]

- slowly-varying phase
- weak attenuation

• Problem:

→ Combine several distances ('holotomography') [8, 9]

Motivation: Low frequency noise

• **Problem:** transfer function goes to 0 in the low frequencies

• **Motivation**
  - Simulation of artefacts e.g. LF noise
  - Test new reconstruction algorithms
  - Reduce need for synchrotron beam time
  - Optimize the experimental acquisition parameters

• **Previously:** Deterministic simulation
  - Wave-object interaction
  - Propagation
Simulation: Wave-object interaction

- Object described by 3D complex refractive index
  \[ n(x,y,z) = 1 - \delta_n(x,y,z) + i\beta(x,y,z), \]

- Wave-object interaction described by a transmittance function:
  \[ u_0(x) = T(x)u_{inc}(x) \]

- Induces amplitude (absorption) and phase modulation:
  \[ T(x) = A(x)\exp[i\phi(x)] = \exp[-B(x)]\exp[i\phi(x)]. \]

- Both amplitude and phase modulation are projections through \( n(x) \)
  \[ B(x) = \left(\frac{2\pi}{\lambda}\right)\int_0^L \beta(x,y,z)\,dz \quad \phi(x) = -\left(\frac{2\pi}{\lambda}\right)\int_0^L \delta_n(x,y,z)\,dz \]
Simulation: Propagation

- Propagation over finite $D$ is described by Fresnel diffraction.
- Propagation is a linear system w.r.t. the wave.
- Convolution of wave with propagator:
  \[ u_D(x) = P_D(x) \ast u_0(x) \quad P_D(x) = \frac{1}{i\lambda D} \exp\left(i \frac{\pi}{\lambda D} |x|^2 \right) \]
- Fourier domain: Multiplication with propagator:
  \[ \tilde{P}_D(f) = \exp(-i\pi\lambda D |f|^2) \]
- Non-linear w.r.t intensity: squared modulus of wave:
  \[ I_D(x) = |u_D(x)|^2. \]
- Quantitative relationship phase -> contrast
In-line phase contrast simulation tool on VIP

- Implementation on the Virtual Imaging Platform (VIP, Creatis, Villeurbanne), an imaging simulation platform [27]
  - MRI
  - PET
  - X-rays
  - Ultrasounds

In-line phase contrast simulation tool on VIP

Propagation models:
- CTF
- Fresnel

STEP 1: Numerical phantoms
- Existing phantoms
- Voxellised objects

STEP 2: Projections
- Analytical
- Radon transform

STEP 3: Noisy propagated images at $D_k$
Deterministic simulation: results

- LF noise not recreated

- Hypothesis: due to scattered radiation
  - Can be simulated using Monte Carlo
  - But...

- Diffraction is a wave phenomenon, scattering is a particle phenomenon
Ray optical approach

- Not straight-forward to combine diffraction and scattering

- What can we implement using standard Monte Carlo?
  - MSc Zhenjie Cen

- Refraction
- Reflection

- Implemented in Geant4

Deterministic process on each ray
Ray optics: example

Figure 3.7: The phantom is an aluminium wire (blue) which has a radius of 15.208 μm. The refractive index decrement of aluminium at 19 keV is $\delta = 2.0 \times 10^{-6}$. To capture the image, we use a flat panel detector (yellow) with a pixel size of 1 μm. For the sake of simplicity, only one photon’s movement is showed (green).
Wave optical approach

- Implemented in GATE (for comparison)
- Uses ITK for computations

**Figure 3.2:** A schematic of the Fresnel diffraction actor algorithm.
Comparison ray/wave optical approaches

Figure 3.8: Comparison of the profiles of the stochastic model and the analytical model. The green curve is obtained using the Monte Carlo refraction model. The blue curve is obtained using the analytical Fresnel diffraction model.
Perspectives: refraction on voxellised phantoms

- Refraction currently limited to analytical phantoms
- Extension to voxellised phantoms
  - Calculation of refractive index gradients

Figure 4.4: Schematic of the local envelope solution.
Perspectives: combine wave and particle effects

\[ W(x, p) = u_0(x + y/2)u_0^*(x - y/2)e^{-ip\cdot y}dy \]

- Phase as optical path length of each ray
  - Propagate with Fresnel propagator

- Sample Wigner distribution as initialisation of MC simulation
  - Phase and absorption as line integrals
  - Sample \( W \) for initial position \( x \) and momentum \( p \) of photons
  - Scattering and propagation in MC
Conclusions

• Simulation of X-ray phase contrast imaging

• Wave-optical approach implemented in VIP and GATE

• Ray-optical refraction approach implemented in GEANT4

• Available through VIP and GATELab

• Uses EGI

• Perspectives: Unify wave and ray optical approaches
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