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Diffraction Tomography, Fourier Reconstruction, and Full Waveform Inversion

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Abstract

In this paper, we study the mathematical imaging problem of diffraction tomography (DT), which is an inverse scattering technique used to find material properties of an object by illuminating it with probing waves and recording the scattered waves. Conventional DT relies on the Fourier diffraction theorem, which is applicable under the condition of weak scattering. However, if the object has high contrasts or is too large compared to the wavelength, it tends to produce multiple scattering, which complicates the reconstruction. We give a survey on diffraction tomography and compare the reconstruction of low and high contrast objects. We also implement and compare the reconstruction using the full waveform inversion method which, contrary to the Born and Rytov approximations, works with the total field and is more robust to multiple scattering.

1. INTRODUCTION

Diffraction tomography (DT) is a technique for reconstructing the scattering potential of an object from measurements of waves scattered by that object. DT can be understood as an alternative to, or extension of, classical computerized tomography. In computerized tomography a crucial assumption is that the radiation, X-rays for instance, essentially propagates along straight lines through the object. The attenuated rays are recorded and can be related to material properties f of the object by means of the Radon, or X-ray, transform. A central result for the inversion of this relation is the Fourier slice theorem. Roughly speaking, it says that the Fourier transformed

measurements are equal to the Fourier transform of f evaluated along slices through the origin, [47].

The straight ray assumption of computerized tomography can be considered valid as long as the wavelength of the incident field is much smaller than the size of the relevant details in the object. As soon as the wavelength is similar to or greater than those details, for instance in situations where X-rays are replaced by visible light, diffraction effects are no longer negligible. As an example of a medical application, an optical diffraction experiment in [57] utilized a red laser of wavelength 633 nm to illuminate human cells of diameter around 10 μm , which include smaller subcellular organelles. One way to achieve better reconstruction quality in such cases is to drop the straight ray assumption and adopt a propagation model based on the wave equation instead.

The theoretical groundwork for DT was laid more than half a century ago [63]. The central result derived there, sometimes called the *Fourier diffraction theorem*, says that the Fourier transformed measurements of the scattered wave are equal to the Fourier transform of the scattering potential evaluated along a hemisphere. This result relies on a series of assumptions: (i) the object is immersed in a homogeneous background, (ii) the incident field is a monochromatic plane wave, (iii) the scattered wave is measured on a plane in \mathbb{R}^3 , and (iv) the first Born approximation of the scattered field is valid.

On the one hand the Born approximation greatly simplifies the relationship between scattered wave and scattering potential. On the other hand, however, it generally requires the object to be weakly scattering, thus limiting the applicability of the Fourier diffraction theorem. An alternative is to assume validity of the first Rytov approximation instead [31]. While mathematically this amounts to essentially the same reconstruction problem, the underlying physical assumptions are not identical to those of the Born approximation, leading to a different range of applicability in general [7, 56]. Nevertheless, the restriction to weakly scattering objects remains.

Full waveform inversion (FWI) is a different approach that can overcome some of the limitations of the first-order methods, typically at the cost of being computationally more demanding. It relies on the iterative minimization of a cost functional which penalizes the misfit between measurements and forward simulations of the total field, cf. [2, 40, 53, 58, 61]. Here, the forward model consists of the solution of the full wave equation, without simplification of first-order approximations. It results in a nonlinear minimization problem to be solved, typically with Newton-type methods [61, 49].

In practical experiments, there are sometimes only measurements of the intensity, i.e., the absolute value of the complex-valued wave, available. Different phase retrieval methods were investigated, e.g., in [42, 23, 29, 5]. For this paper, we assume that both the phase and amplitude information is present, which can be achieved by interferometry, cf. [62].

Contribution and outline. In this paper, we present a numerical comparison of three reconstruction approaches for diffraction tomography on simulated data, based on (i) the Born approximation, (ii) the Rytov approximation, and (iii) FWI. The setting we use for this comparison is 2D transmission imaging in a homogeneous background with (approximate) plane wave irradiation. The object is assumed to make a full turn during the experiment, providing measurements for a uniform set of incidence angles. In addition we investigate how providing additional data by varying the wavelength affects the reconstruction. The scattering potentials considered here are test phantoms of varying sizes, shapes, and contrasts. Moreover, for data generation purposes we compare several forward models.

For numerical reconstruction under the Born and Rytov approximations a well-known method is the backpropagation algorithm [11], which is widely used in practice, cf. [46] and also [14]. Our algorithms rely on the nonuniform discrete Fourier transform (NDFT), which was used in 3D Fourier diffraction tomography yielding better results than discrete backpropagation [37]. Our FWI-based reconstruction uses an iterative Newton-type method on an L^2 distance between data and simulations. Here, the discretization of the partial differential equations associated with the wave propagation uses the hybridizable discontinuous Galerkin method (HDG), [9, 20]. It is implemented, together with the inverse procedure, in the open-source parallel software **hawen**¹, [16].

The outline of this paper is as follows. The conceptual experiment is detailed in Section 2. Forward models are presented in Section 3, and their numerical performance is compared in Section 4. The Fourier diffraction theorem is formulated and discussed in Section 5. Further, Section 6 covers the reconstruction algorithms used for the numerical experiments, which are presented in Section 7. A concluding discussion of our findings is given in Section 8.

2. EXPERIMENTAL SETUP

We consider the tomographic reconstruction of a two-dimensional object taking into account diffraction of the incident field. The object is assumed to be embedded in a homogeneous background and illuminated or insonified by a monochromatic plane wave. In fact, for the computational experiments, we implement and compare several approaches to approximate the incident plane wave, see Section 3 and Section 4. We restrict ourselves to transmission imaging, where the incident field propagates in direction $\mathbf{e}_2 = (0, 1)^\top$ and the resulting field is measured on the line $x_2 = r_M$. The distance between the measurement line and the origin, $r_M > 0$, is sufficiently large so that it does not intersect the object. From the measurements, we aim to reconstruct the object's scattering properties. In order to improve the reconstruction quality, we generate additional data by rotating the object or changing the incident field's wavelength. See Figure 1 for an illustration of the experimental setup.

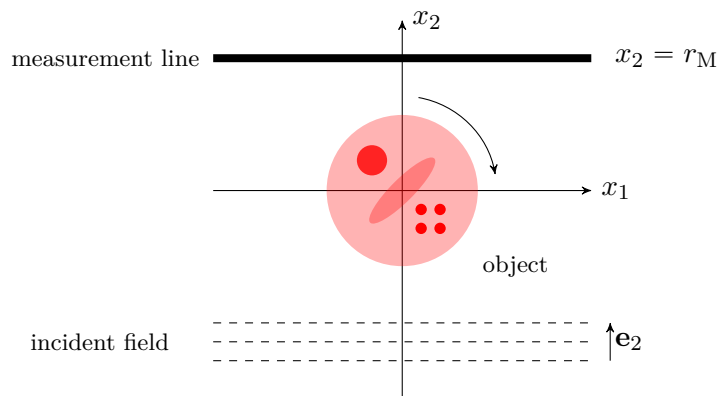


FIGURE 1. *Experimental setup.*

We now introduce the physical quantities needed subsequently. Let $\lambda > 0$ denote the *wavelength* of the incident wave and $k_0 = 2\pi/\lambda$ the background *wave number*. Furthermore, let $n(\mathbf{x})$ denote

¹<https://ffaucher.gitlab.io/hawen-website/>

the *refractive index* at position $\mathbf{x} \in \mathbb{R}^2$ and n_0 the constant refractive index of the background. From these quantities, we define the wave number

$$k(\mathbf{x}) := k_0 \frac{n(\mathbf{x})}{n_0}.$$

Furthermore, the wave number k can be equivalently expressed in terms of the angular frequency ω and the wave speed c such that

$$k(\mathbf{x}) = \frac{\omega}{c(\mathbf{x})} \quad \text{and} \quad k_0 = \frac{\omega}{c_0}, \quad (2.1)$$

where c_0 is the constant wave speed in the background. The *scattering potential* f is obtained by subtracting the background wave number k_0 :

$$f(\mathbf{x}) := k^2(\mathbf{x}) - k_0^2 = k_0^2 \left(\frac{n(\mathbf{x})^2}{n_0^2} - 1 \right). \quad (2.2)$$

Note that, for all practical purposes, f can be assumed to be bounded and compactly supported in the disk $\mathcal{B}_{r_M} = \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| < r_M\}$.

In our subsequent reconstructions with Born and Rytov approximations, f is the quantity to be reconstructed from the measured data and k_0 is known. On the other hand, with FWI, we reconstruct c , see [Remark 6.1](#). These two quantities can be related to each other via

$$c(\mathbf{x}) = \sqrt{\frac{\omega^2}{k_0^2 + f(\mathbf{x})}}. \quad (2.3)$$

3. FORWARD MODELS

In this section, we propose several forward models for the experiment presented above. For all of them, the starting point is the system of equations

$$\left. \begin{aligned} (-\Delta - k(\mathbf{x})^2) u^{\text{tot}}(\mathbf{x}) &= g(\mathbf{x}), \\ (-\Delta - k_0^2) u^{\text{inc}}(\mathbf{x}) &= g(\mathbf{x}), \\ u^{\text{tot}}(\mathbf{x}) &= u^{\text{inc}}(\mathbf{x}) + u^{\text{sca}}(\mathbf{x}), \end{aligned} \right\} \mathbf{x} \in \mathbb{R}^2. \quad (3.1)$$

Here, u^{inc} is the given *incident field*, the *total field* u^{tot} is what is recorded on the measurement line $\{\mathbf{x} \in \mathbb{R}^2 : x_2 = r_M\}$, and the difference between the two constitutes the *scattered field* u^{sca} . We describe different sources g in the following subsections. The scattered field u^{sca} is assumed to satisfy the Sommerfeld radiation condition which requires that

$$\lim_{\|\mathbf{x}\| \rightarrow \infty} \sqrt{\|\mathbf{x}\|} \left(\frac{\partial u^{\text{sca}}}{\partial \|\mathbf{x}\|} - ik_0 u^{\text{sca}} \right) = 0$$

uniformly for all directions $\mathbf{x}/\|\mathbf{x}\|$. It guarantees that u^{sca} is an outgoing wave. Further details concerning derivation and analytical properties of problems like [Equation 3.1](#) can be found, for instance, in [\[10\]](#).

The models considered below are based on the following specifications of [Equation 3.1](#). Their numbers agree with the corresponding subsection numbers, where the models will be explained in more detail.

1. Plane wave No source ($g = 0$) and u^{inc} is an ideal plane wave, see [Equation 3.2](#).

1.1 Born model No source, u^{inc} is an ideal plane wave and u^{sca} satisfies the Born approximation.

1.2 Rytov model No source, u^{inc} is an ideal plane wave and u^{sca} satisfies the Rytov approximation.

In addition we propose the following two models with sources.

2.1 Point source g represents a point source located far from the object.

2.2 Line source g represents simultaneous point sources positioned along a straight line. We refer to this configuration as a ‘line source’.

[Section 4](#) contains a numerical comparison of these forward models.

The proposed selection of equations is motivated in part by the availability of methods for their numerical inversion. While the Born and Rytov models can be inverted using nonuniform Fourier methods, the point and line source models are well-suited for FWI.

3.1. Incident plane wave. *Monochromatic plane waves* are basic solutions u of the homogeneous Helmholtz equation

$$(-\Delta - k_0^2)u = 0.$$

They take the form $u(\mathbf{x}) = e^{ik_0\mathbf{x}\cdot\mathbf{s}}$, where the unit vector \mathbf{s} specifies the direction of propagation of u . Plane waves are widely studied in imaging applications and theory and we refer to [\[10, 12, 32\]](#) for further information.

In the first model we consider the incident field is a monochromatic plane wave propagating in direction \mathbf{e}_2

$$u^{\text{inc}}(\mathbf{x}) = e^{ik_0x_2}. \quad (3.2)$$

In this case, we obtain from [Equation 3.1](#) the following equation for the scattered field

$$(-\Delta - k(\mathbf{x})^2)u^{\text{sca}}(\mathbf{x}) = f(\mathbf{x})e^{ik_0x_2}. \quad (3.3)$$

3.1.1. The Born approximation. [Equation 3.3](#) can be written as

$$(-\Delta - k_0^2)u^{\text{sca}}(\mathbf{x}) = f(\mathbf{x})\left(e^{ik_0x_2} + u^{\text{sca}}(\mathbf{x})\right).$$

If the scattered field u^{sca} is negligible compared to the incident field $e^{ik_0x_2}$, we can ignore u^{sca} on the right-hand side and obtain

$$(-\Delta - k_0^2)u^{\text{Born}}(\mathbf{x}) = f(\mathbf{x})e^{ik_0x_2}, \quad (3.4)$$

where u^{Born} is the (*first-order*) *Born approximation* to the scattered field. Supplementing this equation with the Sommerfeld radiation condition we have a unique solution corresponding to an outgoing wave [\[10\]](#). It can be written as a convolution

$$u^{\text{Born}}(\mathbf{x}) = \int_{\mathbb{R}^2} G(\mathbf{x} - \mathbf{y})f(\mathbf{y})e^{ik_0y_2}d\mathbf{y}, \quad (3.5)$$

where G is the outgoing Green's function for the Helmholtz equation. In \mathbb{R}^2 , it is given by

$$G(\mathbf{x}) = \frac{i}{4} H_0^{(1)}(k_0 \|\mathbf{x}\|), \quad \mathbf{x} \in \mathbb{R}^2 \setminus \{\mathbf{0}\}, \quad (3.6)$$

where $H_0^{(1)}$ denotes the zeroth order Hankel function of the first kind, see [10, Sect. 3.4]. We note that, in spite of a singularity at the origin, G is locally integrable in \mathbb{R}^2 .

The second-order Born approximation can be obtained by replacing the plane wave $e^{ik_0 y_2}$ in Equation 3.5 by the sum $e^{ik_0 y_2} + u^{\text{Born}}(\mathbf{y})$. Iterating this procedure yields Born approximations of arbitrary order. For more details we refer to [32, Sect. 6.2.1] and [12].

3.1.2. The Rytov approximation. In this subsection, we derive an alternative approximation for the scattered field. Introducing the complex phases φ^{inc} , φ^{tot} and φ^{sca} according to

$$u^{\text{tot}} = e^{\varphi^{\text{tot}}}, \quad u^{\text{inc}} = e^{\varphi^{\text{inc}}}, \quad \varphi^{\text{tot}} = \varphi^{\text{inc}} + \varphi^{\text{sca}}, \quad (3.7)$$

one can derive from Equation 3.1, with $g = 0$, the following relation

$$(-\Delta - k_0^2)(u^{\text{inc}} \varphi^{\text{sca}}) = \left(f + (\nabla \varphi^{\text{sca}})^2 \right) u^{\text{inc}}, \quad (3.8)$$

where $(\nabla \varphi^{\text{sca}})^2 = (\partial \varphi^{\text{sca}} / \partial x_1)^2 + (\partial \varphi^{\text{sca}} / \partial x_2)^2$. The details of this derivation can be found, for instance, in [32, Sect. 6.2.2]. Neglecting $(\nabla \varphi^{\text{sca}})^2$ in Equation 3.8 we obtain

$$(-\Delta - k_0^2)(u^{\text{inc}} \varphi^{\text{Rytov}}) = f u^{\text{inc}}, \quad (3.9)$$

where φ^{Rytov} is the *Rytov approximation* to φ^{sca} . Note that we still assume u^{inc} to be a monochromatic plane wave, as given in Equation 3.2. Thus the product $u^{\text{inc}} \varphi^{\text{Rytov}}$ solves the same equation as u^{Born} . If we define the Rytov approximation to the scattered field, u^{Rytov} , in analogy to Equation 3.7 via

$$u^{\text{Rytov}} = e^{\varphi^{\text{Rytov}} + \varphi^{\text{inc}}} - u^{\text{inc}},$$

and replace φ^{Rytov} by $\frac{u^{\text{Born}}}{u^{\text{inc}}}$, we obtain a relation between the two approximate scattered fields that can be expressed as

$$u^{\text{Born}} = u^{\text{inc}} \log \left(\frac{u^{\text{Rytov}}}{u^{\text{inc}}} + 1 \right). \quad (3.10)$$

The relation between Born and Rytov in Equation 3.10 is not unique because of the multiple branches of the complex logarithm. In practical computations, this is addressed by a phase unwrapping as we will see in Equation 6.8.

Remark 3.1 There have been many investigations about the validity of the Born and Rytov approximations, see, e.g., [7, 56] or [32, chap. 6]. The Born approximation is reasonable only for a relatively (to the wavelength) small object. In particular, for a homogeneous cylinder of radius a , the Born approximation is valid if $a(n - n_0) < \lambda/4$, where λ is the wavelength of the incident wave and n is the constant refractive index inside the object. In contrast, the Rytov approximation only requires that $n - n_0 > (\nabla \varphi^{\text{sca}})^2 / k_0^2$, i.e., the phase change of the scattered phase φ^{sca} , see Equation 3.7, is small over one wavelength, but it has no direct requirements on the object size and is therefore applicable for a larger class of objects. The latter is also observed in numerical simulations in [7]. However, for objects that are small and have a low contrast $n - n_0$, the Born and Rytov approximation produce approximately the same results.

3.2. Modeling the total field using line and point sources. As an alternative to ideal incident plane waves we consider models with one or several point sources. If arranged the right way, the resulting incident field can resemble a monochromatic plane wave. We refer to [Section 4](#) for a numerical comparison of the different models presented here.

3.2.1. Point source far from object. In this case the right-hand side in [Equation 3.1](#) is a Dirac delta function so that we obtain

$$\begin{cases} (-\Delta - k(\mathbf{x})^2) u_{\text{P}}^{\text{tot}}(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0), \\ (-\Delta - k_0^2) u_{\text{P}}^{\text{inc}}(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0). \end{cases} \quad (3.11)$$

If the position of the source is given by $\mathbf{x}_0 = -r_0 \mathbf{e}_2$ with $r_0 > 0$ sufficiently large, then, after appropriate rescaling, $u_{\text{P}}^{\text{inc}}$ approximates a plane wave with wave number k_0 and propagation direction \mathbf{e}_2 in a neighborhood of $\mathbf{0}$.

3.2.2. Line source. Alternatively, we let g be a sum of Dirac functions and consider

$$\begin{cases} (-\Delta - k(\mathbf{x})^2) u_{\text{L}}^{\text{tot}}(\mathbf{x}) = \sum_{j=1}^{N_{\text{sim}}} \delta(\mathbf{x} - \mathbf{x}_j), \\ (-\Delta - k_0^2) u_{\text{L}}^{\text{inc}}(\mathbf{x}) = \sum_{j=1}^{N_{\text{sim}}} \delta(\mathbf{x} - \mathbf{x}_j), \end{cases} \quad (3.12)$$

where the number N_{sim} of simultaneous point sources should be sufficiently large. Moreover, the positions \mathbf{x}_j should be arranged uniformly along a line perpendicular to the propagation direction \mathbf{e}_2 of the plane wave. This is illustrated in [Section 4.2](#).

4. NUMERICAL COMPARISON OF FORWARD MODELS

In this section, we numerically compare the forward models presented above. For the discretization of partial differential equations, several approaches exist, we mention for instance the finite differences that approximates the problem on a nodal grid (e.g., [\[60\]](#)), or methods that use the variational formulation, such as finite elements [\[44\]](#) or discontinuous Galerkin methods, [\[25\]](#). In our work, we use the *hybridizable discontinuous Galerkin method* (HDG) for the discretization and refer to [\[9, 36, 20\]](#) for more details. The implementation precisely follows the steps prescribed in [\[20\]](#), and it is carried out in the open-source parallel software **hawen**, see [\[16\]](#) and [footnote 1](#). While the propagation is assumed on infinite space, the numerical simulations are performed on a finite discretization domain $\Omega \subset \mathbb{R}^2$, with absorbing boundary conditions [\[13\]](#) implemented to simulate free-space. It corresponds to the following Robin-type condition applied on the boundary Γ of the discretization domain Ω :

$$-i k(\mathbf{x}) u(\mathbf{x}) + \partial_n u(\mathbf{x}) = 0, \quad \text{for } x \text{ on } \Gamma. \quad (4.1)$$

where $\partial_n u$ denotes the normal derivative of u . The test sample used below is a homogeneous medium encompassing a circular object of radius 4.5 around the origin with contrast $f = 1$. This corresponds to the characteristic function

$$\mathbf{1}_a^{\text{disk}}(\mathbf{x}) := \begin{cases} 1, & \mathbf{x} \in \mathcal{B}_a, \\ 0, & \mathbf{x} \in \mathbb{R}^2 \setminus \mathcal{B}_a, \end{cases} \quad (4.2)$$

of the disk \mathcal{B}_a with radius $a > 0$. The incident plane wave has wave number $k_0 = 2\pi$.

4.1. Modeling the scattered field assuming incident plane waves. We consider the solutions u^{sca} of Equation 3.3 and u^{Born} of Equation 3.4, both satisfying boundary condition Equation 4.1, and simulated following the HDG discretization indicated above. As an alternative for computing the Born approximation u^{Born} , we discretize the convolution Equation 3.5 with the Green's function G given in Equation 3.6. In particular, applying an $N \times N$ quadrature on the uniform grid $\mathcal{R}_N = \{-r_M, -r_M + 2r_M/N, \dots, r_M - 2r_M/N\}^2$ to Equation 3.5, we obtain

$$u^{\text{Born}}(\mathbf{x}) \approx u_{\text{conv},N}^{\text{Born}}(\mathbf{x}) := \left(\frac{2r_M}{N}\right)^2 \sum_{\mathbf{y} \in \mathcal{R}_N} G(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) e^{ik_0 y_2}, \quad \mathbf{x} \in \mathbb{R}^2. \quad (4.3)$$

In Figure 2, we illustrate the solutions obtained with the different formulations. We observe that the transmission waves contain the most energy, that is, waves that “cross” the object. On the other hand, the solution has very low amplitude elsewhere, including the reflected waves. In Figure 2d, we see that the Born approximation leads to an incorrect amplitude of the solution, in particular the imaginary part. In addition, the imaginary part of $u_{\text{conv},200}^{\text{Born}}$ does not match the one of u^{Born} .

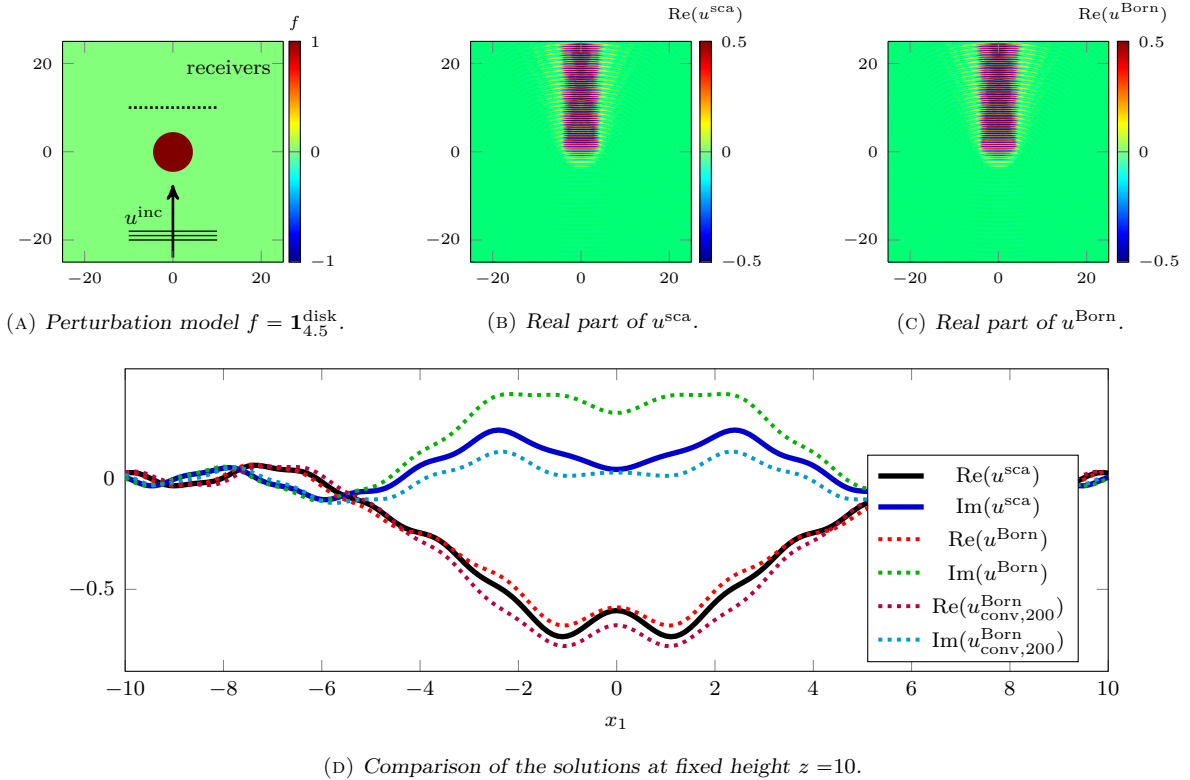


FIGURE 2. Comparison of the scattered wave u^{sca} and the Born approximation u^{Born} . The computations are performed on a domain $[-25, 25] \times [-25, 25]$ with boundary conditions given in Equation 4.1. Further, we display $u_{\text{conv},200}^{\text{Born}}$ which is the Born approximation obtained by the convolution Equation 4.3.

4.2. Modeling the total field using line and point sources. The objective is to evaluate how considering line and point sources differs from using incident plane waves, and if the data obtained with both approaches are comparable. To compare the scattered fields obtained from Equation 3.11 and Equation 3.12 with the solution u^{sca} of Equation 3.3, one needs to rescale

according to

$$\begin{aligned} u_{\text{P}}^{\text{sca}} &= \alpha_{\text{P}} (u_{\text{P}}^{\text{tot}} - u_{\text{P}}^{\text{inc}}), \\ u_{\text{L}}^{\text{sca}} &= \alpha_{\text{L}} (u_{\text{L}}^{\text{tot}} - u_{\text{L}}^{\text{inc}}), \end{aligned}$$

where α_{P} and α_{L} are constants depending only on the number and positions of the point sources \mathbf{x}_j . We illustrate in Figure 3, where the line source is positioned at fixed height $x_2 = -15$ and composed of 441 points between $x_1 = -22$ and $x_1 = 22$. For the case of a point source, we have to consider a very wide domain, namely $[-500, 500] \times [-500, 500]$, and the point source is positioned in $(x_1 = 0, x_2 = -480)$. In Figure 3g, we plot the corresponding solutions on a line at height $x_2 = 10$, i.e., for measurements of transmission waves.

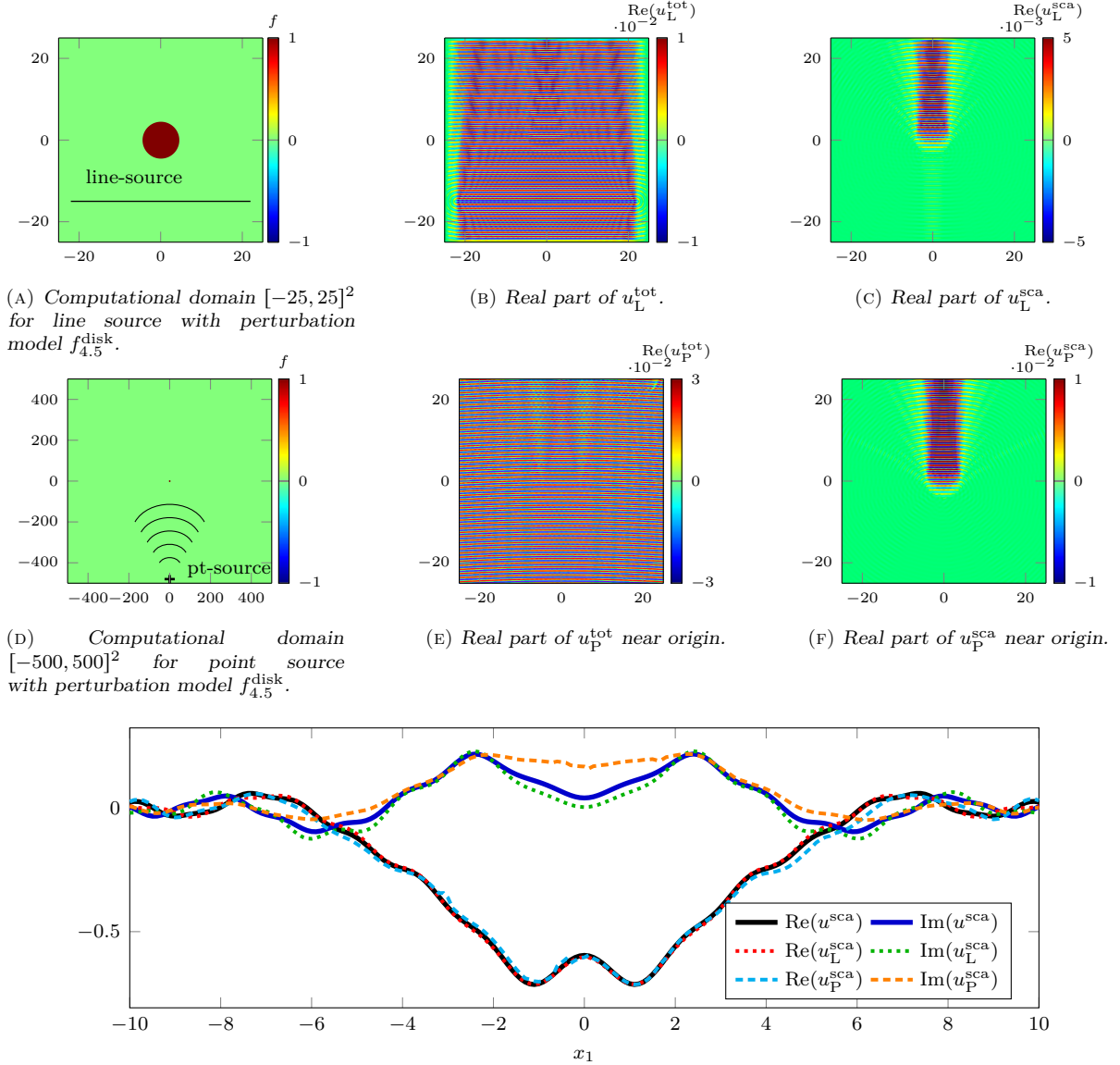


FIGURE 3. Total field $u_{\text{L}}^{\text{tot}}$ and scattered field $u_{\text{L}}^{\text{sca}}$ (line source) and total field $u_{\text{P}}^{\text{tot}}$ and scattered field $u_{\text{P}}^{\text{sca}}$ (point source). The line source is composed of $N_{\text{sim}} = 441$ points at fixed height $x_2 = -15$. The computational domain for the point source is very large such that the perturbation is barely visible and the source is positioned in $\mathbf{x}_0 = (0, -480)^\top$.

We see that the simulation using the line source is very close to the original solution u^{sca} , in fact, it is a more accurate representation than the Born approximation pictured in Figure 2. The

simulation using a point source positioned far away is also accurate, except for the middle area of the imaginary part. Furthermore, the major drawback of using a single point source is that it necessitates a very big domain, hence largely increasing the computational cost.

5. FOURIER DIFFRACTION THEOREM

In this section we discuss the inverse problem of recovering the scattering potential from measurements of the scattered wave under the Born or Rytov approximations. Before stating the fundamental result in this context, see [Theorem 5.1](#) below, we have to introduce further notation.

We denote by \mathcal{F} the two-dimensional Fourier transform and by \mathcal{F}_1 the partial Fourier transform with respect to the first coordinate,

$$\begin{aligned}\mathcal{F}\phi(\mathbf{k}) &= (2\pi)^{-1} \int_{\mathbb{R}^2} \phi(\mathbf{x}) e^{-i\mathbf{x}\cdot\mathbf{k}} d\mathbf{x}, & \mathbf{k} \in \mathbb{R}^2, \\ \mathcal{F}_1\phi(k_1, x_2) &= (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} \phi(\mathbf{x}) e^{-ik_1x_1} dx_1, & (k_1, x_2)^\top \in \mathbb{R}^2.\end{aligned}$$

For $k_1 \in [-k_0, k_0]$, we define

$$\kappa(k_1) := \sqrt{k_0^2 - k_1^2}.$$

We can now formulate the Fourier diffraction theorem, see for instance [\[32, Sect. 6.3\]](#), [\[48, Thm. 3.1\]](#) or [\[63\]](#).

Theorem 5.1 *Let f be bounded with $\text{supp } f \subset \mathcal{B}_{r_M}$. For $k_1 \in (-k_0, k_0)$, we have*

$$\mathcal{F}_1 u^{\text{Born}}(k_1, r_M) = \sqrt{2\pi} \frac{ie^{i\kappa r_M}}{2\kappa} \mathcal{F} f(k_1, \kappa - k_0). \quad (5.1)$$

According to the Fourier diffraction theorem, [Theorem 5.1](#), the measurements of the scattered wave u^{Born} can be related to the scattering potential f on a semicircle in k -space. Below we discuss how this so-called *k-space coverage* of the experiment is affected by (i) rotating the object and (ii) varying the wave number k_0 of the incident field u^{inc} .

5.1. Rotating the object. Suppose the object rotates around the origin during the experiment. Then the resulting orientation-dependent scattering potential can be written as

$$f^\alpha(\mathbf{x}) = f(R_\alpha \mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2,$$

where α ranges over a (continuous or discrete) set of angles $A \subset [0, 2\pi]$ and

$$R_\alpha = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix}$$

is a rotation matrix. If we let u^α be the Born approximation to the wave scattered by f^α , the collected measurements are given by

$$u^\alpha(x_1, r_M), \quad x_1 \in \mathbb{R}, \quad \alpha \in A.$$

Exploiting the rotation property of the Fourier transform, $\mathcal{F}(f \circ R_\alpha) = (\mathcal{F}f) \circ R_\alpha$, we obtain from Equation 5.1

$$\mathcal{F}_1 u^\alpha(k_1, r_M) = \sqrt{2\pi} \frac{ie^{i\kappa r_M}}{2\kappa} \mathcal{F}f(R_\alpha(k_1, \kappa - k_0)^\top).$$

Thus the k-space coverage, that is, the set of all spatial frequencies $\mathbf{y} \in \mathbb{R}^2$ at which $\mathcal{F}f$ is accessible via the Fourier diffraction theorem, is given by

$$\mathcal{Y} = \{\mathbf{y} = R_\alpha(k_1, \kappa - k_0)^\top \in \mathbb{R}^2 : |k_1| < k_0, \alpha \in A\}.$$

It consists of rotated versions (around the origin) of the semicircle $(k_1, \kappa - k_0)^\top$, $|k_1| < k_0$, see Figure 4.

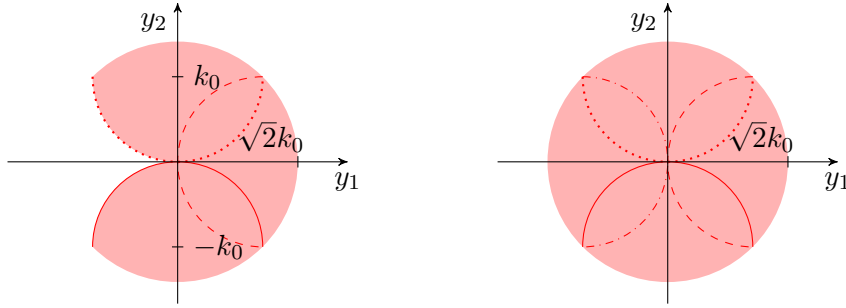


FIGURE 4. k -space coverage for a rotating object. Left: half turn, $A = [0, \pi]$. Right: full turn, $A = [0, 2\pi]$. The k -space coverage (light red) is a union of infinitely many semicircles, each corresponding to a different orientation of the object. Some of the semicircles are depicted in red: solid arc ($\alpha = 0$), dashed ($\alpha = \pi/2$), dotted ($\alpha = \pi$), dash-dotted ($\alpha = 3\pi/2$).

5.2. Varying wave number. Now suppose the object is illuminated or insonified by plane waves with wave numbers ranging over a set $K \subset (0, +\infty)$. Recall the definition of the scattering potential $f_{k_0} = k_0^2(n^2/n_0^2 - 1)$ from Equation 2.2, but note that we have now added a subscript to indicate the dependence of f on k_0 . If the variation of the object's refractive index n with $k_0 \in K$ is negligible, we can write

$$f_{k_0}(\mathbf{x}) = k_0^2 f_1(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2. \quad (5.2)$$

If no confusion arises, we may write $f = f_1$. Denoting by u_{k_0} the Born approximation to the wave scattered by f_{k_0} , the resulting collection of measurements is

$$u_{k_0}(x_1, r_M), \quad x_1 \in \mathbb{R}, \quad k_0 \in K.$$

Then, according to Equation 5.1, we have

$$\mathcal{F}_1 u_{k_0}(k_1, r_M) = \sqrt{2\pi} \frac{ie^{i\kappa r_M}}{2\kappa} k_0^2 \mathcal{F}f_1(k_1, \kappa - k_0).$$

Notice that now κ also varies with k_0 . The resulting k -space coverage

$$\mathcal{Y} = \left\{ \mathbf{y} = (k_1, \kappa - k_0)^\top \in \mathbb{R}^2 : k_0 \in K, |k_1| < k_0 \right\}$$

is a union of semicircles scaled and shifted (in direction of $-\mathbf{e}_2$) according to $k_0 \in K$.

Consider, for example, $K = [k_{\min}, k_{\max}]$. Then the k-space coverage consists of all points $(y_1, y_2)^\top \in \mathbb{R}^2$ such that $|y_1| \leq k_{\max}$ and

$$\sqrt{k_{\max}^2 - y_1^2} - k_{\max} \geq y_2 \geq \begin{cases} -|y_1|, & |y_1| \geq k_{\min}, \\ \sqrt{k_{\min}^2 - y_1^2} - k_{\min}, & \text{otherwise,} \end{cases}$$

see [Figure 5](#). Note that, in contrast to the scenarios of [Section 5.1](#), there are large missing parts near the origin.

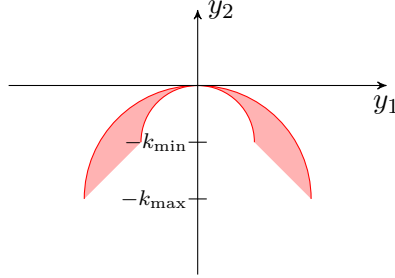


FIGURE 5. k -space coverage for k_0 covering the interval $[k_{\min}, k_{\max}]$.

5.3. Rotating the object with multiple wave numbers. We combine the two previous observations by picking a finite set of wave numbers $K \subset (0, \infty)$ and performing a full rotation of the object for each $k_0 \in K$. Let $u_{k_0}^\alpha$ be the Born approximation to the wave scattered by $f_{k_0}^\alpha = k_0^2 f_1 \circ R_\alpha$. Then the full set of measurements is given by

$$u_{k_0}^\alpha(x_1, r_M), \quad x_1 \in \mathbb{R}, \quad \alpha \in [0, 2\pi], \quad k_0 \in K, \quad (5.3)$$

and the Fourier diffraction theorem yields

$$\mathcal{F}_1 u_{k_0}^\alpha(k_1, r_M) = \sqrt{2\pi} \frac{ie^{i\kappa r_M}}{2\kappa} k_0^2 \mathcal{F} f_1 (R_\alpha(k_1, \kappa - k_0)^\top). \quad (5.4)$$

We deduce from [Section 5.1](#) and [Section 5.2](#) that the resulting k-space coverage \mathcal{Y} is the union of disks with radii $\sqrt{2}k_0$, all centered at the origin. Hence, \mathcal{Y} is just the largest disk, that is, the one corresponding to the largest wave number $\max K$. However, smaller disks in k-space are covered more often, which might improve reliability of the reconstruction for noisy data.

6. RECONSTRUCTION METHODS

In the following, we assume data generated by line-sources according to the setup described in [Section 4.2](#). We simulate the total fields solutions to [Equation 3.12](#), which are the synthetic data used for the reconstruction.

6.1. Reconstruction using Full Waveform Inversion. For the identification of the physical properties of the medium, the *Full Waveform Inversion* (FWI) relies on an iterative minimization of a misfit functional which evaluates a distance between numerical simulation and measurements of the total field. The Full Waveform Inversion method arises in the context of seismic inversion for sub-surface Earth imaging, cf. [\[2, 40, 58, 53, 61\]](#), where the measured seismograms are compared to simulated waves.

With FWI, we invert with respect to the wave speed c , from which the wave number is defined according to [Equation 2.1](#). It further connects with the model perturbation f according to [Equation 2.3](#). In our experiment, c_0 is used as an initial guess (i.e., we start from constant background) and then c is inverted rather than f , as discussed in [Remark 6.1](#). Given some measurements \mathbf{d} of the total field, the quantitative reconstruction of the wave speed c is performed following the minimization of the misfit functional \mathcal{J} such that

$$\min_c \mathcal{J}(c), \quad \mathcal{J} = \text{dist}\left(\mathcal{R}u^{\text{tot}}, \mathbf{d}\right), \quad \text{where } u \text{ solves } \text{Equation 3.12}. \quad (6.1)$$

Here, $\text{dist}(\cdot)$ is a distance function to evaluate the difference between the measurements and the simulations, and \mathcal{R} is a linear operator to restrict the solution to the positions of the receivers. For simplicity, we do not encode a regularization term in [Equation 6.1](#) and refer the readers to, e.g., [\[21, 33\]](#) and the references therein.

Several formulations of the distance function have been studied for FWI (in particular for seismic applications), such as a logarithmic criterion, [\[55\]](#), the use of the signal's phase or amplitude, [\[4, 54\]](#), the use of the envelope of the signal, [\[22\]](#), criteria based upon cross-correlation, [\[41, 59, 17, 19\]](#), or optimal transport distance, [\[43\]](#). Here, we rely on a least-squares approach where the misfit functional is defined as the L^2 distance between the data and simulations:

$$\mathcal{J}(c) := \frac{1}{2} \sum_{\omega \in c_0 K} \sum_{\alpha \in A} \|\mathcal{R}u^{\text{tot}}(c, \omega, \alpha) - \mathbf{d}(\omega, \alpha)\|_{L^2(-l_M, l_M)}^2, \quad (6.2)$$

where $\mathbf{d}(\omega, \alpha)$ refers to the measurement data of the total field at the measurement plane with respect to the object rotated with angle α , and $u^{\text{tot}}(c, \omega, \alpha)$ is the solution of [Equation 3.12](#) with $k(\mathbf{x}) = \omega/c(R_\alpha^\top \mathbf{x})$. The last term $R_\alpha^\top \mathbf{x}$ encodes the rotation of the object. We note that a rotation of the object is equivalent of the rotation of both the measurement line and the direction of the incident field. We have encoded a sum over the frequencies ω , which are chosen in accordance with the frequency content available in measurements. In the computational experiments, we further investigate uni- and multi-frequency reconstructions.

The minimization of the misfit functional [Equation 6.2](#) follows an iterative Newton-type method as depicted in [Algorithm 1](#). Due to the computational cost, we use first-order information and avoid the Hessian computation, [\[61\]](#): Namely, we rely on the nonlinear conjugate gradient method for the model update, cf. [\[49, 15\]](#). Furthermore, to avoid the formation of the dense Jacobian, the gradient of the misfit functional is computed using the adjoint-state method, cf. [\[53, 50, 3, 20\]](#). In [Algorithm 1](#), we further implement a progression in the frequency content, which is common to mitigate the ill-posedness of the nonlinear inverse problem, [\[6\]](#). We further invert each frequency independently, from low to high, as advocated by [\[3, 18\]](#). For the implementation details using the HDG discretization, we refer to [\[20\]](#).

Remark 6.1 In the computational experiments, the reconstruction with FWI assumes the availability of the total fields which are solutions to [Equation 3.12](#), and we invert with respect to the (frequency independent) wave speed c defined in [Equation 2.3](#). We could instead use the representation with relation $k^2 = k_0^2 + f$, and invert with respect to the perturbation f , imposing the (known) smooth background c_0 . Inverting with respect to c rather than f is mainly motivated by consistency with existing literature in FWI [\[61\]](#), in which the background model (c_0) is usually unknown. Nonetheless, reformulating the minimization with respect to f and imposing c_0 could improve the efficiency of FWI, as advocated by the data-space reflectivity inversion of [\[8, 18\]](#).

6.2. Reconstruction based on the Born and Rytov approximations. In this section, we present numerical methods for the computation of the Born and Rytov approximations from

Input: Initial wave speed model c_0 .
 Initiate global iteration number $\ell := 1$;
for frequency $\omega \in c_0 K$ **do**
 for iteration $j = 1, \dots, n_{iter}$ **do**
 Compute the solution to the wave equation using current wave speed model c_ℓ and frequency ω , that is, the solution to Equation 3.12 with $k(\mathbf{x}) = \omega/c_\ell(\mathbf{x})$;
 Evaluate the misfit functional \mathcal{J} in Equation 6.2;
 Compute the gradient of the misfit functional using the adjoint-state method;
 Update the wave speed model using nonlinear conjugate gradient method to obtain $c_{\ell+1}$;
 Update global iteration number $\ell \leftarrow \ell + 1$;
 end
end
Output: Approximate wave speed c , from which the scattering potential f can be computed via Equations 2.2 and 2.1.

Algorithm 1: Iterative reconstruction of the wave speed model following the minimization of the misfit functional. At each iteration, the total field solution to Equation 3.12 is computed and the gradient of the misfit functional is used to update the wave speed model. The algorithm stops when the prescribed number of iterations is performed for all of the frequencies of interest.

Equation 3.4 and Equation 3.9, respectively, as well as the reconstruction of the scattering potential. We concentrate on the case of full rotations of the object using incident waves with different wave numbers $k_0 \in K$, see Section 5.3. The tomographic reconstruction is based on the Fourier diffraction theorem, Theorem 5.1, and the nonuniform discrete Fourier transform. Nonuniform Fourier methods have also been applied in computerized tomography [52], magnetic resonance imaging [38], spherical tomography [27, 28] or surface wave tomography [26].

In the following, we describe the discretization steps we apply. For $N \in 2\mathbb{N}$, let

$$\mathcal{I}_N := \left\{ -\frac{N}{2} + j : j = 0, \dots, N-1 \right\}.$$

We sample the scattering potential f on the uniform grid $\mathcal{R}_N := \frac{2r_s}{N}\mathcal{I}_N^2$ in the square $[-r_s, r_s]^2$ for some $r_s > 0$. We assume that we are given measurements of the Born approximation

$$u_{k_0}^\alpha(x_1, r_M), \quad x_1 \in [-l_M, l_M],$$

for $\alpha \in A \subset [0, 2\pi]$ and $k_0 \in K$, cf. Equation 5.3. We want to reconstruct the scattering potential $f = f_1$, recall Equation 5.2, utilizing Equation 5.4. We adapt the reconstruction approach of [37], which is written for the 3D case. First, we need to approximate the partial Fourier transform

$$\mathcal{F}_1 u_{k_0}^\alpha(k_1, r_M) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u_{k_0}^\alpha(x_1, r_M) e^{-ix_1 k_1} dx_1, \quad k_1 \in [-k_0, k_0]. \quad (6.3)$$

The *discrete Fourier transform* (DFT) of $u(\cdot, r_M)$ on m equispaced points $x_1 \in (2l_M/m)\mathcal{I}_m$ can be defined by

$$\mathbf{F}_{1,m} u(k_1, r_M) := \frac{1}{\sqrt{2\pi}} \frac{2l_M}{m} \sum_{x_1 \in \frac{2l_M}{m}\mathcal{I}_m} u(x_1, r_M) e^{-ix_1 k_1}, \quad k_1 \in \frac{\pi}{l_M}\mathcal{I}_m, \quad (6.4)$$

which gives an approximation of Equation 6.3. Then Equation 5.4 yields

$$k_0^2 \mathcal{F} f (R_\alpha(k_1, \kappa - k_0)^\top) = -i \sqrt{\frac{2}{\pi}} \kappa e^{-i\kappa r_M} \mathcal{F}_1 u_{k_0}^\alpha(k_1, r_M) \quad (6.5)$$

for $|k_1| \leq k_0$. Considering that we sample the angle α on the equispaced, discrete grid $A = (2\pi/n_A)\{0, 1, \dots, n_A - 1\}$ and some finite set $K \subset (0, \infty)$, [Equation 6.4](#) provides an approximation of $\mathcal{F}f$ on the non-uniform grid

$$\mathcal{Y}_{m,n_A} := \left\{ R_\alpha(k_1, \kappa - k_0)^\top : \right. \\ \left. k_1 \in \frac{\pi}{l_M} \mathcal{I}_m, |k_1| \leq k_0, \alpha \in \frac{2\pi}{n_A} \{0, 1, \dots, n_A - 1\}, k_0 \in K \right\}$$

in k -space, from which we want to reconstruct the scattering potential f .

Let M be the cardinality of \mathcal{Y}_{m,n_A} . The two-dimensional *nonuniform discrete Fourier transform* (NDFT) is the linear operator $\mathbf{F}_N: \mathbb{R}^{N^2} \rightarrow \mathbb{R}^M$ defined for the vector $\mathbf{f}_N := (f(\mathbf{x}))_{\mathbf{x} \in \mathcal{R}_N}$ elementwise by

$$\mathbf{F}_N \mathbf{f}_N(\mathbf{y}) := \frac{1}{2\pi} \frac{(2r_s)^2}{N^2} \sum_{\mathbf{x} \in \mathcal{R}_N} f(\mathbf{x}) e^{-i\mathbf{x} \cdot \mathbf{y}}, \quad \mathbf{y} \in \mathcal{Y}_{m,n_A}, \quad (6.6)$$

see [\[51, Section 7.1\]](#). It provides an approximation of the Fourier transform

$$\mathcal{F}f(\mathbf{y}) \approx \mathbf{F}_N \mathbf{f}_N(\mathbf{y}), \quad \mathbf{y} \in \mathcal{Y}_{m,n_A}. \quad (6.7)$$

Solving an equation $\mathbf{F}_N \mathbf{f}_N(\mathbf{y}) = \mathbf{b}$ for \mathbf{f}_N amounts to applying an *inverse NDFT*, which usually utilizes an iterative method such as the conjugate gradient method on the normal equations (CGNE), see [\[39\]](#) and [\[51, Section 7.6\]](#). One should be aware that the notation regarding conjugate gradient algorithms varies in the literature: the algorithm called CGNE in [\[24\]](#), is known as CGNR in [\[39\]](#). Conversely, the algorithm CGME in [\[24\]](#) is known as CGNE in [\[39\]](#).

In conclusion, our method for computing f given the Born approximation u^{Born} is summarized in [Algorithm 2](#).

Input: Measurement data

$$u_{k_0}^\alpha(x_1, r_M), \quad x_1 \in \frac{2l_M}{m} \mathcal{I}_m, \quad \alpha \in A = \frac{2\pi}{n_A} \{0, \dots, n_A - 1\}, \quad k_0 \in K.$$

for $k_0 \in K$ **do**

for $\alpha \in A$ **do**

 Compute $-i\sqrt{\frac{2}{\pi}} \kappa e^{-i\kappa r_M} \mathbf{F}_{1,m} u_{k_0}^\alpha(k_1, r_M)$, $k_1 \in \frac{\pi}{l_M} \mathcal{I}_m$, with a DFT in [Equation 6.4](#);

end

end

Solve [Equation 6.5](#) with [Equation 6.7](#) for \mathbf{f}_N using the conjugate gradient method;

Output: Approximate scattering potential $\mathbf{f}_N \approx (f(\mathbf{x}))_{\mathbf{x} \in \mathcal{R}_N}$.

Algorithm 2: Iterative reconstruction of the scattering potential f based on the Born approximation using an inverse NDFT.

The Rytov approximation u^{Rytov} , see [Equation 3.9](#), is closely related to the Born approximation, but it has a different physical interpretation. Assuming that the measurements arise from the Rytov approximation, we apply [Equation 3.10](#) to obtain u^{Born} from which we can proceed to recover f as shown above. We note that the actual implementation of [Equation 3.10](#) requires a phase unwrapping because the complex logarithm is unique only up to adding $2\pi i$, cf. [\[46\]](#). In particular, we use in the two-dimensional case

$$u^{\text{Born}} = u^{\text{inc}} \left(i \text{unwrap} \left(\arg \left(\frac{u^{\text{Rytov}}}{u^{\text{inc}}} + 1 \right) \right) + \ln \left| \frac{u^{\text{Rytov}}}{u^{\text{inc}}} + 1 \right| \right), \quad (6.8)$$

where \arg denotes the principle argument of a complex number and unwrap denotes a standard unwrapping algorithm. For the reconstruction with the Rytov approximation, we can use [Algorithm 2](#) as well, but we have to preprocess the data u by [Equation 6.8](#).

7. NUMERICAL EXPERIMENTS

In this section, we carry out numerical experiments comparing the reconstruction obtained with FWI ([Section 6.1](#)) and Born and Rytov approximations ([Section 6.2](#)), using single and multi-frequency data-sets. We consider different media with varying shapes and amplitude for the embedded objects. Our experiments use synthetic data with added noise: Firstly, synthetic simulations are carried out for the known wave speeds using the software `hawen` [[16](#)]. The discretization relies on a fine mesh (usually a few hundred thousands cells in the discretized domain) and polynomials of order 5 to ensure accuracy. Then, white Gaussian noise is incorporated in the synthetic data, with a signal-to-noise ratio of 50 dB. The reconstruction with FWI also relies on software `hawen`, but uses different discretization setups to foster the computational time: the discretization mesh is coarser (usually a few tens of thousand cells) and the polynomial order varies with the cells, depending on the (local to the cell) wavelength, in order to remain as small as possible, as detailed in [[20](#)]. The computational cost of FWI is further discussed in [Section 7.4](#).

We perform a full rotation of the object for a single or for multiple frequencies ω and thus wave numbers k_0 , cf. [Section 5.3](#). For different frequencies, the scattering potential is scaled according to [Equation 5.2](#). We always reconstruct the rescaled scattering potential f_1 , which we will simply denote by f in the following. In all numerical experiments, we rely on forward data generated with the forward model of line sources in [subsection 3.2.2](#).

We compare the reconstruction quality based on the *peak signal-to-noise ratio* (PSNR) of the reconstruction \mathbf{g} with respect to the ground truth \mathbf{f} determined by

$$\text{PSNR}(\mathbf{f}, \mathbf{g}) := 10 \log_{10} \frac{\max_{\mathbf{x} \in \mathcal{R}_N} |\mathbf{f}(\mathbf{x})|^2}{N^{-2} \sum_{\mathbf{x} \in \mathcal{R}_N} |\mathbf{f}(\mathbf{x}) - \mathbf{g}(\mathbf{x})|^2},$$

where higher values indicate a better reconstruction quality.

7.1. Reconstruction of circular contrast with various amplitudes and sizes. For the initial reconstruction experiments, we consider a circular object in a homogeneous background, namely the scattering potential f of [Equation 4.2](#). We investigate different sizes and contrasts for the object, as shown in [Figure 6](#). The data are generated for $n_A = 40$ angles of incidence equally partitioned between 0° to 351° , every 9° , and the measurement line is sampled on the 200 point uniform grid $10^{-1} \mathcal{I}_{200} \subset [-l_M, l_M]$ with $l_M = 10$. Let us note that in this context of a circularly symmetric object, the data of each angle are similar and correspond to that of [Figure 3](#) for $f = \mathbf{1}_{4.5}^{\text{disk}}$.

7.1.1. Reconstruction using FWI with single-frequency data-sets. We first only use data at frequency $\omega/(2\pi) = 1$, that is, wave number $k_0 = 2\pi$ for the reconstruction of the different perturbations illustrated in [Figure 6](#). With the background $k_0 = 2\pi$ (i.e., wave speed of 1), it means that we only rely on waves with wavelength 1 when propagating in the (homogeneous)

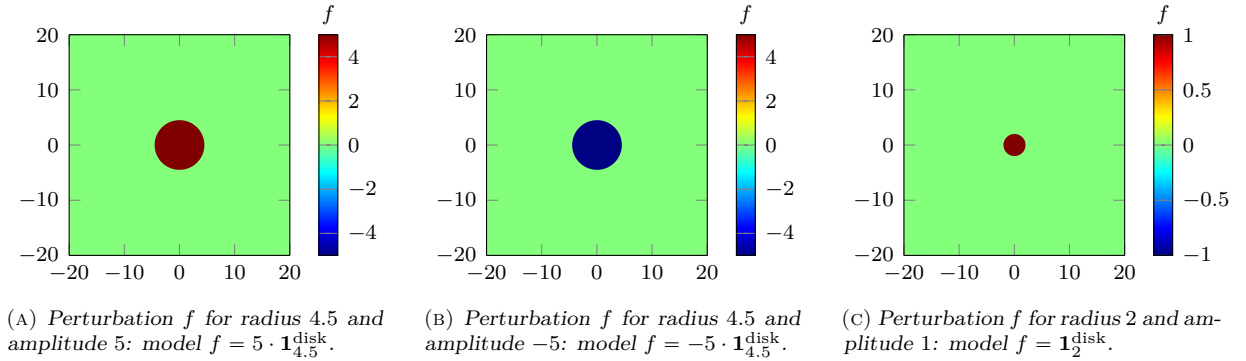


FIGURE 6. Different perturbation models f used for the computational experiments, given for frequency $\omega/(2\pi) = 1$, with the relation to the wave speed given in Equation 2.3. Both the size and contrast vary: we consider two radii (4.5 and 2) and three contrasts (1, 5 and -5 with corresponding wave speeds $c = 0.9876$, $c = 0.9421$ and $c = 1.0701$, respectively), for a total of six configurations. The computations are carried out on the domain $[-50, 50] \times [-50, 50]$, i.e., a slightly larger setup than Figure 3, and we only picture the area near the origin for clearer visualization.

background. Then all measurements in \mathbf{x} are in multiples of the wavelength. In the case of a single frequency, only the inner loop remains in Algorithm 1, and we perform 50 iterations. In Figure 7, we picture the reconstruction obtained for the six different perturbations f . We observe that the reconstructions of the smaller object of radius 2 (Figures 7a, 7b and 7c) are more accurate, both in terms of the circular shape, and in terms of amplitude. In the case of the larger object, the mild amplitude (Figure 7d) is accurately recovered, while the stronger contrasts (Figures 7e and 7f) are only partially retrieved. Here, the outer part of the disk appears, but the amplitude is incorrect with a ring effect and incorrect values in the inner area. Therefore, the reconstruction using single-frequency data is limited and its success depends on two factors: the size of the object and its contrast.

7.1.2. Reconstruction using FWI with multiple frequency data-sets. The difficulty of recovering a large object with a strong contrast can be mitigated by the use of multi-frequency data-sets, allowing a multi-scale reconstruction [6, 18]. We carry out the iterative reconstruction using increasing frequencies, starting with $\omega/(2\pi) = 0.2$ and up to $\omega/(2\pi) = 1$. Following [18], we use a sequential progression, that is, every frequency is inverted separately. The reconstructions for the object of radius 4.5 and contrast $f = \pm 5$ are pictured in Figure 8. Contrary to the case of a single frequency (see Figure 7d), the reconstruction is now accurate and stable: the amplitude is accurately retrieved and the circular shape is clear, avoiding the circular artifacts observed in Figures 7e and 7f.

Remark 7.1 It is possible to recover the model with a single frequency, that needs to be carefully chosen depending on the size of the object and the amplitude of the contrast. We have seen in Figure 7 that the frequency $\omega/(2\pi) = 1$ is sufficient for the object of radius 2 but for the radius 4.5, we need a lower frequency (i.e., larger wavelength) to uncover the larger object. We illustrate in Figure 9 the reconstruction using data at only $\omega/(2\pi) = 0.7$, where we see that the shape and contrast are retrieved accurately. Nonetheless, it is hard to predict this frequency a-priori and we believe it remains more natural to use multiple frequencies (when available in the data), to ensure the robustness of the algorithm.

7.1.3. Reconstruction using Born and Rytov approximations. For the reconstruction with Algorithm 2, which relies on the Born or Rytov approximation, we use the same data as

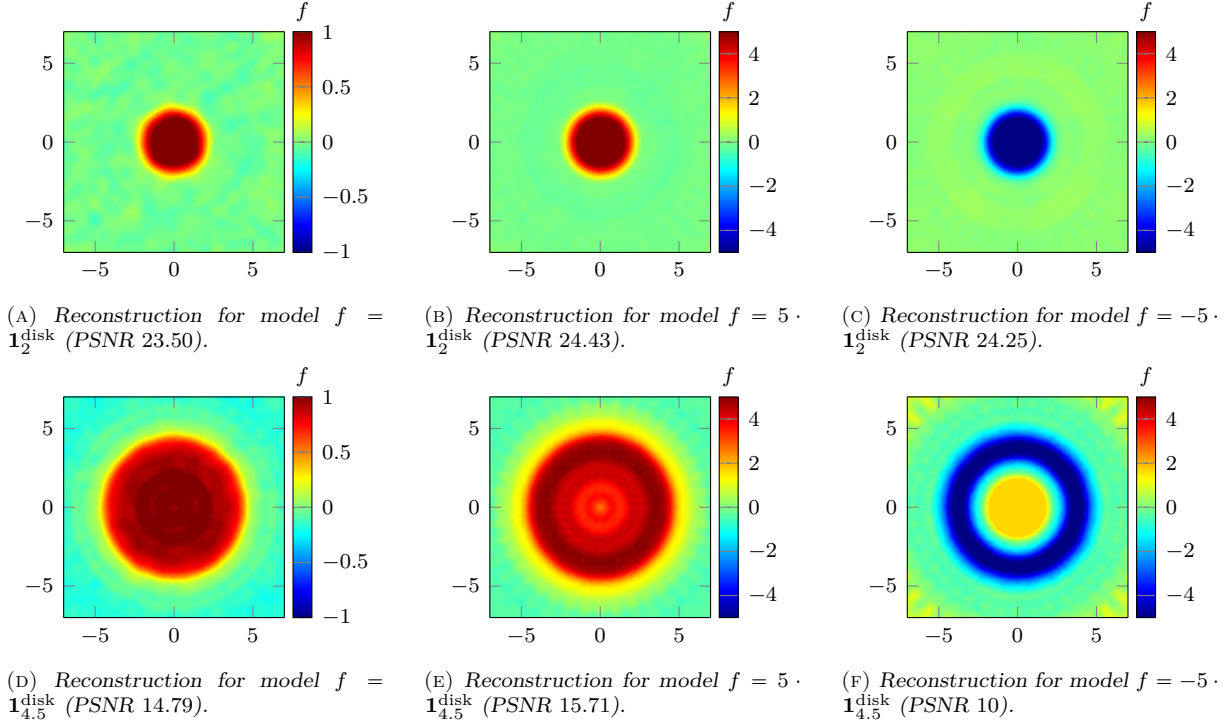


FIGURE 7. Reconstruction using iterative minimization using data of frequency $\omega/(2\pi) = 1$ only. In each cases, 50 iterations are performed and the initial model consists in a constant background where $k_0 = 2\pi$. The data consist of $n_A = 40$ different angles of incidence from 0° to 351° .

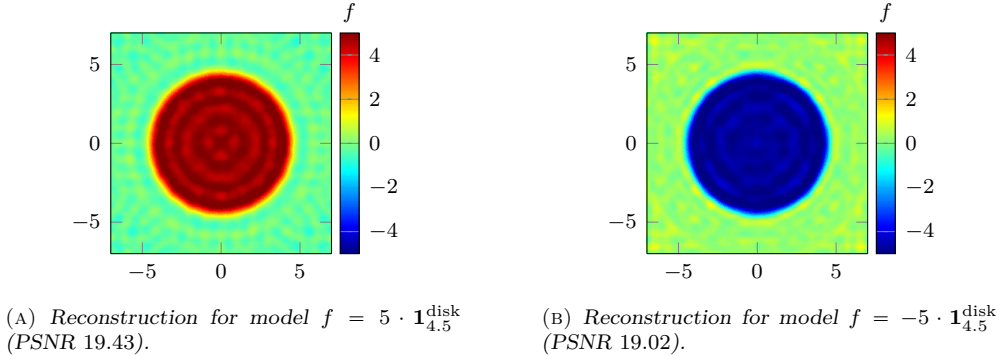


FIGURE 8. Reconstruction using multi-frequency data from $\omega/(2\pi) = 0.2$ to $\omega/(2\pi) = 1$. The initial model consists in a constant wave speed $c_0 = 1$. The data consist of $n_A = 40$ different angles of incidence from 0° to 351° .

in the above experiment. We use a grid with $N = 240$ and $r_s = N/(8\sqrt{2}) \approx 10$. The numerical results indicate that r_s should not be smaller than l_M . Since we have $k_1^2 \leq k_0^2$ and the distance between two grid points of k_1 is π/l_M , only around $2k_0 l_M/\pi \approx 40$ of them contribute to the data of the inverse NDFE.

In the following reconstructions, we use a fixed number of 20 iteration steps in the conjugate gradient method. Initially, we use the frequency $\omega/(2\pi) = 1$ of the incident wave, therefore $k_0 = 2\pi$. Reconstructions of the circular model $f = \mathbf{1}_a^{\text{disk}}$ are shown in Figure 10. We note that all reconstructions are reasonably good, where the Rytov reconstruction looks slightly better inside the object.

For a higher amplitude of the model function f , the limitations of the linear models become

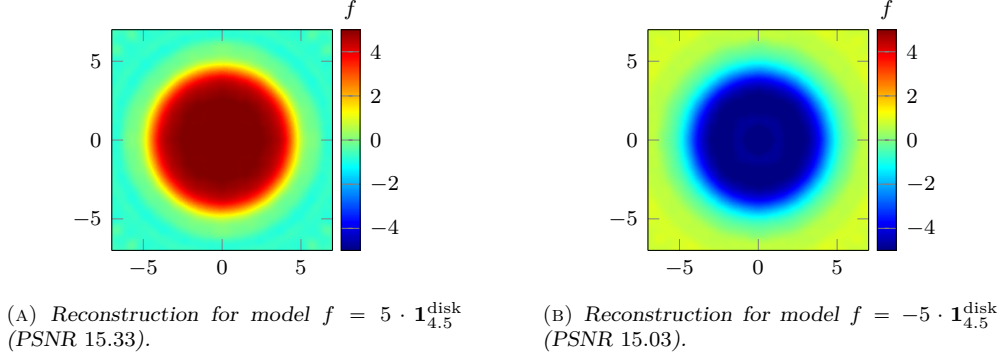


FIGURE 9. Reconstruction using frequency $\omega/(2\pi) = 0.7$. The initial model consists in a constant wave speed $c_0 = 1$. The data consist of $n_A = 40$ different angles of incidence from 0° to 351° .

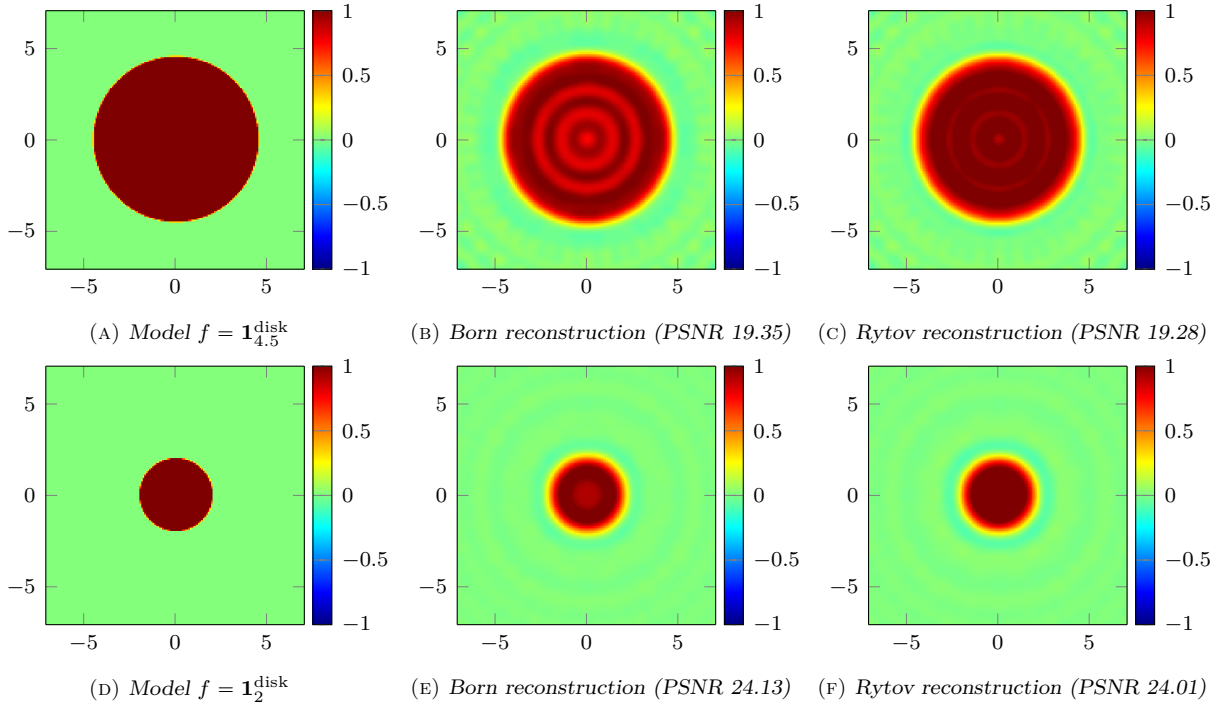


FIGURE 10. Reconstructions with the Born and Rytov approximation, where the data $u(\cdot, r_M)$ is generated with the line source model. The incident field has the frequency $\omega/(2\pi) = 1$. Visible is only the cut out center, where we compute the PSNR.

apparent. In Figure 11, we see that the Born reconstruction of the larger object fails, and for the smaller object only the Rytov approximation yields a good reconstruction, which is consistent with Remark 3.1. With the Born approximation, we recognize the object's shape but not its amplitude, which is consistent with the observations in [45]. However, as we see in Figure 7, even the FWI reconstruction makes a considerable error in the object's interior, and we cannot expect the linear models to be better.

We see that the FWI and the Born/Rytov reconstructions contain different kinds of artifacts. Therefore, a comparison of the visual image quality perception does not necessarily yield the same conclusions as for the computed PSNR values. Furthermore, the size of the object has a considerable effect on the PSNR, e.g., the images in Figure 11 (c) and (f) show a comparable visual quality, but the latter's PSNR is considerably better because of the lower error in the

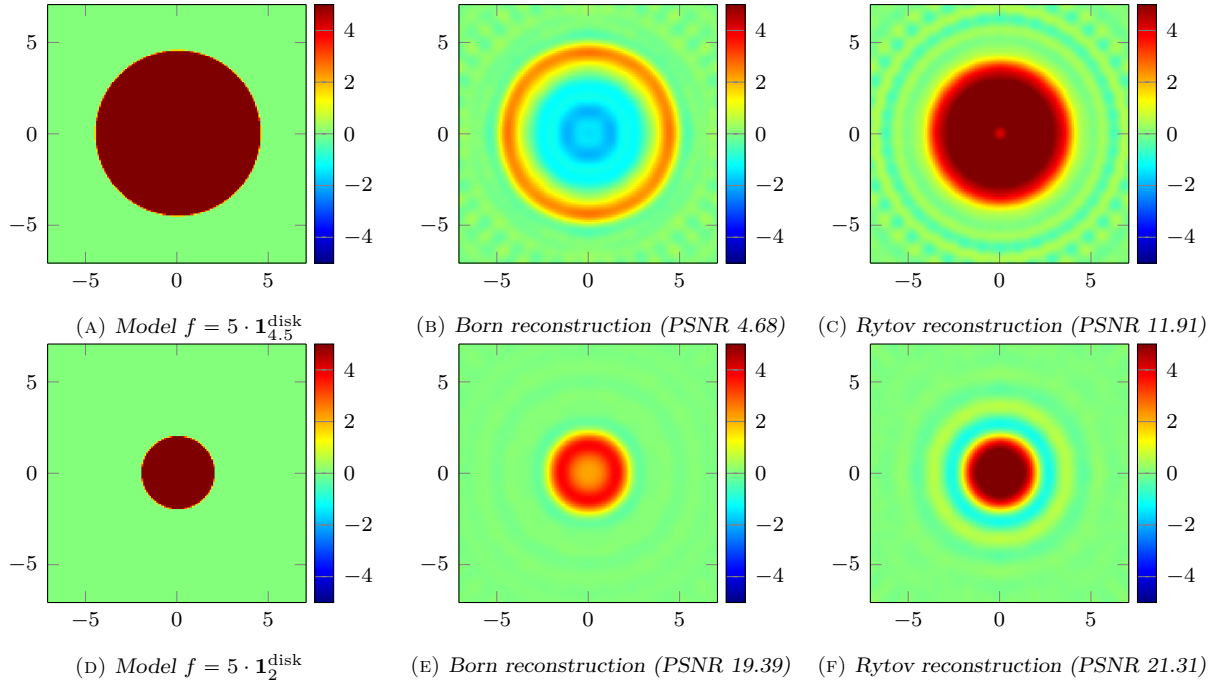


FIGURE 11. Same setting as in Figure 10, but with a higher amplitude of 5.

background farther away from the object, see also [30] for a study on the PSNR.

In Figure 12, we use the same setup as before, but with the frequency $\omega/(2\pi) = 0.7$ instead of $\omega/(2\pi) = 1$ and thus the wave number $k_0 = \omega$. Apparently, the reconstruction becomes worse with lower frequency, because it provides a smaller k-space coverage.

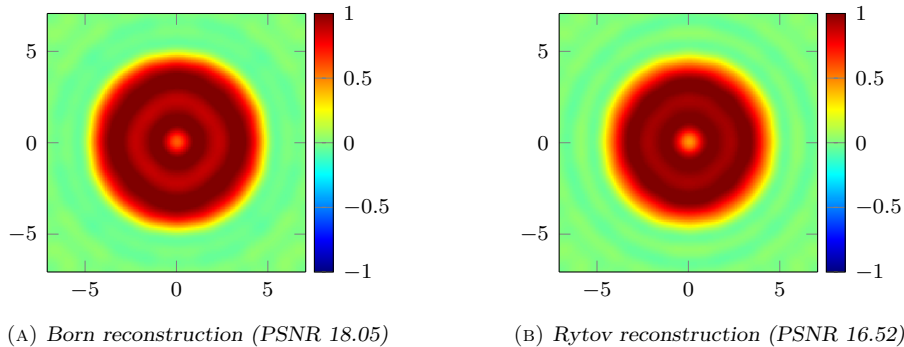
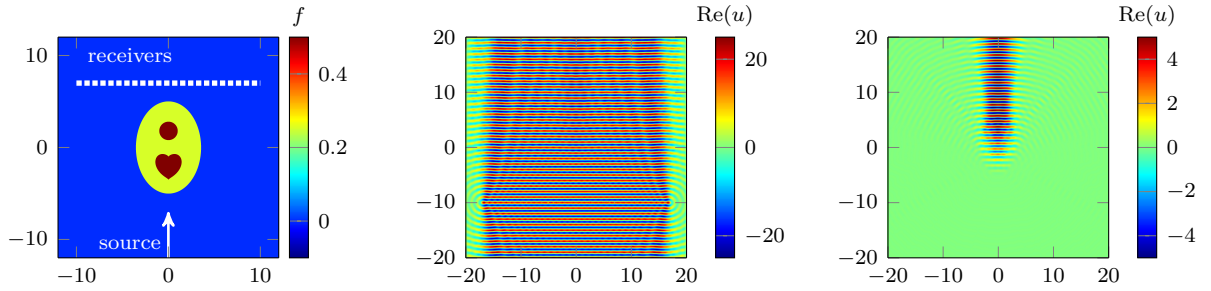


FIGURE 12. Reconstructions of $\mathbf{1}_{4.5}^{\text{disk}}$, where the incident field has the frequency $\omega/(2\pi) = 0.7$ instead of 1. The rest of the setting is from Figure 10.

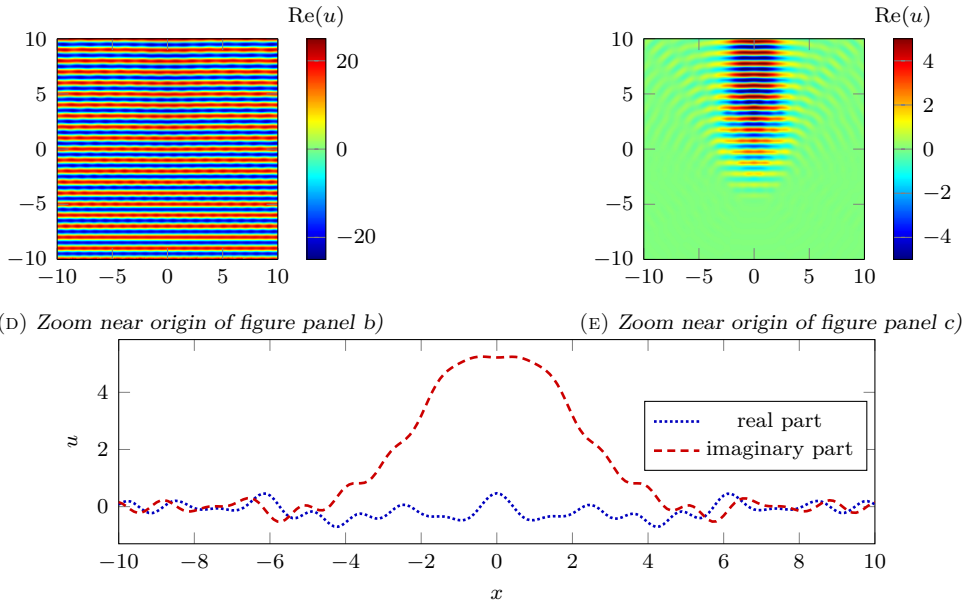
7.2. Reconstruction of embedded shapes: Phantom 1. We consider a more challenging scenario with shapes embedded in the background medium. In Figure 13a, we picture the perturbation f consisting of a disk and heart included in an ellipse, with f varying from 0 to 0.5. The computational domain corresponds to $[-20, 20] \times [-20, 20]$, with line-sources positioned at a distance $R = 10$ and receivers in $r_M = 6$ to capture the data. The data are generated using $n_A = 100$ incidence angles α equispaced on $[0, 2\pi]$, following the steps described in Section 4.2. This is illustrated in Figure 13.



(A) Perturbation model at frequency $\omega/(2\pi) = 1$, the wave speed is equal to 1 in the background. The positions of the source and the receivers recording transmission data are pictured in white.

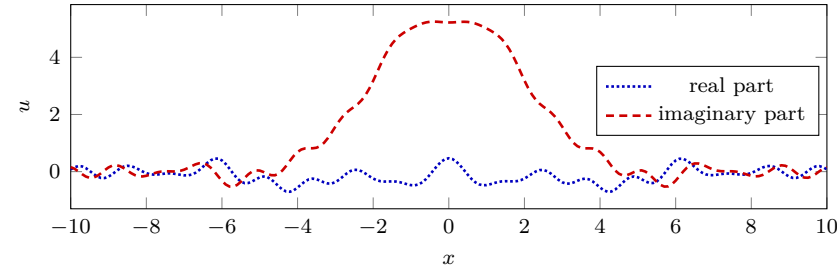
(B) Real part of the global solution to Equation 3.12 at frequency $\omega/(2\pi) = 1$, the source is discretized by $N_{\text{sim}} = 1361$ simultaneous excitations at fixed height $x_2 = -10$.

(C) Real part of the scattering solution at frequency $\omega/(2\pi) = 1$.



(D) Zoom near origin of figure panel b)

(E) Zoom near origin of figure panel c)



(F) Scattered solution measured at the 201 receivers positioned at fixed height $x_2 = 6$.

FIGURE 13. Illustration of the acquisition setup and generated data. The computations are carried out on the domain $[-20, 20] \times [-20, 20]$. While FWI uses the total field, the reconstruction based upon Born and Rytov approximations use the scattered solutions, obtained after removing a reference solution corresponding to a propagation in an homogeneous medium, cf. Section 3.

7.2.1. Reconstruction using FWI. We carry out the reconstruction following Algorithm 1, and the results are pictured in Figure 14, where we compare the use of single and multi-frequency data. In this example, we see that with relatively low frequency data (i.e., relatively large wavelength), such as for frequency $\omega/(2\pi) = 0.7$ and $\omega/(2\pi) = 1$, the reconstruction is smooth, see Figure 14a and Figure 14b, and one needs to use smaller wavelengths to obtain a better reconstruction, see Figure 14c and Figure 14d. In Figure 14e, we see that multi-frequency data gives the best reconstruction, it is also the most robust as one does not need to anticipate the appropriate wavelength before carrying out the reconstruction. Here both the shapes and contrast in amplitude are accurately obtained. We notice some oscillatory noise in the reconstructed models, which could certainly be reduced by incorporating a regularization criterion in the minimization [21].

In Figure 15, we conduct a similar computational experiment, but increasing the contrast in the included heart shape where f has now a value of 2, see Figure 15a. We provide single

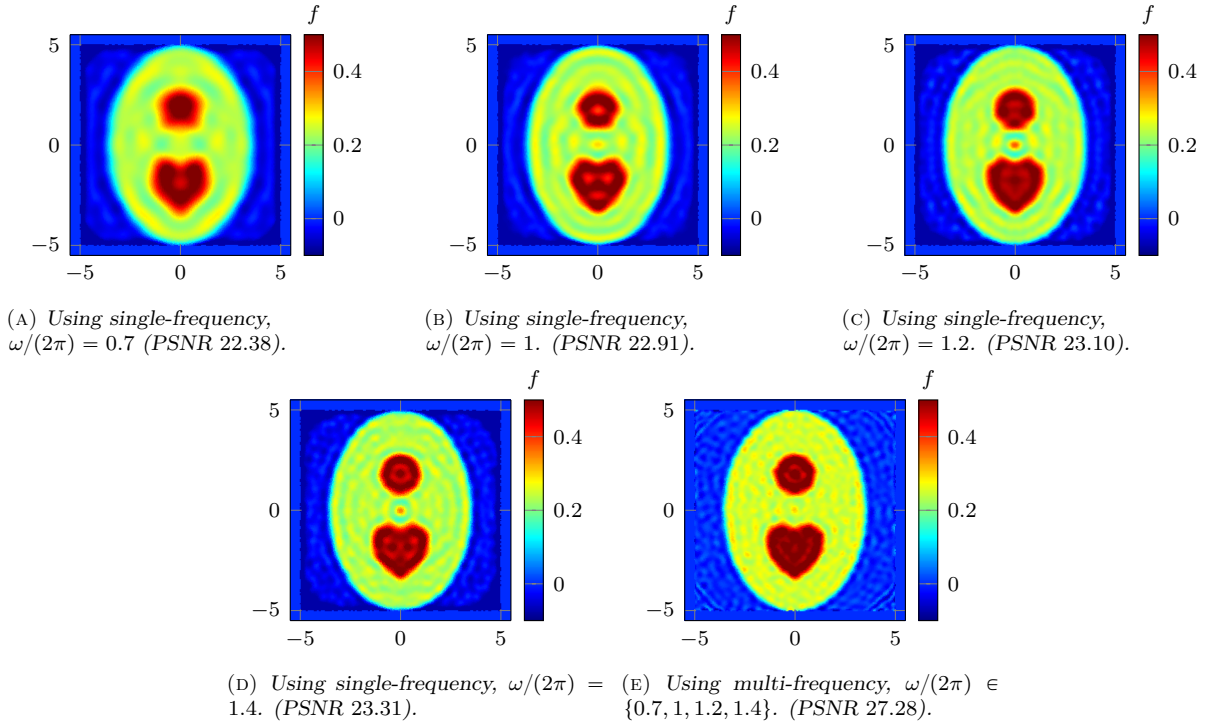


FIGURE 14. Reconstruction of the model [Figure 13a](#) with FWI and starting from a homogeneous background with $f = 0$. The models are given at frequency $\omega/(2\pi) = 1$ and the wave speed is equal to 1 in the background.

and multi-frequency reconstructions, and observe that large wavelengths still provide a smooth reconstruction. The high contrast in the heart is well recovered.

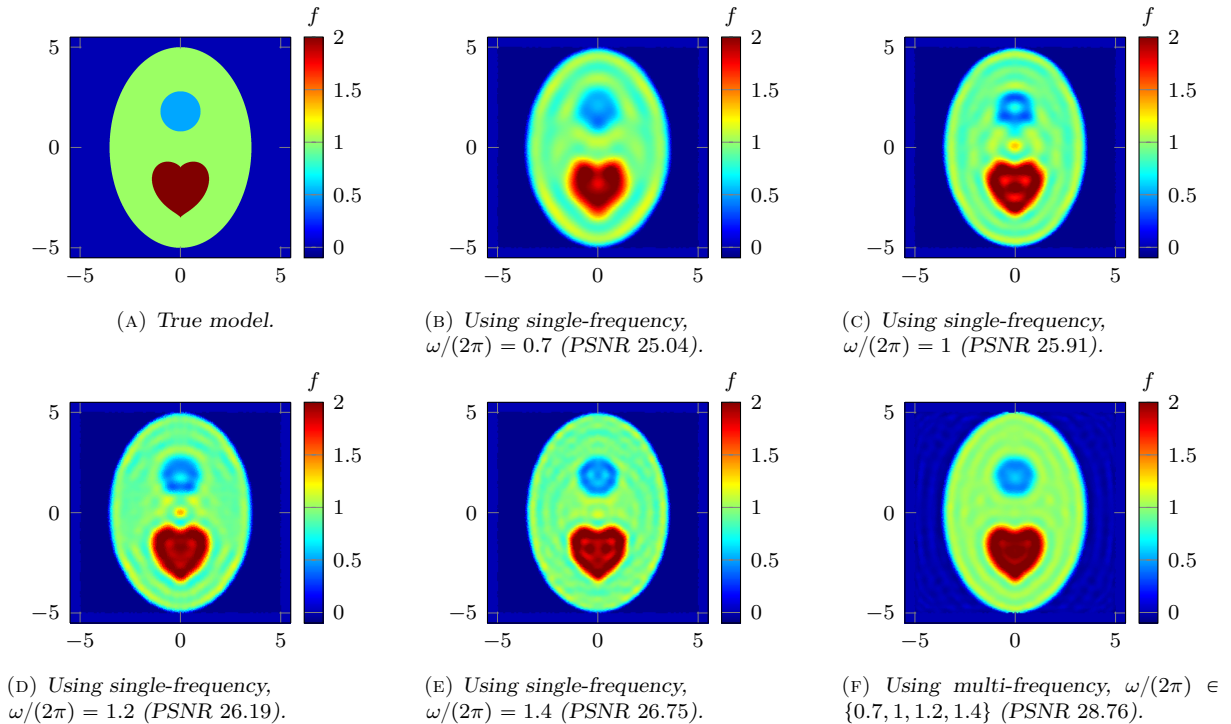


FIGURE 15. Reconstruction with FWI starting from a homogeneous background with $f = 0$. The models are given at frequency $\omega/(2\pi) = 1$ and the wave speed is equal to 1 in the background.

7.2.2. Reconstruction using Born and Rytov approximations. We perform the reconstruction with Algorithm 2 of the test model f from Figure 13. In the following tests, we discretize f on a finer grid of resolution $N = 720$, which covers the radius $r_s = 15/\sqrt{2}$. The PSNR is computed only on the central part of the grid that is visible in the image. Since we know that the f is real-valued, we take only the real part of the reconstruction. For simplicity, we use a constant number of 12 iterations in the conjugate gradient method of the inverse NDFT.

The Born and Rytov reconstructions are shown in Figure 16, where the data u is the same as in subsection 7.2.1. The reconstruction with a higher frequency of the incident wave is more accurate, since it provides a larger k-space coverage, which is the disk of radius $\sqrt{2}k_0 = \sqrt{2}\omega$, see Section 5. Moreover, the multi-frequency reconstruction is shown in Figure 16 (g) and (h). Even though the multi-frequency setup covers the same disk in k-space, it still seems superior because we have more data points of the Fourier transform $\mathcal{F}f$.

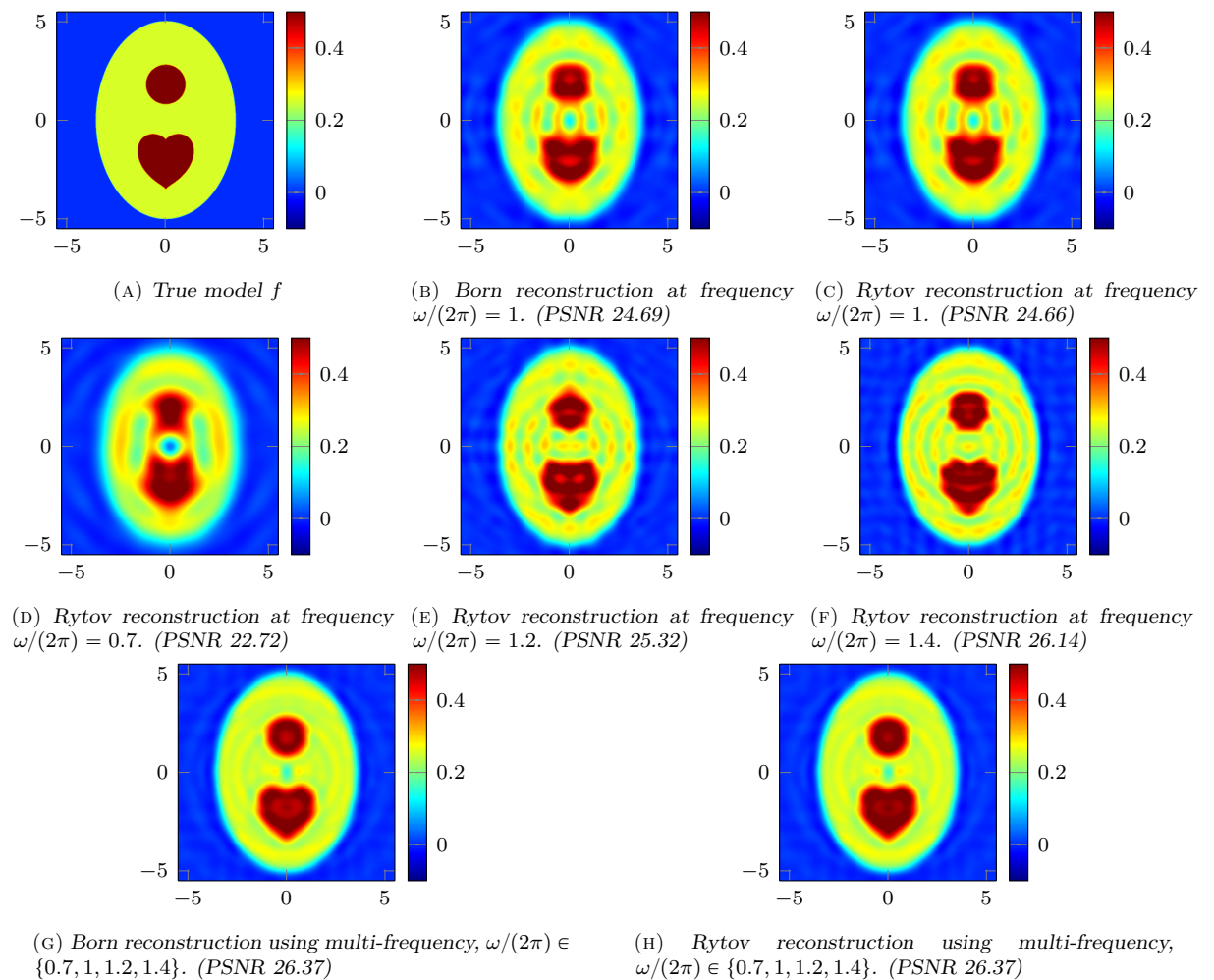


FIGURE 16. Reconstructions for different frequencies of the incident wave. The PSNR is computed on the visible part of the grid for the real part of the reconstruction, since we know that f must be real.

For the similar model from Figure 15a with a higher contrast, the reconstructions with Born and Rytov approximation differ more from the FWI reconstruction because of the more severe scattering, see Figure 17. In general, we can expect the FWI reconstruction to be better since it is a numerical approximation of the wave equation, of which the Born or Rytov approximations are just linearizations.

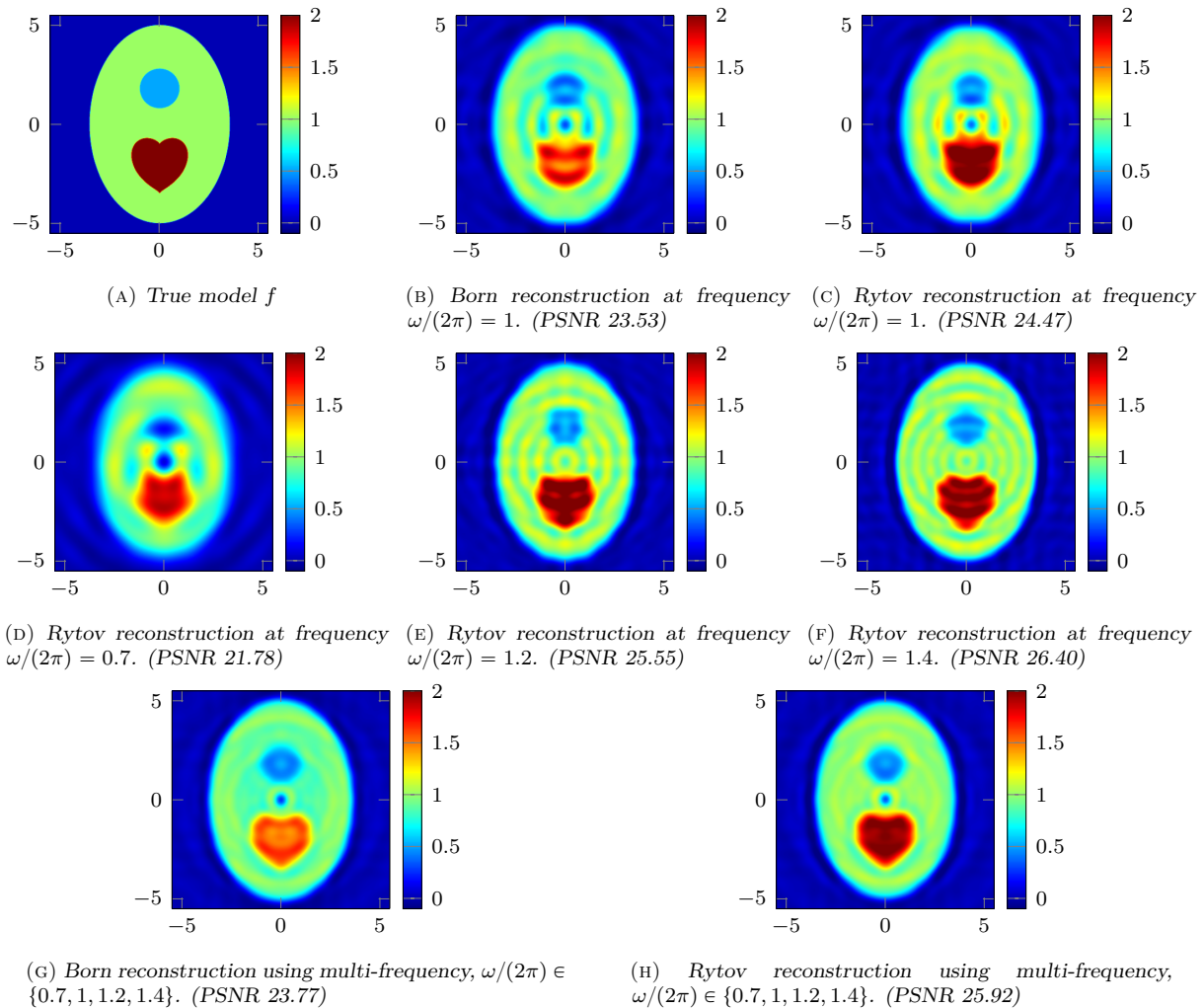


FIGURE 17. Reconstructions with a higher contrast, where the rest of the setting is the same as in Figure 16.

7.3. Reconstruction of embedded shapes: Phantom 2. We now consider the case with combinations of smaller convex and non-convex shapes included in the background medium.

7.3.1. Reconstruction using FWI. In Figure 18 and Figure 19, we show the model perturbation, which consist in small objects buried in the background. FWI is carried out with single and multiple frequencies, while we investigate a mild contrast in Figure 18 (where f is at most 0.5) and a stronger contrast in Figure 19 (where f is at most 2). We see that the model can be recovered using a single frequency, which has to be selected depending on the contrast. As an alternative, multi-frequency data appears to be a robust candidate and always provides a good reconstruction, for both the object's shape and amplitude. The reconstruction quality with high contrast in Figure 19 seems to be of a similar level as with low contrast.

7.3.2. Reconstruction using Born and Rytov approximations. In Figure 20, we show the reconstruction using Born and Rytov approximations. Here, we can clearly see that we need a higher frequency in order to resolve small features of the object. However, the reconstructions are still inferior to the FWI.

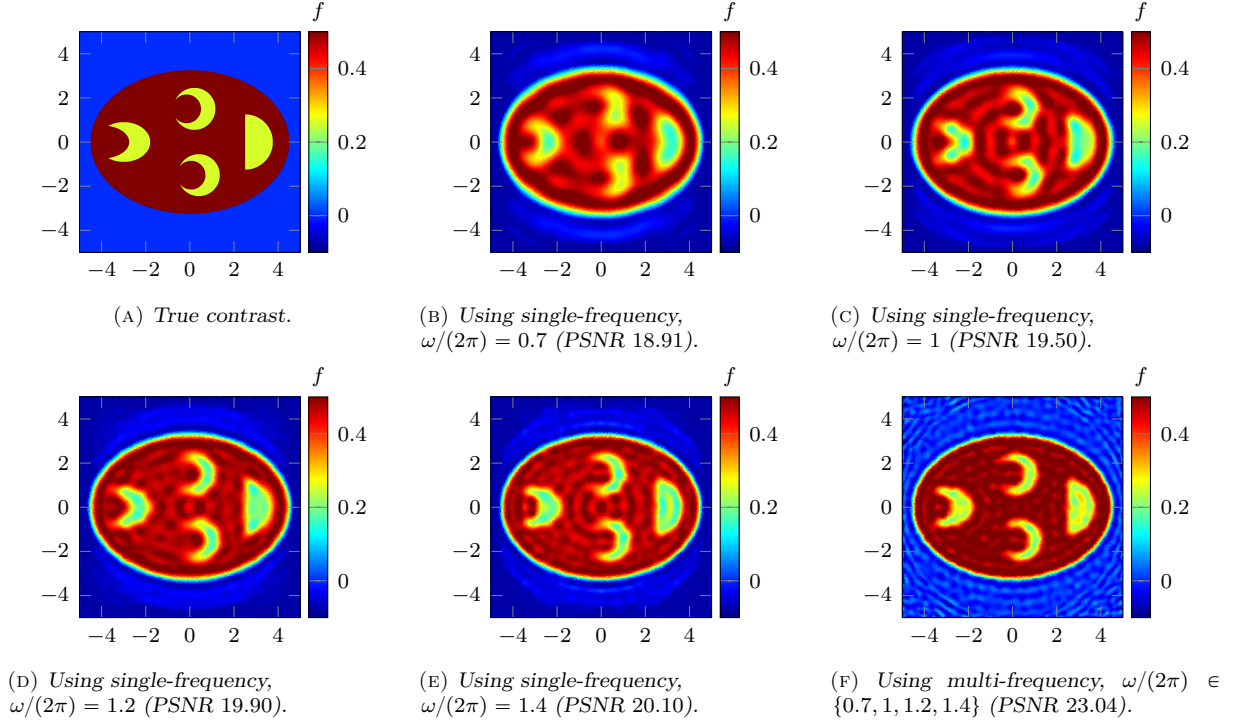


FIGURE 18. Reconstruction with FWI starting from a homogeneous background with $f = 0$. The models are given at frequency $\omega/(2\pi) = 1$ and the wave speed is equal to 1 in the background.

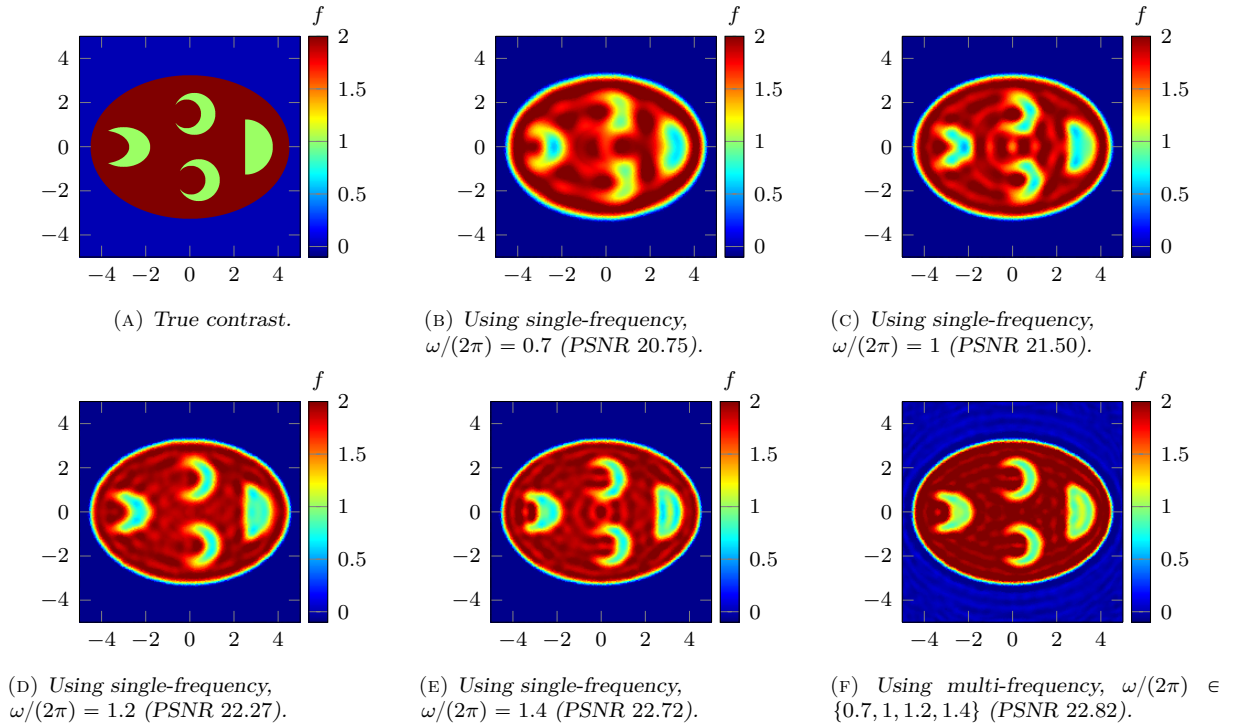


FIGURE 19. Reconstruction with FWI starting from a homogeneous background with $f = 0$. The models are given at frequency $\omega/(2\pi) = 1$ and the wave speed is equal to 1 in the background.

With a higher contrast, the reconstruction with the Rytov approximation is considerably better than the one with the Born approximation, see Figure 21. This is consistent with Remark 3.1.

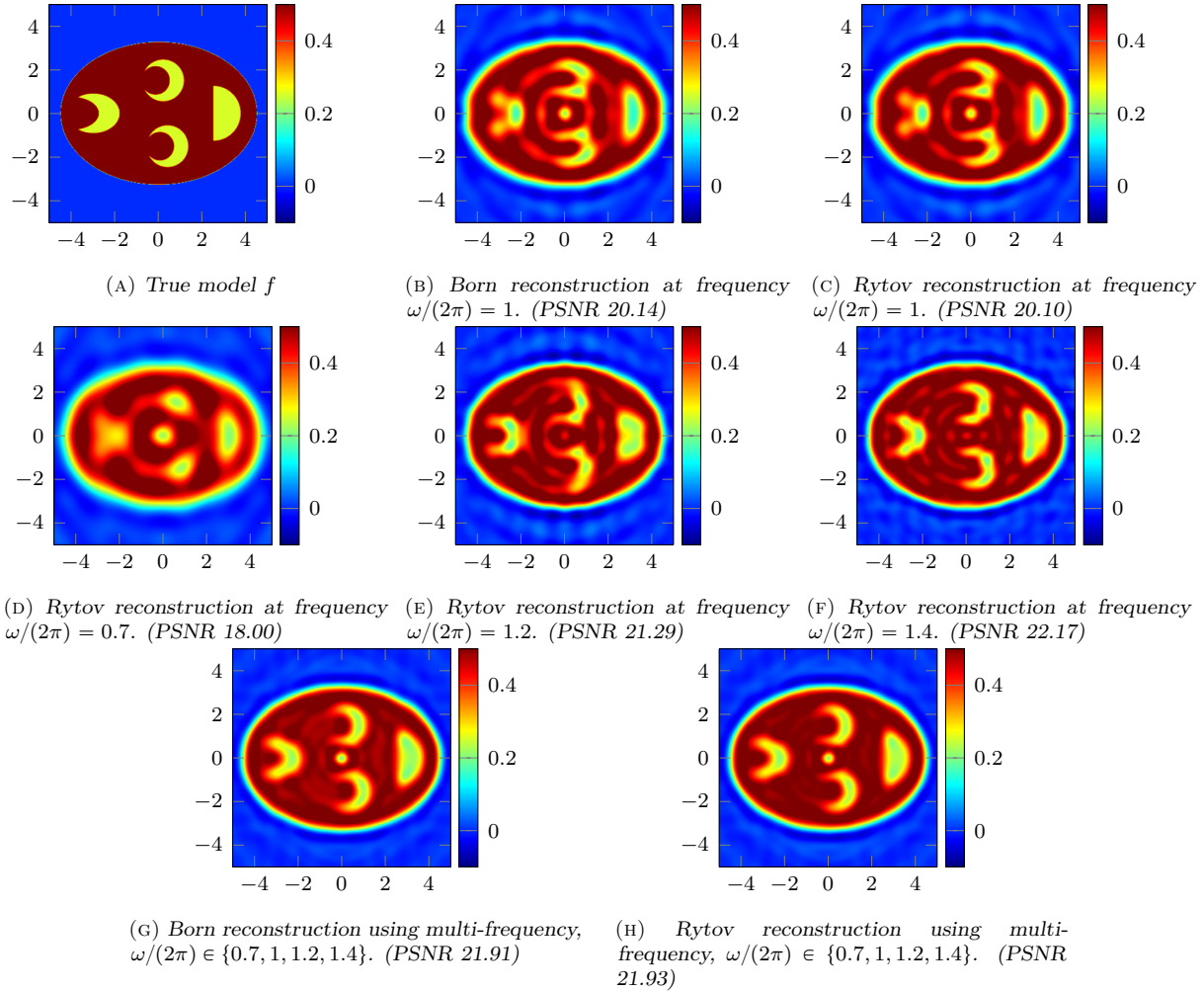


FIGURE 20. Reconstructions of the more complicated shapes. The models are given at frequency $\omega/(2\pi) = 1$.

Interestingly, the shapes reconstruction in high contrast barely profits from taking frequencies higher than 1, even though the k-space coverage is larger. In this situation, the Rytov reconstruction is almost comparable to the one with lower contrast, but still worse than the FWI.

7.4. Computational costs.

Computational cost of FWI. The computational cost of FWI comes from the discretization and resolution of the wave problem Equation 3.12 for each of the sources in the acquisition, coupled with the iterative procedure of Algorithm 1. In our numerical experiments, we use the software `hawen` for the iterative inversion, [16], footnote 1, which relies on the Hybridizable discontinuous Galerkin discretization, [9, 20]. The number of degrees of freedom for the discretization depends on the number of cells in the mesh, and the polynomial order. In the inversion experiments, we use a fixed mesh for all iterations, with about fifty thousands cells. On the other hand, the polynomial order is selected depending on the wavelength on each cell. That is, each of the cells in the mesh is allowed to have a different order (here between 3 to 7), see [20]. Then, when the frequency changes, while the mesh remains the same, the order of the polynomial evolves accordingly to the change of wavelength. Once the wave equation, Equation 3.12, is discretized, we obtain a linear system which size is the number of degrees of freedom, that must be solved for the different sources (i.e., the different incident angles). We rely on the direct solver MUMPS,

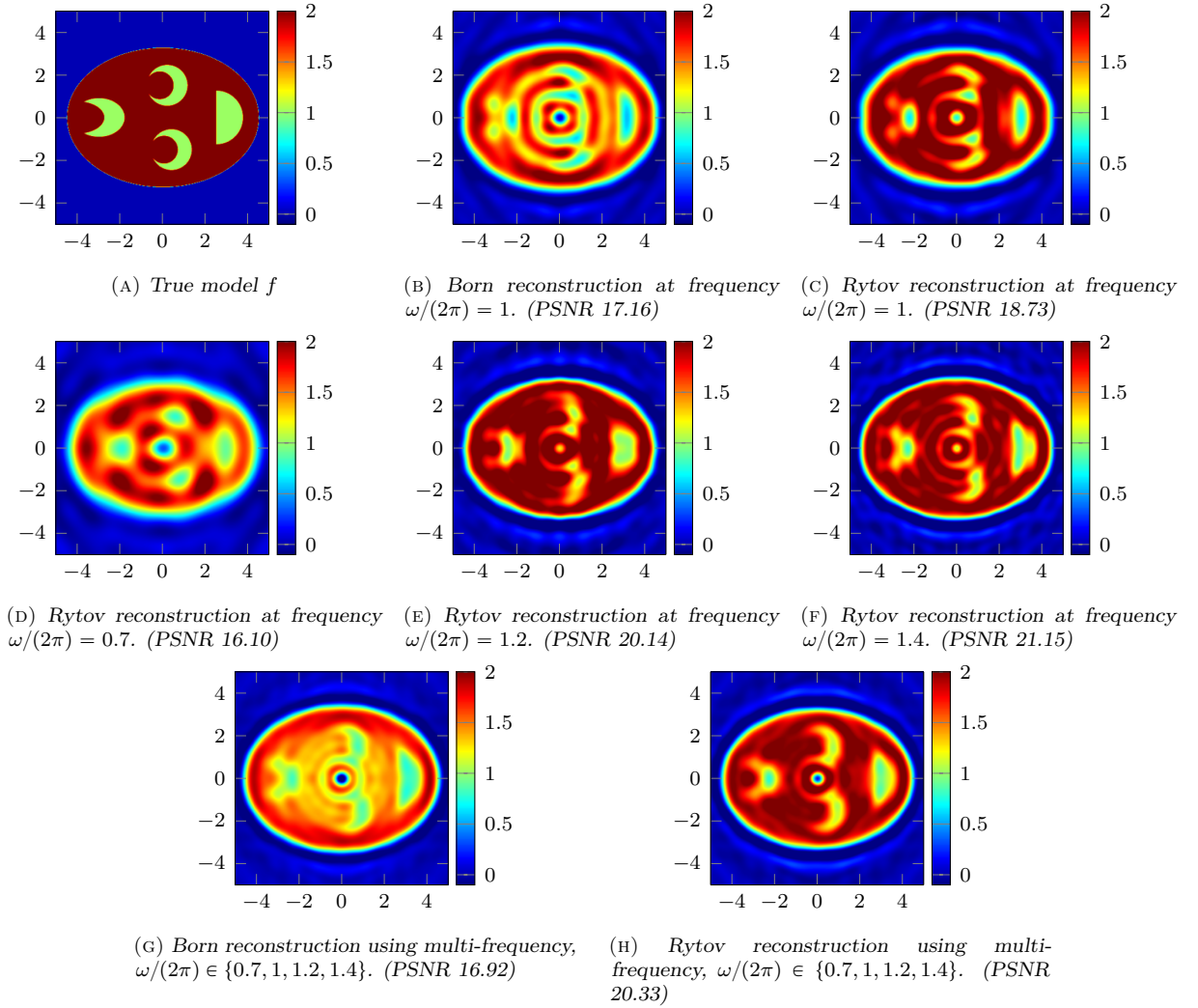


FIGURE 21. Reconstructions of the more complicated shapes with a higher contrast than in Figure 20. The models are given at frequency $\omega/(2\pi) = 1$.

[1], such that once the matrix factorization is computed, the numerical cost of having several sources (i.e., multiple right-hand sides in the linear system) is drastically mitigated, motivating the use of a direct solver instead of an iterative one.

Our numerical experiments have been carried out on the Vienna Scientific Cluster VSC-4², using 48 cores. For the reconstructions of Figure 14, Figure 15, Figure 18 and Figure 19, the size of the computational domain is 40×40 , with about 350 000 degrees of freedom. Using single-frequency data, 50 iterations are performed in Algorithm 1 and the total computational time is of about 40 min. In the case of multiple frequencies, we have a total of 120 iterations and the computational time is of about 1 h 45 min.

Computational cost of Born and Rytov approximations. The conjugate gradient method used in the inverse NDFT requires in each iteration step the evaluation of an NDFT Equation 6.6 and its adjoint. We utilize the nonequispaced fast Fourier transform (NFFT) algorithm [35], implemented in the open-source software library `nfft` [34], which can compute an NDFT in $\mathcal{O}(N^2 \log N + M)$ arithmetic operations, which is considerably less than the $\mathcal{O}(N^2 M)$ operations of a straightforward implementation of Equation 6.6.

²<https://vsc.ac.at/>

The numerical simulations of [subsection 7.2.2](#) have been carried out on a 4-core Intel Core i5-6500 processor. We used 12 iterations of the conjugate gradient method and noted that the reconstruction quality hardly benefits from a higher number of iterations. The reconstruction of an image took about one second, with a grid size 720×720 of f and 200×100 data points of u for each frequency. Therefore, the numerical computation of the Born and Rytov approximations is much faster than the FWI.

8. CONCLUSION

We study the imaging problem for diffraction tomography, where wave measurements are used to quantitatively reconstruct the physical properties, i.e., the refractive index. The forward operator that describes the wave propagation corresponds with the Helmholtz equation, which, under the assumption of small background perturbations, can be represented via the Born and Rytov approximations.

Firstly, we have compared different forward models in terms of the resulting measured data u . It highlights that, even in the case of a small circular object, the Born approximation is not entirely accurate to represent the total wave field given by the Helmholtz equation. In addition, the source that initiates the phenomenon (e.g., a point source located very far from the object, or simultaneous point source along a line), also plays an important role as it changes the resulting signals, hence leading to systematic differences depending on the choice of forward model. We found that the line source model approximates the plane wave pretty well.

Secondly, we have carried out the reconstruction using data from the total field u^{tot} , and compared the efficiency of the Full Waveform Inversion method (FWI) with that of the Born and Rytov approximations. FWI works directly with the Helmholtz problem, [Equation 3.12](#), hence giving a robust approach that can be implemented in all configurations, however at the cost of possibly intensive computations. On the other hand, the Born and Rytov are computationally cheap, but lack accuracy when the object is too large or when the contrast is too strong. We have also noted that the Rytov approximation gives better results than the Born one. Furthermore, for all reconstruction methods, we have shown that using data of multiple frequencies allows to improve the robustness of the reconstruction by providing information on multiple wavelengths.

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