## Imaging-SHG Readme

Kui Ren\* Nathan Soedjak<sup>†</sup>

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Overview. This is a MATLAB code for solving an inverse problem in quantitative thermoacoustic tomography in the presence of second harmonic generation (SHG), based on the Helmholtz model for wave propagation. This code accompanies the paper [1], where theoretical results on the inverse problem may also be found. All of the numerical experiments in that paper can be reproduced by simply running the appropriate example file (e.g., Experiment-I\_gamma.m).

**Mathematical Model.** The mathematical model is the following boundary value problem:

$$\begin{array}{rclcrcl} \Delta u + k^2 (1+\eta) u + i k \sigma u & = & 0, & \text{in } \Omega \\ \Delta v + (2k)^2 (1+\eta) v + i 2k \sigma v & = & -(2k)^2 \gamma u^2, & \text{in } \Omega \\ u = g, & v + i 2k \boldsymbol{\nu} \cdot \nabla v & = & 0, & \text{on } \partial \Omega. \end{array}$$

**The Data.** The data we measure is encoded in the map:

$$\Lambda_{\eta,\sigma,\gamma,\Gamma}: g \mapsto H = \Gamma\sigma(|u|^2 + |v|^2).$$

**The Objective.** The objective here is to reconstruct a subset of the four coefficients  $\eta, \sigma, \gamma, \Gamma$  (possibly all) from the data. Theoretically, we know from [1] that we have uniqueness and stability results for this inverse problem.

The Algorithm. We assume that we collect data from  $N_s$  illuminations  $\{g_j\}_{j=1}^{N_s}$ . The system for source  $g_j$  is

$$\begin{array}{rclcrcl} \Delta u_j + k^2 (1+\eta) u_j + ik\sigma u_j & = & 0, & \text{in } \Omega \\ \Delta v_j + (2k)^2 (1+\eta) v_j + i2k\sigma v_j & = & -(2k)^2 \gamma u_j^2, & \text{in } \Omega \\ u_j = g_j, & v_j + i2k \boldsymbol{\nu} \cdot \nabla v_j & = & 0, & \text{on } \partial \Omega. \end{array}$$

<sup>\*</sup>Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027; kr2002@columbia.edu

<sup>&</sup>lt;sup>†</sup>Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027; ns3572@columbia.edu

The corresponding data is  $H_j = \Lambda_{\eta,\sigma,\gamma,\Gamma}(g_j) = \Gamma\sigma(|u_j|^2 + |v_j|^2)$ . We therefore collect the data  $\{(g_j,H_j)\}_{j=1}^{N_s}$ .

Before solving the inverse problem using using standard least-squares optimization, we split into two cases.

 $\Gamma$  is known. In this case, we minimize the usual least-squares functional

$$\Phi(\eta, \sigma, \gamma) := \frac{1}{2} \sum_{j=1}^{N_s} \|\Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\eta} \|\nabla \eta\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\sigma} \|\nabla \sigma\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\gamma} \|\nabla \gamma\|_{L^2(\Omega)}^2.$$

$$\tag{1}$$

 $\Gamma$  is unknown. Due to the fact that  $\Gamma$  only appears in the measurement, not the PDE model, a naive least-squares minimization formulation like the one above will lead to unbalanced sensitivity between  $\Gamma$  and the rest of the parameters. Hence we instead take a two-step reconstruction approach. In the first step, we use the ratio between measurements to eliminate  $\Gamma$ . That is, we minimize the functional

$$\Psi(\eta, \sigma, \gamma) := \frac{1}{2} \sum_{j=2}^{N_s} \left\| \frac{|u_j|^2 + |v_j|^2}{|u_1|^2 + |v_1|^2} - \frac{H_j}{H_1} \right\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\eta} \|\nabla \eta\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\sigma} \|\nabla \sigma\|_{L^2(\Omega)}^2 + \frac{1}{2} \beta_{\gamma} \|\nabla \gamma\|_{L^2(\Omega)}^2.$$

$$\tag{2}$$

It is clear that  $\Psi$  only depends on  $\eta$ ,  $\sigma$ , and  $\gamma$ , not  $\Gamma$ . Once  $\eta$ ,  $\sigma$ , and  $\gamma$  are reconstructed, we can reconstruct  $\Gamma$  as

$$\Gamma = \frac{1}{N_s} \sum_{j=1}^{N_s} \frac{H_j}{\sigma(|u_j|^2 + |v_j|^2)}.$$

The Gradient Calculation. We use the adjoint state method to calculate the gradients of the objective functions  $\Phi$  and  $\Psi$ .

**Gradients of**  $\Phi$ . For  $1 \leq j \leq N_s$ , we introduce the adjoint equations

$$\Delta u_j^{(2)} + k^2 (1+\eta) u_j^{(2)} + ik\sigma u_j^{(2)} = -\Big[\Gamma\sigma(|u_j|^2 + |v_j|^2) - H_j\Big]\Gamma\sigma u_j^*, \text{ in } \Omega$$
 
$$u_j^{(2)} = 0, \qquad \text{on } \partial\Omega$$
 
$$\Delta v_j^{(2)} + (2k)^2 (1+\eta) v_j^{(2)} + i2k\sigma v_j^{(2)} = -\Big[\Gamma\sigma(|u_j|^2 + |v_j|^2) - H_j\Big]\Gamma\sigma v_j^*, \text{ in } \Omega$$
 
$$v_j^{(2)} + i2k\boldsymbol{\nu} \cdot \nabla v_j^{(2)} = 0, \qquad \text{on } \partial\Omega$$
 
$$\Delta u_j^{(3)} + k^2 (1+\eta) u_j^{(3)} + ik\sigma u_j^{(3)} = -2(2k)^2 \gamma u_j v_j^{(2)}, \text{ in } \Omega$$
 
$$u_j^{(3)} = 0, \qquad \text{on } \partial\Omega .$$

It is then straightforward to verify that the Fréchet derivatives of  $\Phi$  with respect to  $\eta$ ,  $\sigma$  and  $\gamma$  are given by

$$\Phi'_{\eta}(\eta, \sigma, \gamma)[\delta \eta] = \sum_{j=1}^{N_s} \int_{\Omega} 2k^2 \Re(u_j u_j^{(2)} + 4v_j v_j^{(2)} + u_j u_j^{(3)}) \delta \eta \, d\mathbf{x} - \beta_{\eta} \int_{\Omega} (\Delta \eta) \delta \eta \, d\mathbf{x} + \beta_{\eta} \int_{\partial \Omega} \frac{\partial \eta}{\partial \nu} \delta \eta \, dS,$$

$$\Phi'_{\sigma}(\eta, \sigma, \gamma)[\delta \sigma] = \sum_{j=1}^{N_s} \int_{\Omega} \left[ \left[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \right] \Gamma(|u_j|^2 + |v_j|^2) + 2k \Re(i u_j u_j^{(2)} + 2i v_j v_j^{(2)} + i u_j u_j^{(3)}) \right] \delta \sigma \, d\mathbf{x}$$

$$- \beta_{\sigma} \int_{\Omega} (\Delta \sigma) \delta \sigma \, d\mathbf{x} + \beta_{\sigma} \int_{\partial \Omega} \frac{\partial \sigma}{\partial \nu} \delta \sigma \, dS,$$

$$\Phi'_{\gamma}(\eta, \sigma, \gamma)[\delta \gamma] = \sum_{j=1}^{N_s} \int_{\Omega} 2(2k)^2 \Re(u_j^2 v_j^{(2)}) \delta \gamma \, d\mathbf{x} - \beta_{\gamma} \int_{\Omega} (\Delta \gamma) \delta \gamma \, d\mathbf{x} + \beta_{\gamma} \int_{\partial \Omega} \frac{\partial \gamma}{\partial \nu} \delta \gamma \, dS.$$

**Gradients of**  $\Psi$ **.** For the Fréchet derivatives of  $\Psi$ , we introduce the adjoint equations

$$\begin{array}{rclcrcl} \Delta u_j^{(2)} + k^2 (1 + \eta) u_j^{(2)} + ik\sigma u_j^{(2)} & = & - \Big[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \Big] \frac{u_j^*}{|u_1|^2 + |v_1|^2}, & \text{in} & \Omega \\ & u_j^{(2)} & = & 0, & & & \text{on} & \partial \Omega \\ \\ \Delta u_1^{(2)} + k^2 (1 + \eta) u_1^{(2)} + ik\sigma u_1^{(2)} & = & - \Big[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \Big] \frac{(|u_j|^2 + |v_j|^2) u_1^*}{(|u_1|^2 + |v_1|^2)^2}, & \text{in} & \Omega \\ & u_1^{(2)} & = & 0, & & & \text{on} & \partial \Omega \\ \\ \Delta v_j^{(2)} + (2k)^2 (1 + \eta) v_j^{(2)} + i2k\sigma v_j^{(2)} & = & - \Big[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \Big] \frac{v_j^*}{|u_1|^2 + |v_1|^2}, & \text{in} & \Omega \\ & v_j^{(2)} + i2k \boldsymbol{\nu} \cdot \nabla v_j^{(2)} & = & 0, & & \text{on} & \partial \Omega \\ \\ \Delta v_1^{(2)} + (2k)^2 (1 + \eta) v_1^{(2)} + i2k\sigma v_1^{(2)} & = & \Big[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \Big] \frac{(|u_j|^2 + |v_j|^2) v_1^*}{(|u_1|^2 + |v_1|^2)^2}, & \text{in} & \Omega \\ & v_1^{(2)} + i2k \boldsymbol{\nu} \cdot \nabla v_1^{(2)} & = & 0, & & \text{on} & \partial \Omega \\ \\ \Delta u_j^{(3)} + k^2 (1 + \eta) u_j^{(3)} + ik\sigma u_j^{(3)} & = & -2(2k)^2 \gamma u_j v_j^{(2)}, & \text{in} & \Omega \\ & u_j^{(2)} & = & 0, & & \text{on} & \partial \Omega \\ \\ \Delta u_1^{(3)} + k^2 (1 + \eta) u_1^{(3)} + ik\sigma u_1^{(3)} & = & -2(2k)^2 \gamma u_1 v_1^{(2)}, & \text{in} & \Omega \\ & u_1^{(2)} & = & 0, & & \text{on} & \partial \Omega. \\ \end{array}$$

It is then straightforward to verify that the Fréchet derivatives of  $\Psi$  with respect to  $\eta$ ,  $\sigma$  and  $\gamma$  are given by

$$\begin{split} \Psi_{\eta}'(\eta,\sigma,\gamma)[\delta\eta] &= \sum_{j=1}^{N_s} \int_{\Omega} 2k^2 \Re(u_j u_j^{(2)} + 4v_j v_j^{(2)} + u_j u_j^{(3)} + u_1 u_1^{(2)} + 4v_1 v_1^{(2)} + u_1 u_1^{(3)}) \delta\eta \, d\mathbf{x} \\ &- \beta_{\eta} \int_{\Omega} (\Delta \eta) \delta\eta \, dx + \beta_{\eta} \int_{\partial \Omega} \frac{\partial \eta}{\partial \nu} \delta\eta \, dS, \\ \Psi_{\sigma}'(\eta,\sigma,\gamma)[\delta\sigma] &= \sum_{j=1}^{N_s} \int_{\Omega} \left[ \left[ \Gamma \sigma(|u_j|^2 + |v_j|^2) - H_j \right] \Gamma(|u_j|^2 + |v_j|^2) \right. \\ &+ 2k \Re(iu_j u_j^{(2)} + 2iv_j v_j^{(2)} + iu_j u_j^{(3)} + iu_1 u_1^{(2)} + 2iv_1 v_1^{(2)} + iu_1 u_1^{(3)}) \right] \delta\sigma \, d\mathbf{x} \\ &- \beta_{\sigma} \int_{\Omega} (\Delta \sigma) \delta\sigma \, dx + \beta_{\sigma} \int_{\partial \Omega} \frac{\partial \sigma}{\partial \nu} \delta\sigma \, dS, \\ \Psi_{\gamma}'(\eta,\sigma,\gamma)[\delta\gamma] &= \sum_{j=1}^{N_s} \int_{\Omega} 2(2k)^2 \Re(u_j^2 v_j^{(2)} + u_1^2 v_1^{(2)}) \delta\gamma \, d\mathbf{x} \\ &- \beta_{\gamma} \int_{\Omega} (\Delta \gamma) \delta\gamma \, dx + \beta_{\gamma} \int_{\partial \Omega} \frac{\partial \gamma}{\partial \nu} \delta\gamma \, dS. \end{split}$$

The Forward/Adjoint Solver. In the minimization process, we solve the forward and adjoint problems with a standard  $P_1$  finite element solver of the MATLAB PDE Toolbox.

## References

[1] K. Ren and N. Soedjak, Recovering coefficients in a system of semilinear Helmholtz equations from internal data, (in preparation).