Data-Compatible T-Matrix Completion (DCTMC)

A new numerical method for solving nonlinear inverse problems

Howard W. Levinson

Department of Mathematics, University of Pennsylvania and University of Michigan (Sept 2016-)

Vadim A. Markel

Institut Fresnel, University of Aix-Marseille

Dept. of Radiology, University of Pennsylvania (on leave)

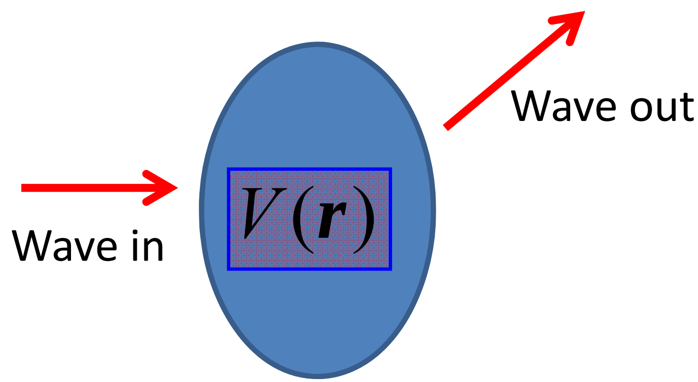
Motivation 1: Local Minima

$$F[V] = \Phi$$

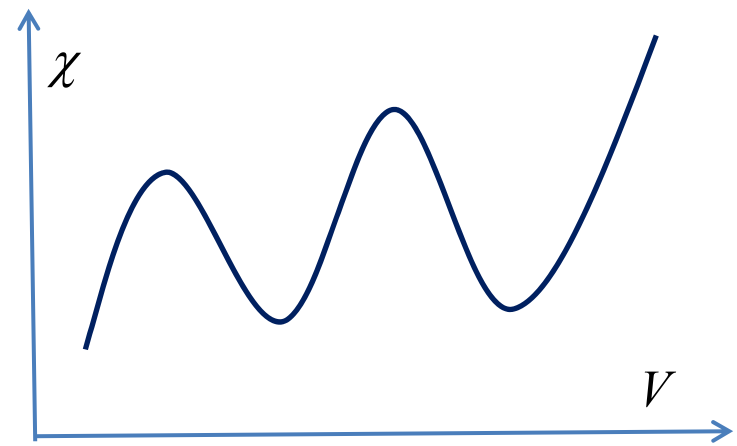
Theoretical model

Object

Data

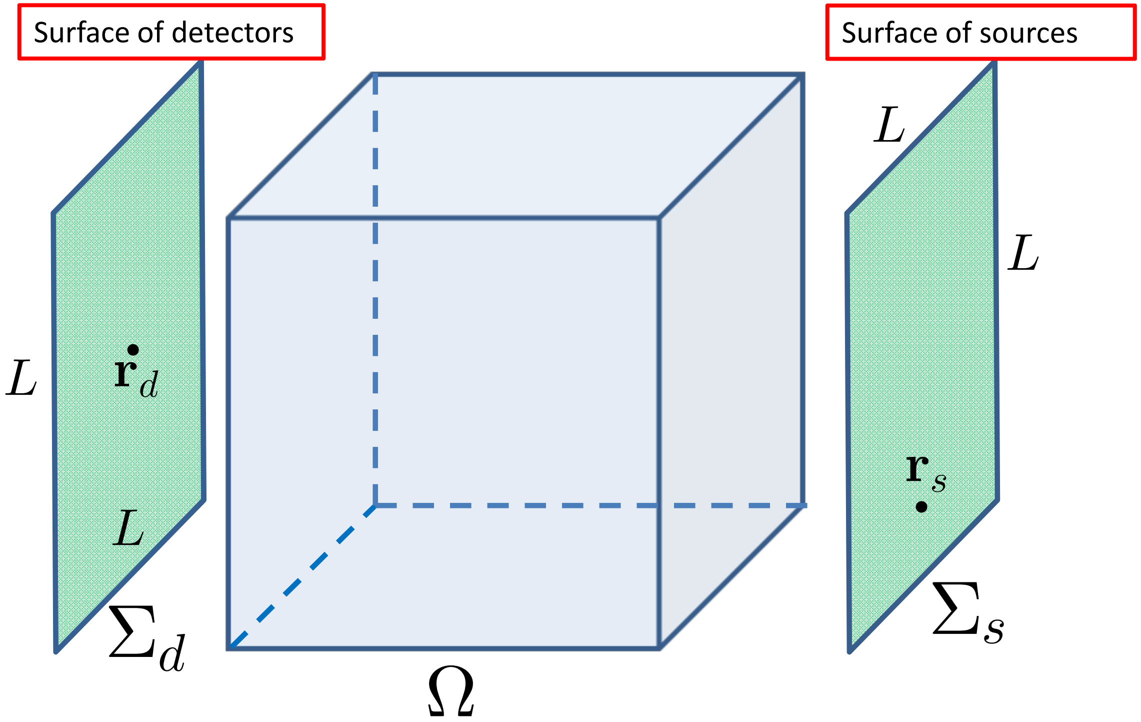


$$\chi = D\left[F[V] - \Phi\right] + \lambda^2 D\left[\Phi - \Phi_{\text{guess}}\right]$$



Motivation 2: Large Data Sets

$$\chi = D\left[F[V] - \Phi\right] + \lambda^2 D\left[\Phi - \Phi_{\text{guess}}\right]$$



$$N_s = L^2$$

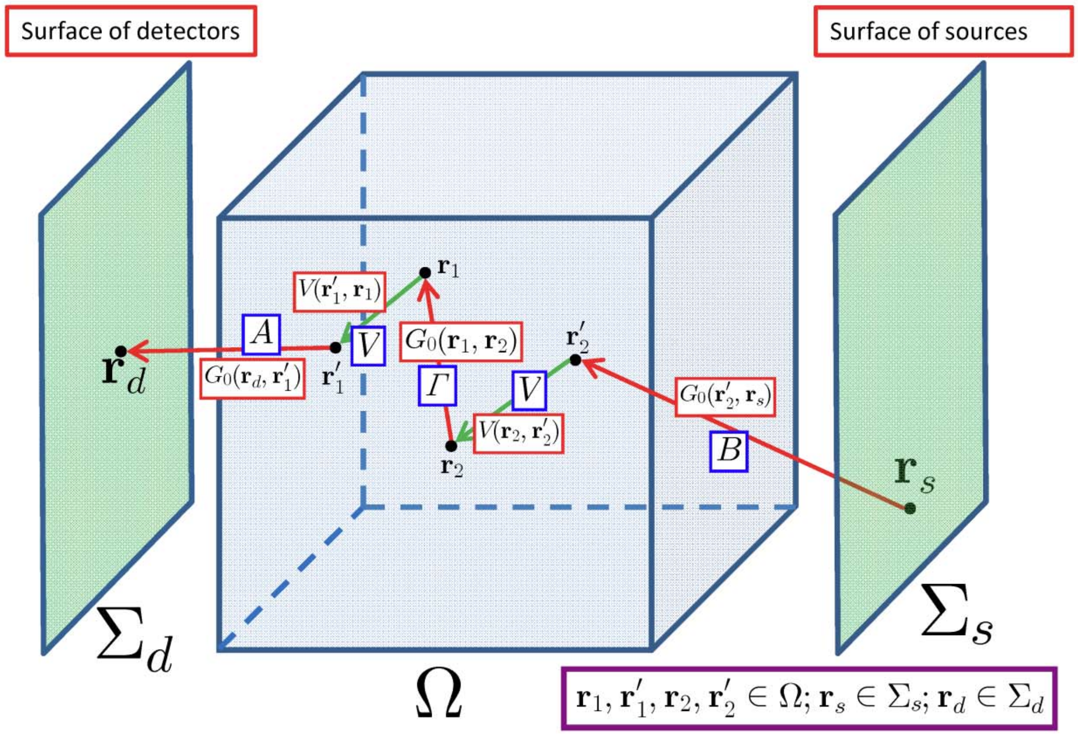
$$N_d = L^2$$

$$N = N_s N_d = L^4$$

Algebraic Structure of the Inverse Problem

$A(I - V\Gamma)^{-1} VB = \Phi$ ⟸ Every variable is a matrix!

A, B, Γ -- different restrictions of the same unperturbed Green's function G_0



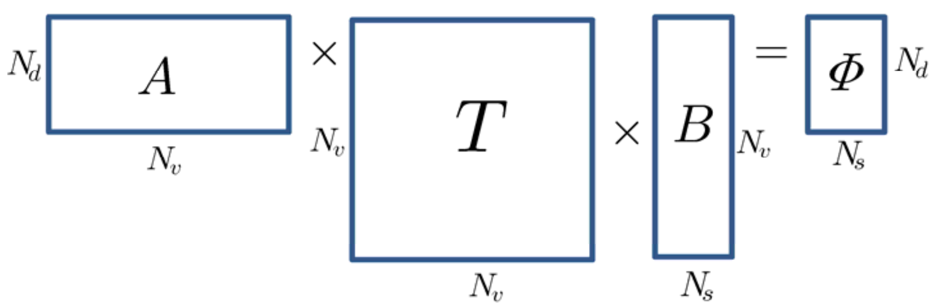
$$A(I - V\Gamma)^{-1}VB = \Phi$$

$$T[V] = (I - V\Gamma)^{-1}V$$

$$V[T] = (I + TV)^{-1}T$$

Let us view T-matrix as the fundamental unknown and use the one-to-one Correspondence between *T* and *V*

$$ATB = \Phi$$



Main Idea

(1) First, we define a class of kernels $V(\mathbf{r}, \mathbf{r}')$ that are compatible with the data. This is the only instance when the data are used, and it turns out that the size of the data set is not a limiting factor for this step.

(2) Then we iteratively reduce the off-diagonal norm of $V(\mathbf{r}, \mathbf{r}')$ while making sure that $V(\mathbf{r}, \mathbf{r}')$ remains within the class of "data-compatible" kernels.

(3) Once the ratio of the off-diagonal and diagonal norms of $V(\mathbf{r}, \mathbf{r}')$ is deemed sufficiently small, we compute $\sigma(\mathbf{r}) = \int V(\mathbf{r}, \mathbf{r}') d^3 r'$. This gives an approximate numerical solution to the nonlinear ISP.

The Experimental T-Matrix

$$A=\sum_{\mu=1}^{N_d}\sigma_\mu^A\left|f_\mu^A\right\rangle\left\langle g_\mu^A\right|$$

$$B=\sum_{\mu=1}^{N_s}\sigma_\mu^B\left|f_\mu^B\right\rangle\left\langle g_\mu^B\right|$$

$$ATB=\Phi$$

$$\sigma_\mu^A\sigma_\nu^B\tilde{T}_{\mu\nu}=\tilde{\Phi}_{\mu\nu}\ ,\quad 1\le\mu\le N_d,\quad 1\le\nu\le N_s$$

$$\tilde{\Phi}_{\mu\nu}=\left\langle f_\mu^A\right|\Phi\left|g_\nu^B\right\rangle,\ 1\le\mu\le N_d\ ,\ 1\le\nu\le N_s$$

$$\tilde{T}_{\mu\nu}=\left\langle g_\mu^A\right|\Phi\left|f_\nu^B\right\rangle,\ 1\le\mu,\nu\le N_\nu$$

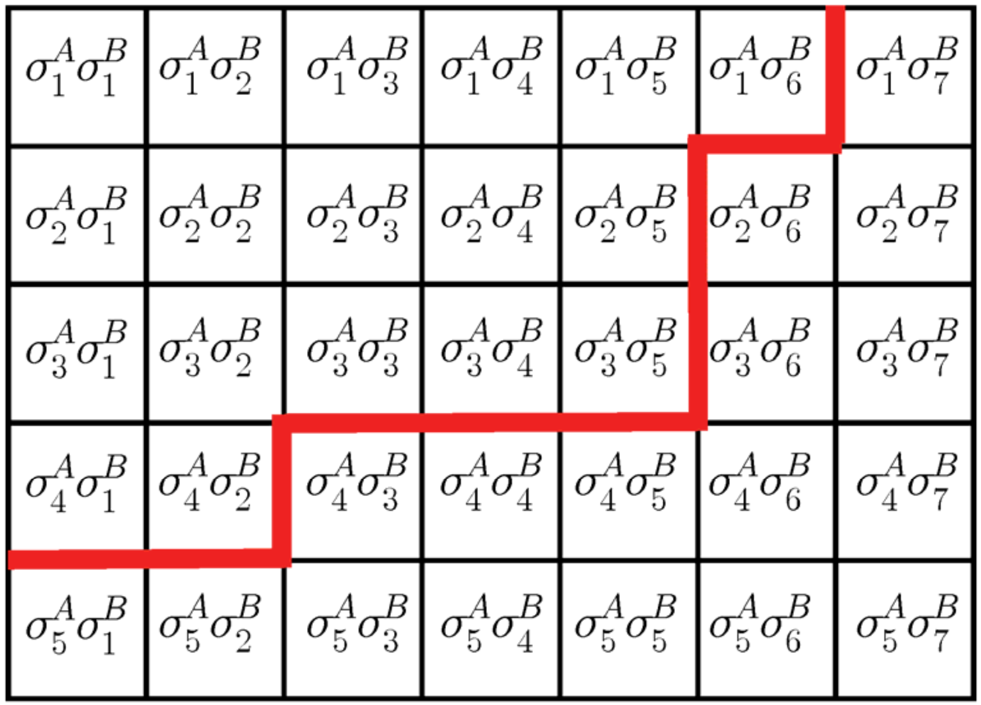
$$\tilde{T}=R_A^*TR_B=\mathscr{R}[T]\ ,\quad T=\mathscr{R}^{-1}[\tilde{T}]$$

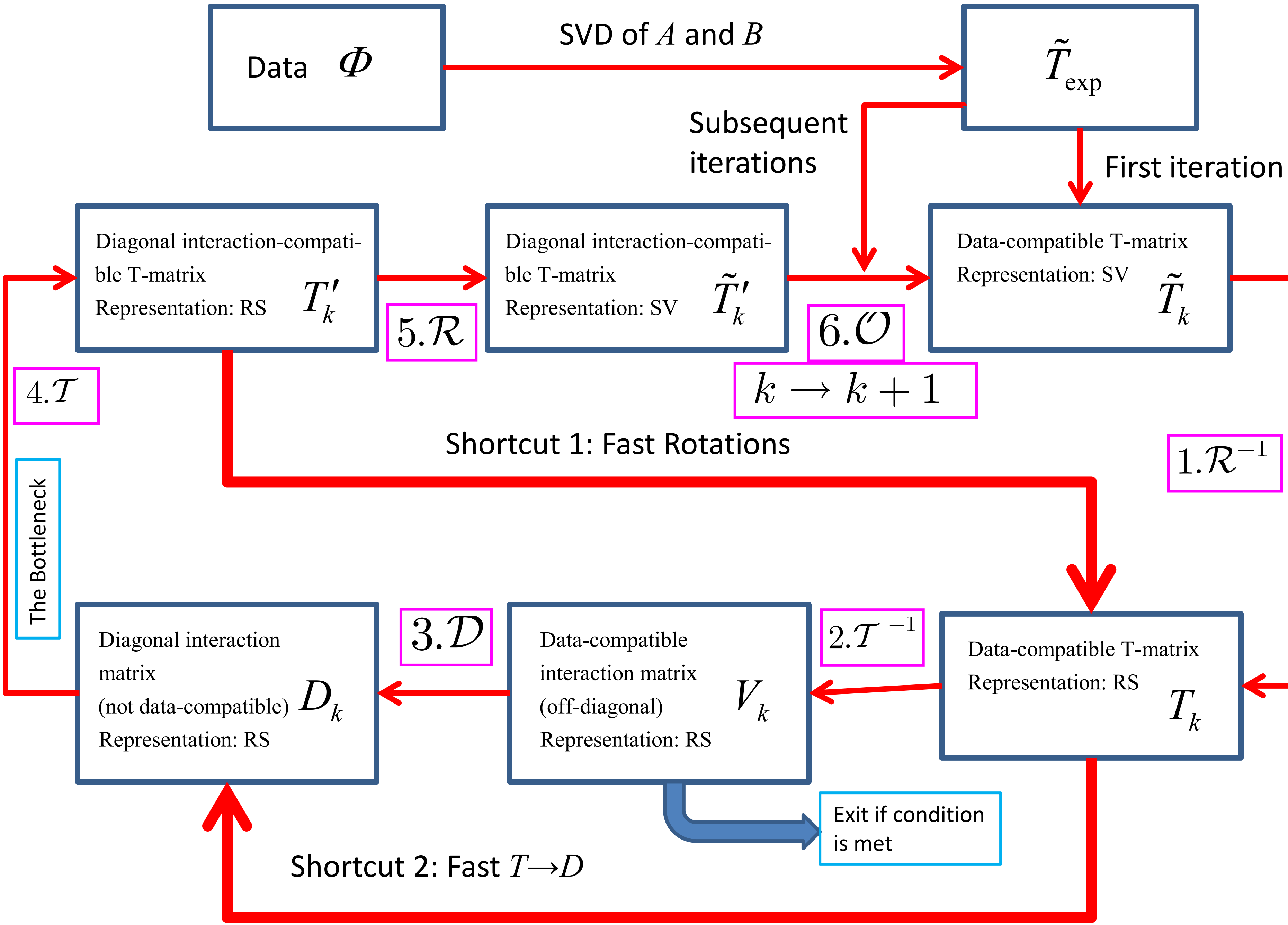
$$\tilde{T}_{\mu\nu}=\begin{cases}\dfrac{1}{\sigma_\mu^A\sigma_\nu^B}\tilde{\Phi}_{\mu\nu}\ , & \text{if}\quad \sigma_\mu^A\sigma_\nu^B>\varepsilon^2\\ \text{Unknown}\ , & \text{otherwise}\end{cases}$$

$$\tilde{T}=\begin{bmatrix}\dfrac{\tilde{\Phi}_{\mu\nu}}{\sigma_\mu^A\sigma_\nu^B}\ (M_A\times M_B) & \text{UNKNOWN}\\ \text{UNKNOWN} & \text{UNKNOWN}\\ \text{UNKNOWN} & \text{UNKNOWN}\end{bmatrix}$$

$$\tilde{T}_{\exp}=\begin{bmatrix}\dfrac{\tilde{\Phi}_{\mu\nu}}{\sigma_\mu^A\sigma_\nu^B}\ (M_A\times M_B) & 0\\ 0 & 0\end{bmatrix}$$

$$T_{\exp}=A^+\Phi B^+$$


$\sigma_1^A\sigma_1^B$ $\sigma_1^A\sigma_2^B$ $\sigma_1^A\sigma_3^B$ $\sigma_1^A\sigma_4^B$ $\sigma_1^A\sigma_5^B$ $\sigma_1^A\sigma_6^B$ $\sigma_1^A\sigma_7^B$
$\sigma_2^A\sigma_1^B$ $\sigma_2^A\sigma_2^B$ $\sigma_2^A\sigma_3^B$ $\sigma_2^A\sigma_4^B$ $\sigma_2^A\sigma_5^B$ $\sigma_2^A\sigma_6^B$ $\sigma_2^A\sigma_7^B$
$\sigma_3^A\sigma_1^B$ $\sigma_3^A\sigma_2^B$ $\sigma_3^A\sigma_3^B$ $\sigma_3^A\sigma_4^B$ $\sigma_3^A\sigma_5^B$ $\sigma_3^A\sigma_6^B$ $\sigma_3^A\sigma_7^B$
$\sigma_4^A\sigma_1^B$ $\sigma_4^A\sigma_2^B$ $\sigma_4^A\sigma_3^B$ $\sigma_4^A\sigma_4^B$ $\sigma_4^A\sigma_5^B$ $\sigma_4^A\sigma_6^B$ $\sigma_4^A\sigma_7^B$
$\sigma_5^A\sigma_1^B$ $\sigma_5^A\sigma_2^B$ $\sigma_5^A\sigma_3^B$ $\sigma_5^A\sigma_4^B$ $\sigma_5^A\sigma_5^B$ $\sigma_5^A\sigma_6^B$ $\sigma_5^A\sigma_7^B$



Data Φ
SVD of A and B
$\tilde{T}_{\exp}$
Subsequent iterations
First iteration
Diagonal interaction-compatible T-matrix
Representation: RS T'_k
5.$\mathcal{R}$
Diagonal interaction-compatible T-matrix
Representation: SV $\tilde{T}'_k$
6.$\mathcal{O}$
$k \to k+1$
Data-compatible T-matrix
Representation: SV $\tilde{T}_k$
4.$\mathcal{T}$
Shortcut 1: Fast Rotations
1.$\mathcal{R}^{-1}$
The Bottleneck
Diagonal interaction matrix
(not data-compatible) D_k
Representation: RS
3.$\mathcal{D}$
Data-compatible interaction matrix
(off-diagonal) V_k
Representation: RS
2.$\mathcal{T}^{-1}$
Data-compatible T-matrix
Representation: RS T_k
Exit if condition is met
Shortcut 2: Fast $T \to D$

Computational Shortcut: Fast Rotations

$$5:\quad \tilde{T}'_k = \mathscr{R}[T'_k]$$

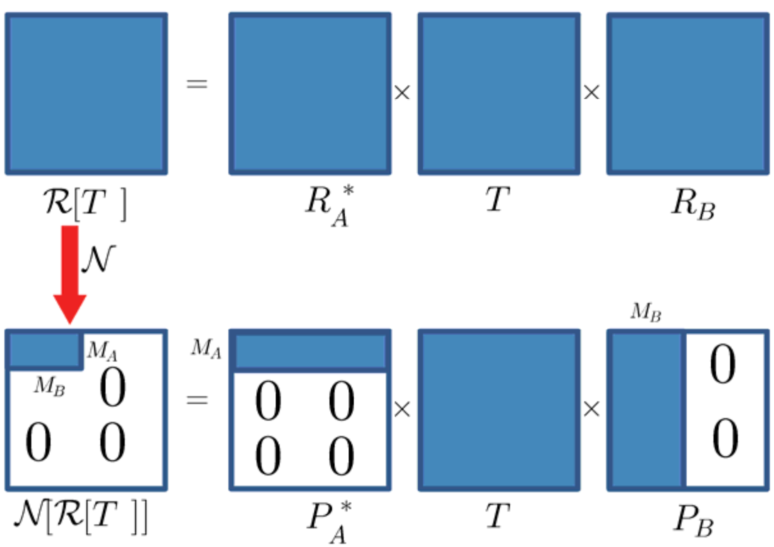
$$6:\quad \tilde{T}_{k+1} = \mathscr{O}[\tilde{T}'_k]$$

$$1:\quad T_{k+1} = \mathscr{R}^{-1}[\tilde{T}_{k+1}]$$

$$\mathscr{O}[\tilde{T}] = \mathscr{M}[\tilde{T}] + \tilde{T}_{\exp} = \tilde{T} - \mathscr{N}[\tilde{T}] + \tilde{T}_{\exp}$$

$$\mathscr{M}[\tilde{T}] + \mathscr{N}[\tilde{T}] = \tilde{T}$$

$$T_{k+1} = \mathscr{R}^{-1}[\mathscr{O}[\mathscr{R}[T'_k]]] = T'_k + T_{\exp} - \mathscr{R}^{-1}[\mathscr{N}[\mathscr{R}[T'_k]]]$$



$$\mathscr{R}^{-1}[\mathscr{N}[\mathscr{R}[T]]] = P_A(P_A^* T P_B)P_B^*$$

Operation of "Diagonalization" and Linear Reconstructions

$$D = \mathcal{D}[V]$$

$$D_{ij} = \delta_{ij} \sum_j w(r_{ij}) V_{ij}$$

If $w(r_{ij}) = \delta_{ij}$, we can analyse the algorithm in the linear regime:

$$\left| v_{k+1} \right\rangle = \left| v_{\exp} \right\rangle + (I - W) \left| v_k \right\rangle$$

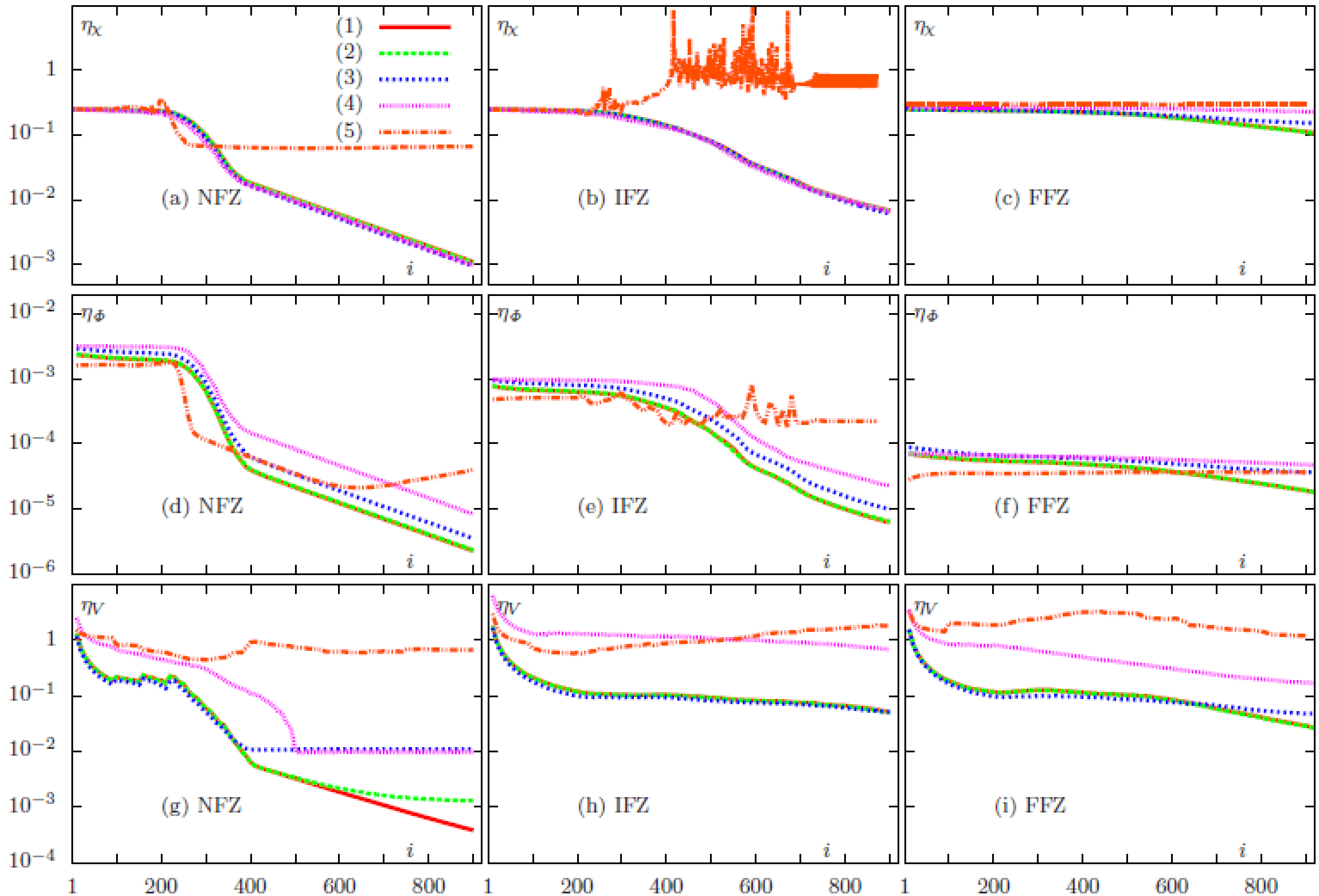
$$W_{ij} = (P_A^* P_A)_{ij} (P_B^* P_B)_{ji}$$

Vector containing the diagonal part of *V*

Fixed point: $\left| v_\infty \right\rangle = W^{-1} \left| v_{\exp} \right\rangle$

Tikhonov regularization: $W \to W + \lambda^2 I$

Practical tip: Richardson iteration is a very slow way to arrive at the linearized solution.
Use direct solver of CG to compute linearized solution and then use this result as an initial guess
For the nonlinear iterations.



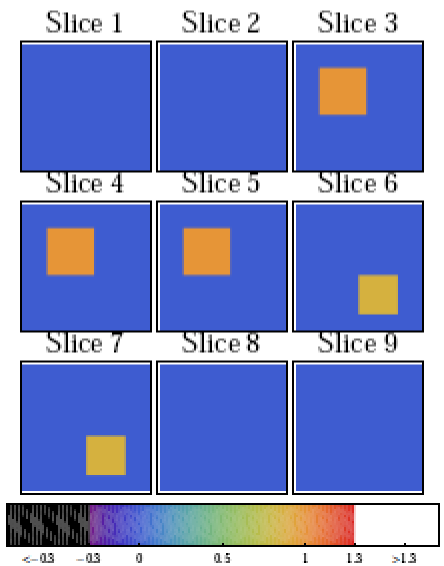
η_X
η_Φ
η_V
(1)
(2)
(3)
(4)
(5)
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
(a) NFZ
(b) IFZ
(c) FFZ
(d) NFZ
(e) IFZ
(f) FFZ
(g) NFZ
(h) IFZ
(i) FFZ
i
1
200
400
600
800

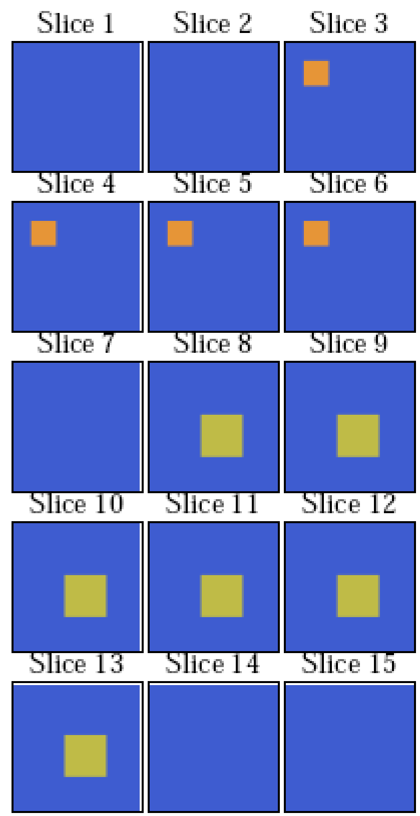
Diffraction tomography:

$$G_0(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp\left(ik\left|\boldsymbol{r}-\boldsymbol{r}'\right|\right)}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|}$$

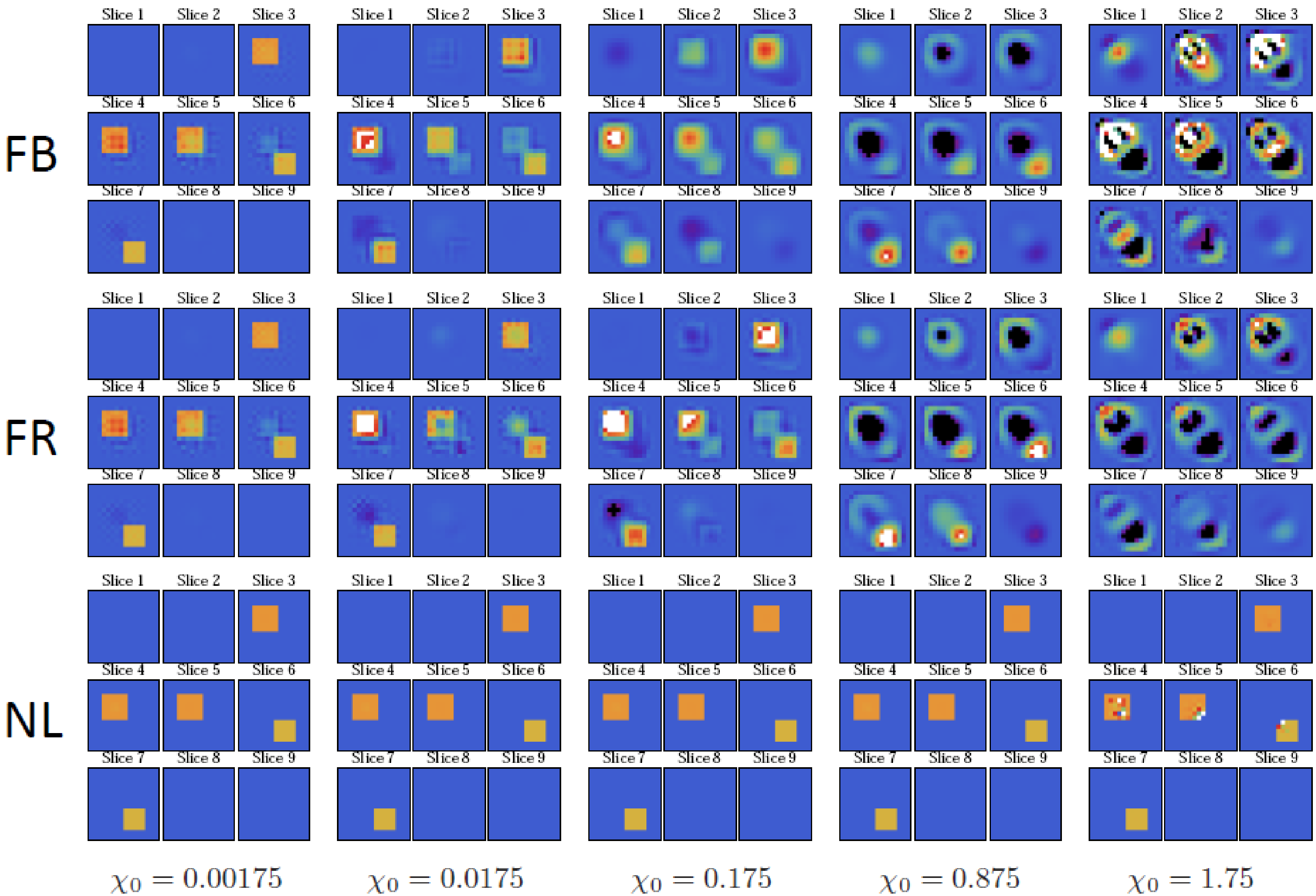
Contrast:

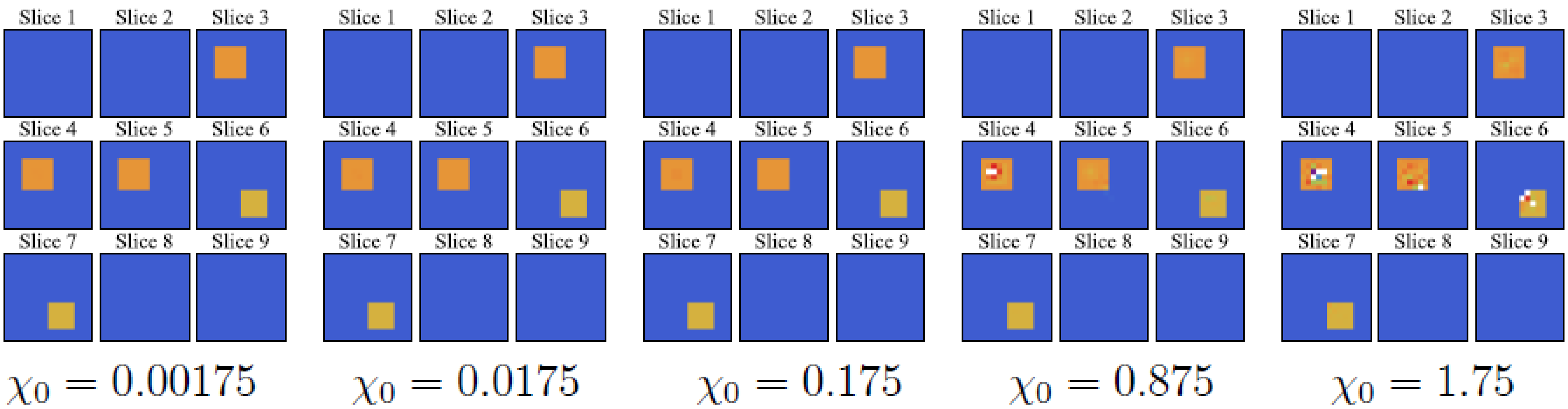
$$\chi(\boldsymbol{r}) = \frac{\varepsilon(\boldsymbol{r})-1}{4\pi}$$





No improvements: 900 iterations





With improvements: 70 iterations

- Start from linearized reconstruction (can be computed fast using our method)
- Use weighted summation to the diagonal for "force-diagonalization"
- Use reciprocity of source-detector pairs to improve symmetry of the experimental T-matrix
- Method starts to break down due to incorrect assignment of non-interacting voxels (this can be avoid altogether – not a problem of convergence)

Diffusion tomography:

$$G_0(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp\left(-k\left|\boldsymbol{r}-\boldsymbol{r}'\right|\right)}{\left|\boldsymbol{r}-\boldsymbol{r}'\right|}$$

Contrast:

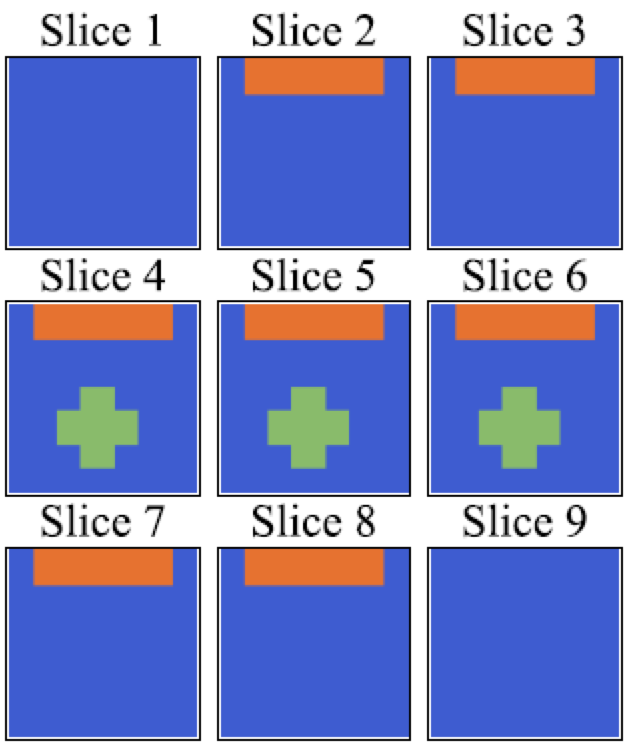
$$\delta\alpha(\boldsymbol{r}) = \frac{\alpha(\boldsymbol{r})-\alpha_0}{\alpha_0}$$

Optical depth:

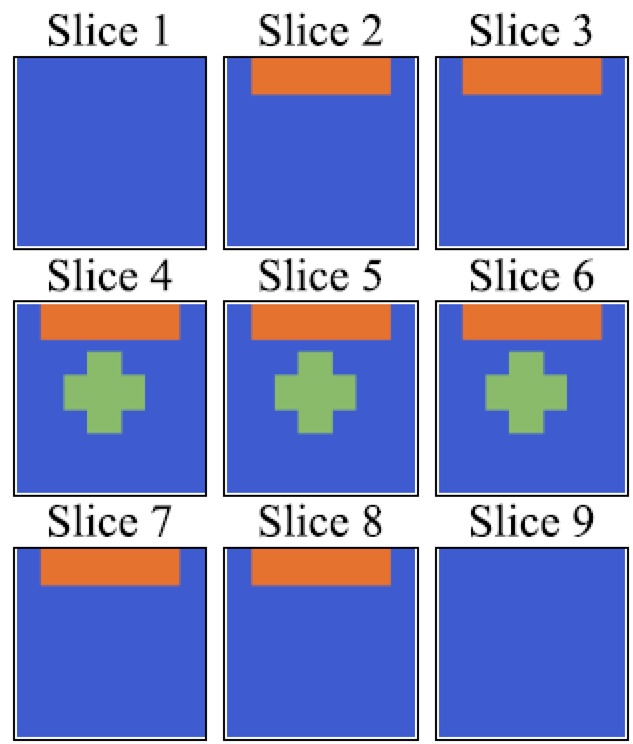
$$kL \approx 2$$

Noise:

2%

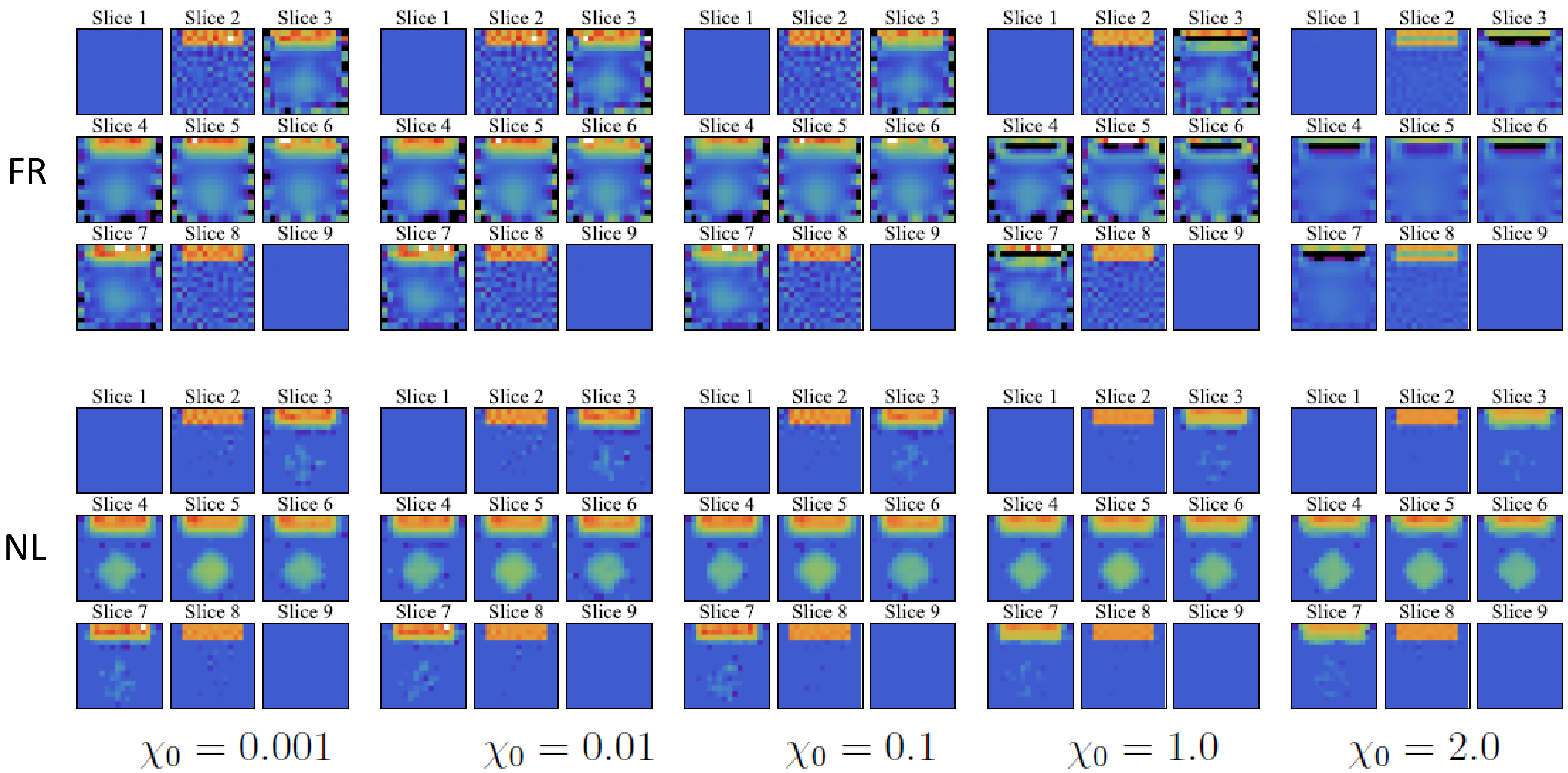


Target far

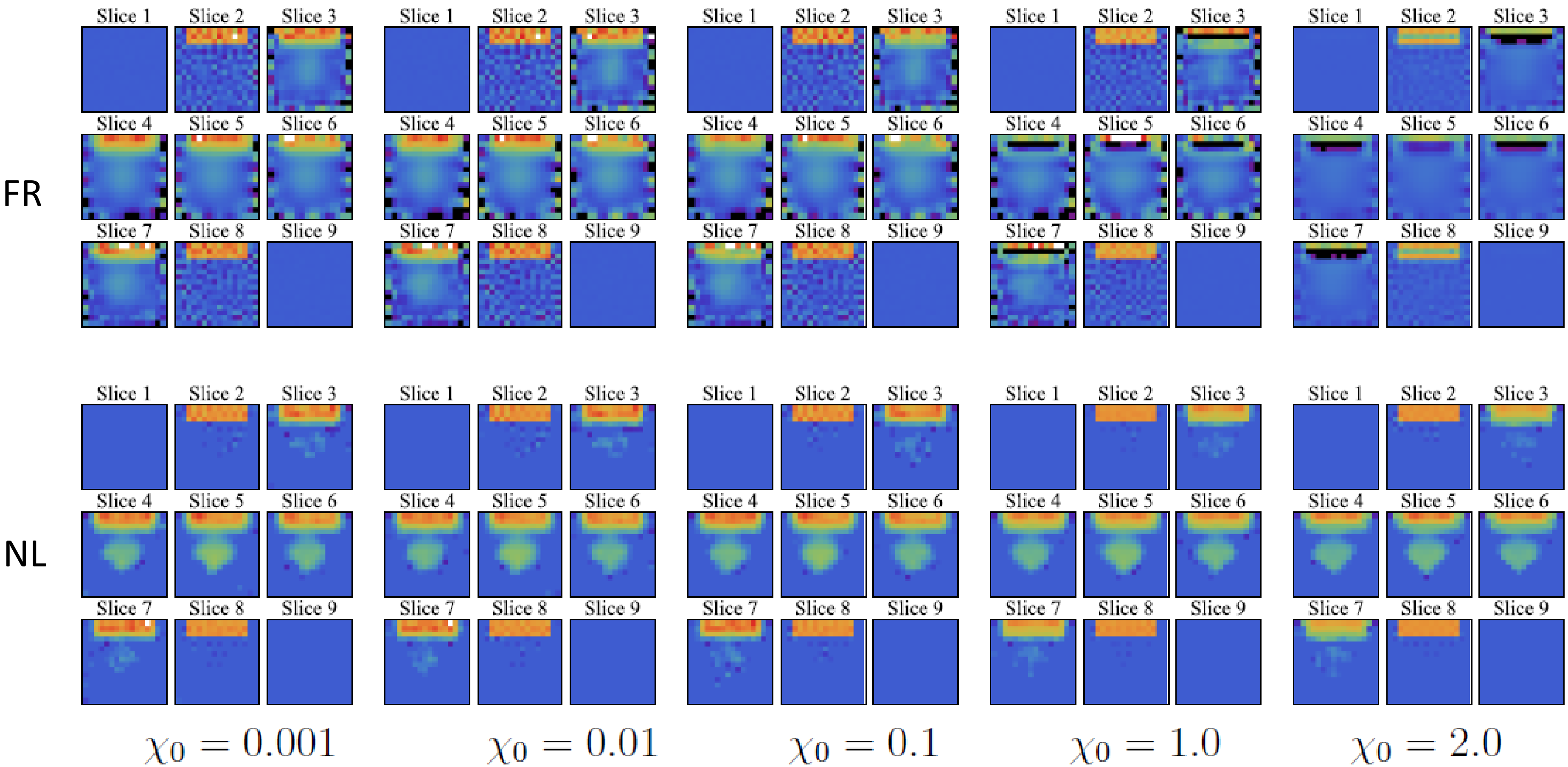


Target near

Target far

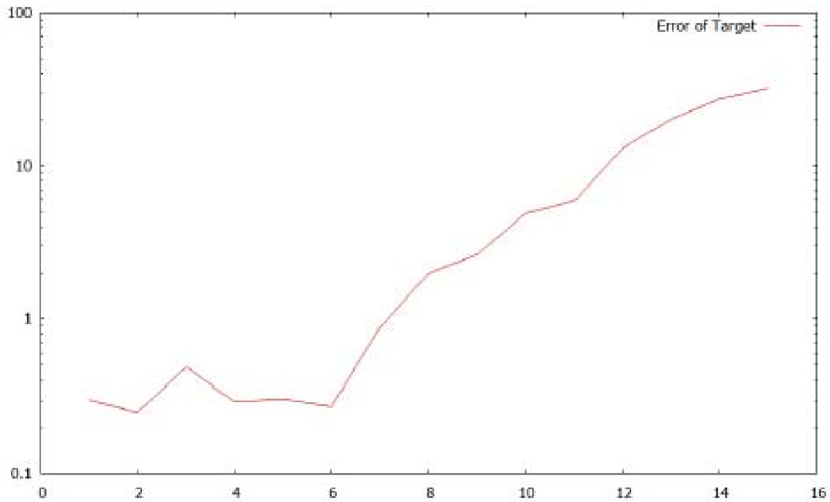

FR
NL
Slice 1
Slice 2
Slice 3
Slice 4
Slice 5
Slice 6
Slice 7
Slice 8
Slice 9
$\chi_0 = 0.001$
$\chi_0 = 0.01$
$\chi_0 = 0.1$
$\chi_0 = 1.0$
$\chi_0 = 2.0$

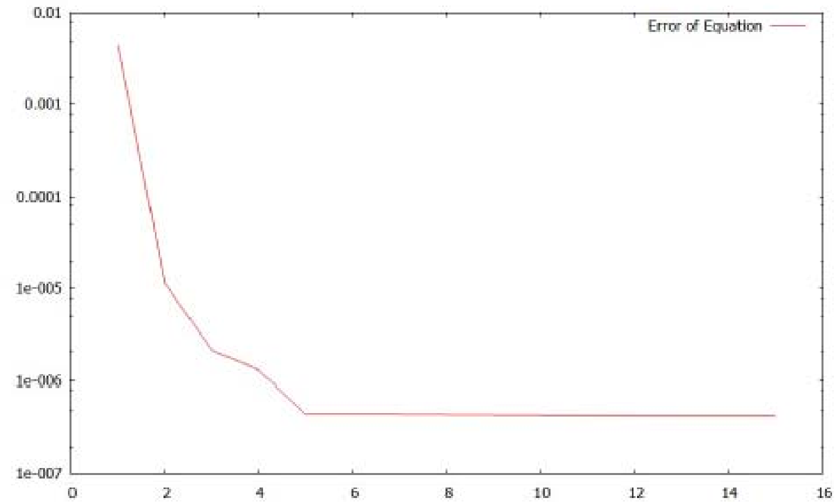
Target near



FR
NL
Slice 1
Slice 2
Slice 3
Slice 4
Slice 5
Slice 6
Slice 7
Slice 8
Slice 9
$\chi_0 = 0.001$
$\chi_0 = 0.01$
$\chi_0 = 0.1$
$\chi_0 = 1.0$
$\chi_0 = 2.0$

DCTMC works when Newton-Gauss fails (Convergence of Levenberg-Marquardt Iterations for the inverse diffraction problem, moderate contrast 0.0175)





CONCLUSIONS

- DCTMC works for nonlinear ISP with fairly strong nonlinearity
- DCTMC is, unfortunately, a complicated method: it requires many tweaks, attention to detail, and good programming to work
- As any other method, DCTMC breaks at some point. Not every nonlinear ISP can be solved!
- Please listen to Howard Levinson at 15:15 today (this room)

Preprints: **arXiv:1401.3319**, **arXiv:1505.06777**
Under consideration in Phys. Rev. E