Learned iterative solvers for the Helmholtz equation

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SLIM

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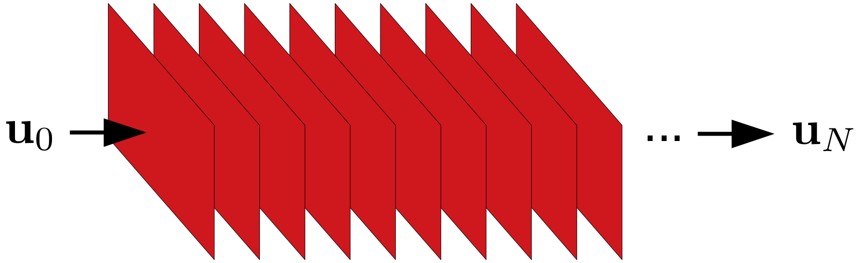
Neural nets and iterative schemes in computational maths

Structural likeness between **neural networks**...



$$\partial_t \mathbf{u}(t) = F(t, \mathbf{u}(t)) \qquad \mathbf{u}(t + \Delta t) \approx \mathbf{u}(t) + a(W(t) * \mathbf{u}(t) + b(t))$$

[Haber and Ruthotto, 2017]

Neural nets and iterative schemes in computational maths

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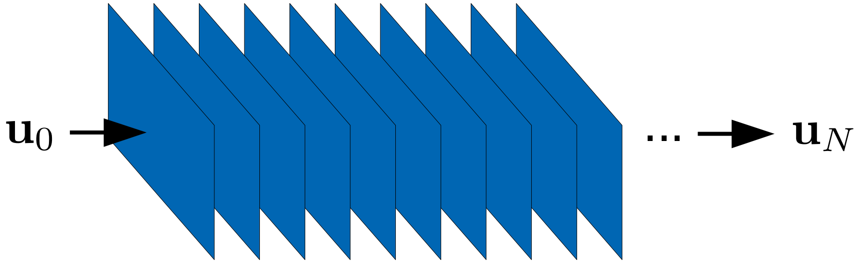

$$\mathbf{m}\,\partial_{tt}\mathbf{u} - \Delta\mathbf{u} = \mathbf{f} \qquad \mathbf{u}(t+\Delta t) \approx 2\mathbf{u}(t) - \mathbf{u}(t-\Delta t) + \Delta t^2/\mathbf{m}\,(\Delta\mathbf{u}(t) + \mathbf{f}(t))$$

...and iterative computational processes such as:

- **time stepping** in finite-differences [Siahkoohi et al., 2018]

Neural nets and iterative schemes in computational maths

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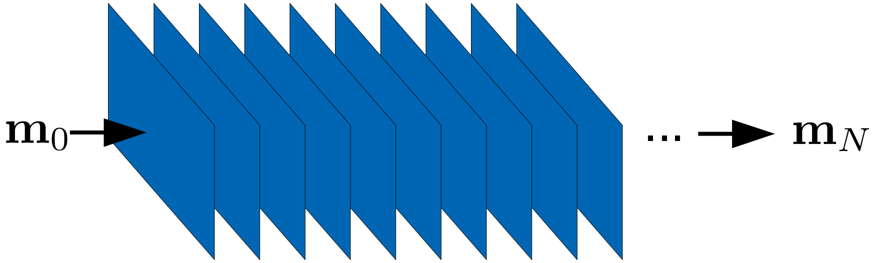


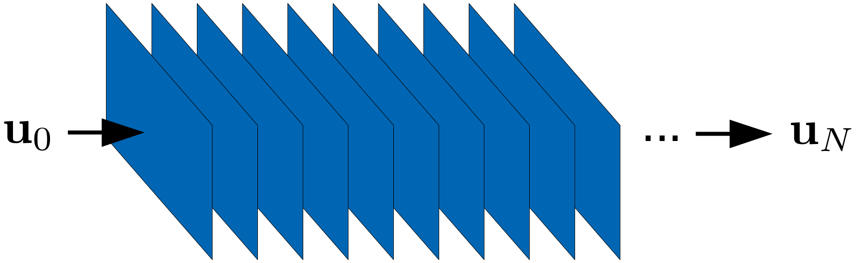
$\min_{\mathbf{m}} J(\mathbf{m}) \qquad \mathbf{m}_{i+1} = \mathbf{m}_i - \alpha \nabla_{\mathbf{m}_i} J$

...and iterative computational processes such as:

- nonlinear optimization in **inverse problems** [Adler and Öktem, 2017]

Neural nets and iterative schemes in computational maths

Structural likeness between **neural networks**...

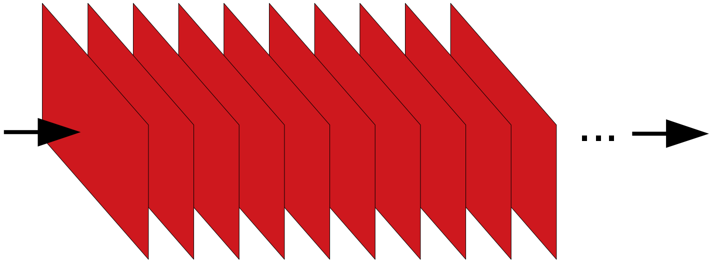


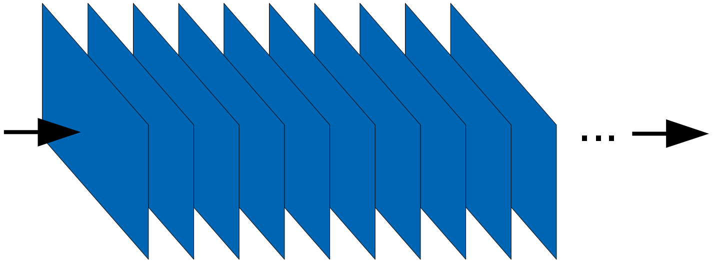
$$A\mathbf{u} = \mathbf{b} \qquad \mathbf{u}_{i+1} = \mathbf{u}_i + \sum_{j \leq i} \alpha_j \mathbf{r}_j$$

...and iterative computational processes such as:

- **iterative solvers** for linear systems (this talk: **Helmholtz** equation)

Neural nets and iterative schemes in computational maths





Neural nets:
generalizes according to *available data*, but potentially *cheaper*

Computational "nets":
general but *expensive*, pre-"trained" by first principles

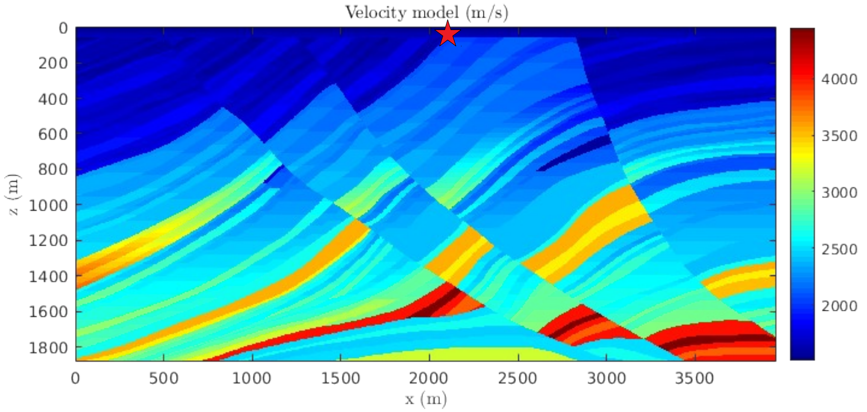
This work:
(neural net)-augmented physics/maths

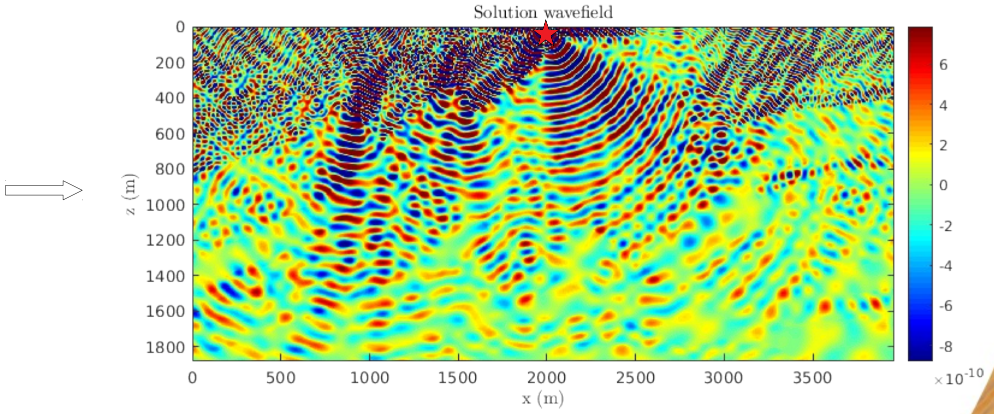
Helmholtz equation

Long-standing problem in frequency-domain **wave equation based imaging**:

- numerical solution of the **Helmholtz** equation (e.g., discretized by finite-differences):

$$H[\mathbf{m}] = -\omega^2 \mathbf{m} - \Delta, \qquad H[\mathbf{m}]\mathbf{u} = \mathbf{f}$$





Helmholtz equation: classical solution methods

Classical solution methods:

- **direct methods**: **LU factorization** (e.g., via nested dissection [George, 1973])

  Big-O complexity [Mulder and Plessix, 2002]:

Complexity	2D	3D
# grid points	n^2	n^3
factorization	$n_f n^3$	$n_f n^6$
application	$n_s n_f n^2 \log n$	$n_s n_f n^4 \log n$

Helmholtz equation: classical solution methods

Classical solution methods:

- **iterative methods**: **Krylov-subspace** schemes for **indefinite** systems (e.g., GMRES, BiCGStab, ... [Saad, 2003]):

$$\mathbf{u}_{i+1} = \mathbf{u}_i + \sum_{j \leq i} \alpha_j \mathbf{r}_j, \quad \mathbf{r}_j = \mathbf{f} - H[\mathbf{m}]\,\mathbf{u}_j$$

Need **pre-conditioning**!

Helmholtz equation: classical solution methods

Classical solution methods:

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Need **pre-conditioning**!

E.g., **shifted-Laplacian** preconditioning by **multigrid** [Erlangga et al., 2006]:

$$H_\beta[\mathbf{m}]\,\mathbf{u} = \mathbf{f}, \quad H_\beta[\mathbf{m}] = -\omega^2(1 - \beta \mathrm{i})\mathbf{m} - \Delta$$

...competitive with time-domain based imaging? # iter grow linearly with frequency [Knibbe et al., 2014]

Helmholtz equation: potential role of machine learning?

Assumptions:

- ultimate goal: solve the inverse problem; **we don't need/want overly "accurate" solutions** (even better, *solve forward and inverse map jointly*?)
- **specialized right-hand sides** (e.g., point sources)
- **prior information** about **model parameter distribution** is often available

Role of machine learning:

- **specialize** classical methods to a restricted class of problems = **accelerate** classical methods for the problem at hand

PDE solution by machine learning: general overview

Ever growing body of work, so far focused on learning solutions which generalize over:

- boundary conditions and domain geometry
- right-hand side
- initial conditions; etc...

Poisson equation	[Tang et al., 2017], [Tompson et al., 2017], [Farimani et al. 2017], [Zhang et al., 2018], [Hsieh et al., 2019]
Laplace equation	[Sharma et al., 2017]
Schrodinger equation	[Mills et al., 2017]
Fluid dynamics	[Guo et al., 2016], [Yang et al., 2016], [Chu and Thuerey, 2017], [Kutz, 2017], [Singh et al., 2017]
Black-Scholes	[Sirignano and Spiliopoulos, 2018]

Helmholtz equation: Krylov net training setup

Goal:

- approximate the Helmholtz **solution map** with a net-based approximation (for a **fixed source and frequency**)

$$F : \mathcal{M} \to \mathcal{U},\; F(\mathbf{m}) = (H[\mathbf{m}])^{-1}\,\mathbf{f} \quad \Longleftrightarrow \quad F_\theta : \mathcal{M} \to \mathcal{U},\; F_\theta(\mathbf{m}) \approx (H[\mathbf{m}])^{-1}\,\mathbf{f}$$

Candidate loss functions:

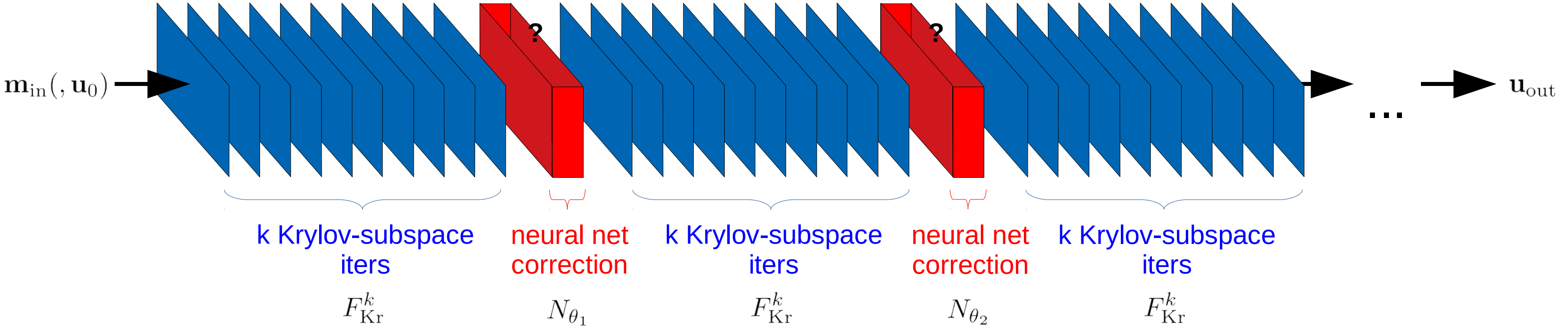
$$F_{\theta^*} = F_{\arg\min_\theta \; L(\theta)},$$

- **supervised**, given solution (this talk): $L(\theta) = \mathbb{E}_{\mathbf{m}\sim p_M} ||F(\mathbf{m}) - F_\theta(\mathbf{m})||_2^2$
- unsupervised: $L(\theta) = \mathbb{E}_{\mathbf{m}\sim p_M} ||\mathbf{f} - H[\mathbf{m}]\, F_\theta(\mathbf{m})||_2^2$

- Training with stochastic gradient descent algorithms (ADAM, [Kingma and Ba, 2015])

Helmholtz equation: Krylov net structure

Main idea: **intersperse** Krylov-subspace “nets” and neural nets...



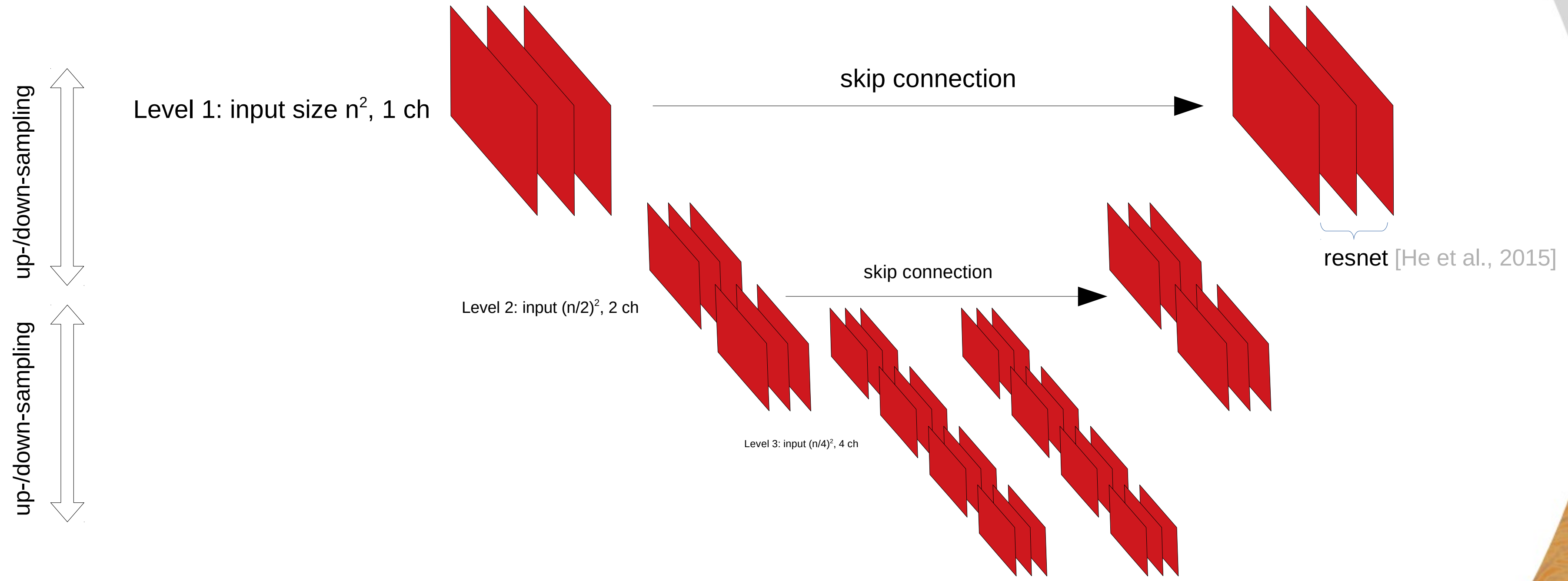
$$F_{(\theta_1,\ldots,\theta_N)} : \mathcal{M} \to \mathcal{U}, \qquad F_{(\theta_1,\ldots,\theta_N)}(\mathbf{m}) = \begin{cases} F^k_{\text{Kr}}(\mathbf{m}, N_{\theta_N} \circ F_{(\theta_1,\ldots,\theta_{N-1})}(\mathbf{m})), & N \geq 1 \\ F^k_{\text{Kr}}(\mathbf{m}, \underbrace{\mathbf{u}_0}_{\text{fixed}}), & N = 0 \end{cases}$$

$$F^k_{\text{Kr}} : \mathcal{M} \times \mathcal{U} \to \mathcal{U}, \quad F^k_{\text{Kr}}(\mathbf{m}, \mathbf{u}) = \mathbf{u} + \sum_{j=0}^{k-1} \alpha_j H[\mathbf{m}]^j\, \mathbf{r}, \ \text{for some } \alpha_j \quad (\in \mathbf{u} + \text{Kr}(H[\mathbf{m}], \mathbf{r}))$$

$$N_{\theta_i} : \mathcal{U} \to \mathcal{U}$$

Helmholtz equation: Krylov net structure

2-D net correction architecture (“Unet”) ~ multigrid
(e.g. [Ke et al., 2017], [He and Xu, 2019]):



Complexity ~ $O(n^2 \log n)$

Helmholtz equation: Krylov net structure

2-D net correction architecture, **two-grid sketch**:

Pre-smoothing (fine grid): $\mathbf{x}^h \leftarrow \mathbf{x}^h + a(W_k^h * \mathbf{x}^h + b_k^h), \quad \text{for } k = 1, \ldots, N$

activation function (e.g., ReLU)

resnet

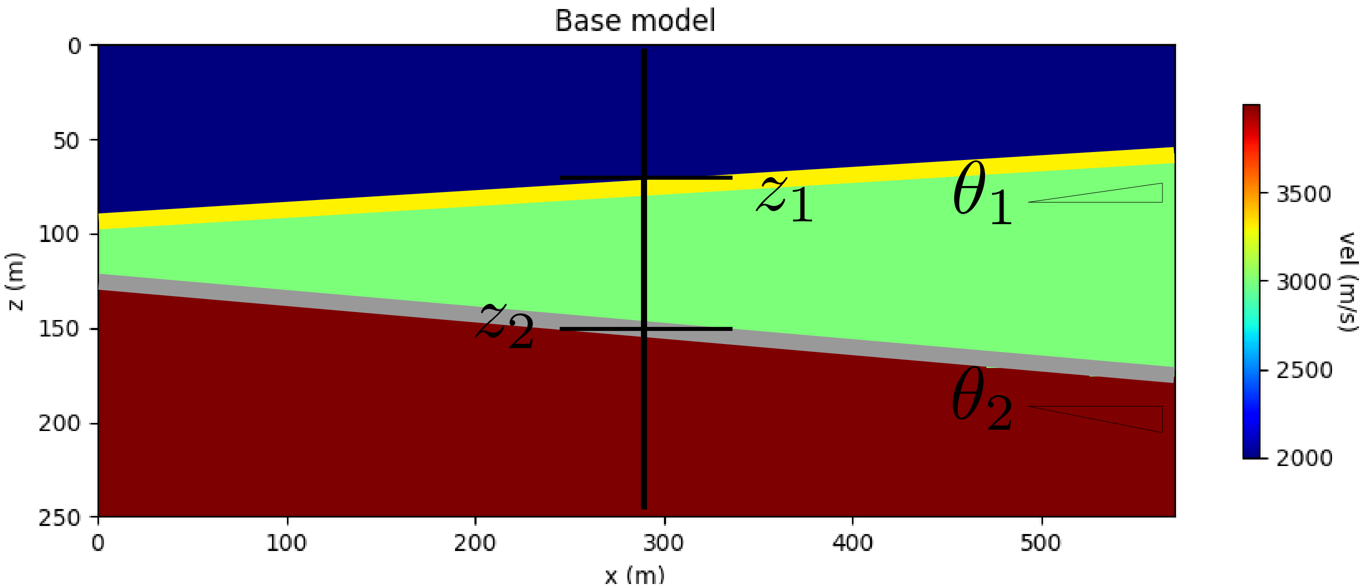
Restriction (many channels!): $\mathbf{x}_{\mathrm{ch}_i}^{2h} \leftarrow R_h^{2h}(W_{\mathrm{ch}_i}^h * \mathbf{x}^h + b_{\mathrm{ch}_i}^h), \quad \text{for } i = 1, \ldots, N_{\mathrm{ch}}$

Smoothing (coarse grid): $\mathbf{x}_{\mathrm{ch}_i}^{2h} \leftarrow \mathbf{x}_{\mathrm{ch}_i}^{2h} + a(\sum_j W_{k,\mathrm{ch}_i,\mathrm{ch}_j}^{2h} * \mathbf{x}_{\mathrm{ch}_j}^{2h} + b_{k,\mathrm{ch}_i}^{2h}), \quad \text{for } i, k, \ldots$

Prolongation: $\mathbf{x}^h \leftarrow \mathbf{x}^h + P_{2h}^h \sum_i (W_{\mathrm{ch}_i}^{2h} * \mathbf{x}_{\mathrm{ch}_i}^{2h} + b_{\mathrm{ch}_i}^{2h})$

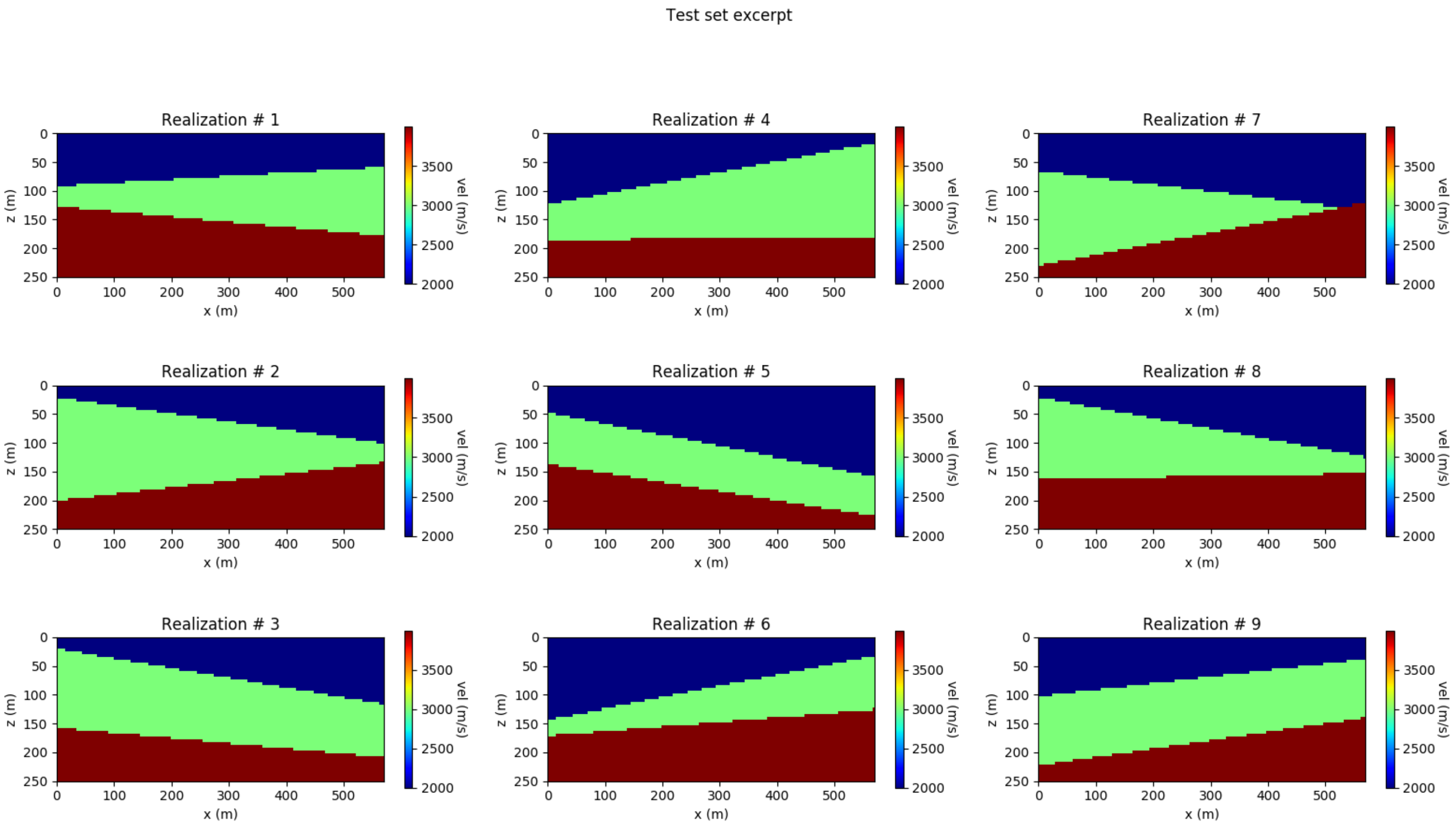
Post-smoothing (fine grid): $\mathbf{x}^h \leftarrow \mathbf{x}^h + a(W_l^h * \mathbf{x}^h + b_l^h), \quad \text{for } l = 1, \ldots, N$

Example 1: layered model distribution (fixed source and frequency)

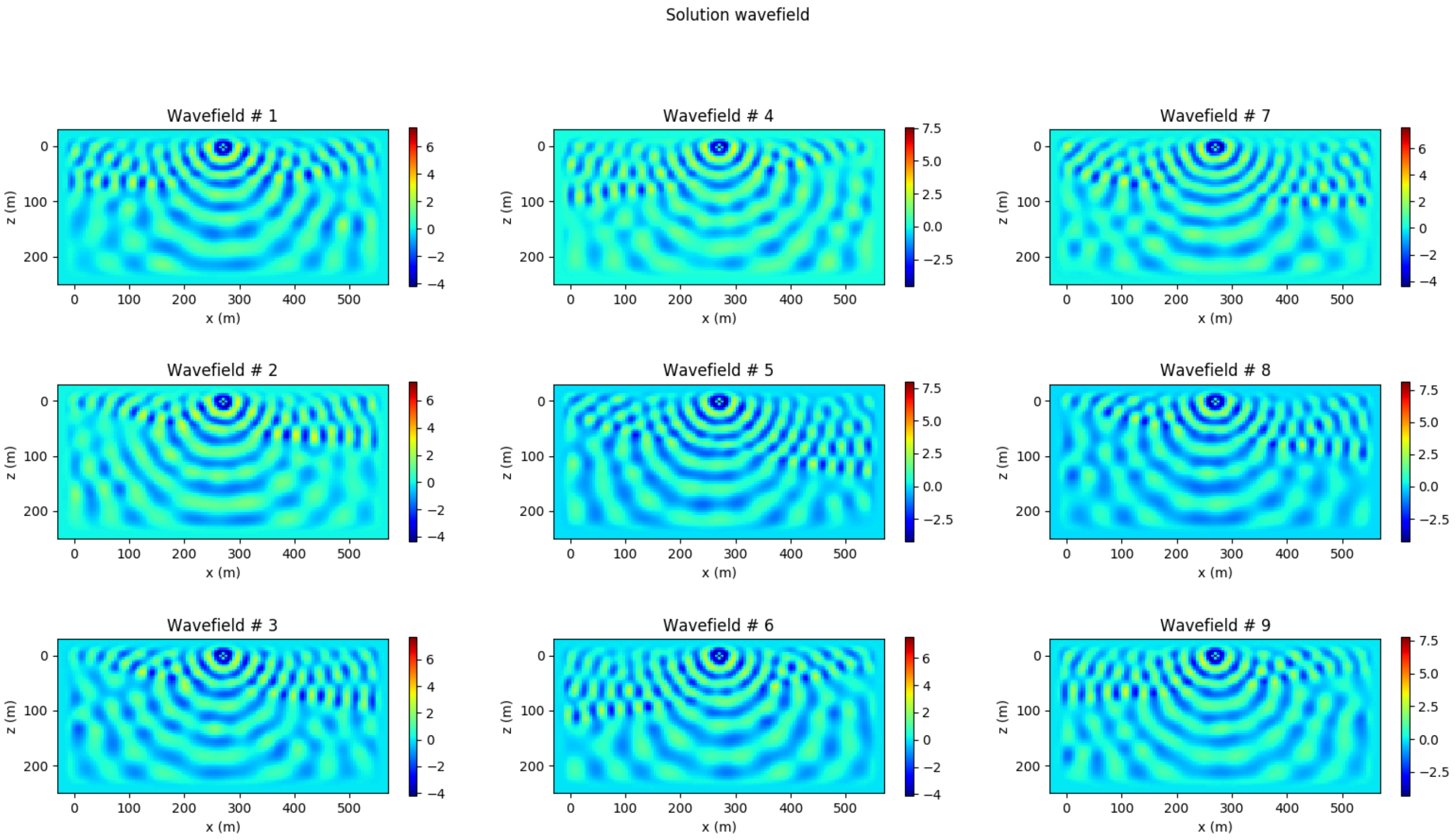


$$z \sim z^0 + U(-a, a) \qquad \theta \sim U(-b, b)$$

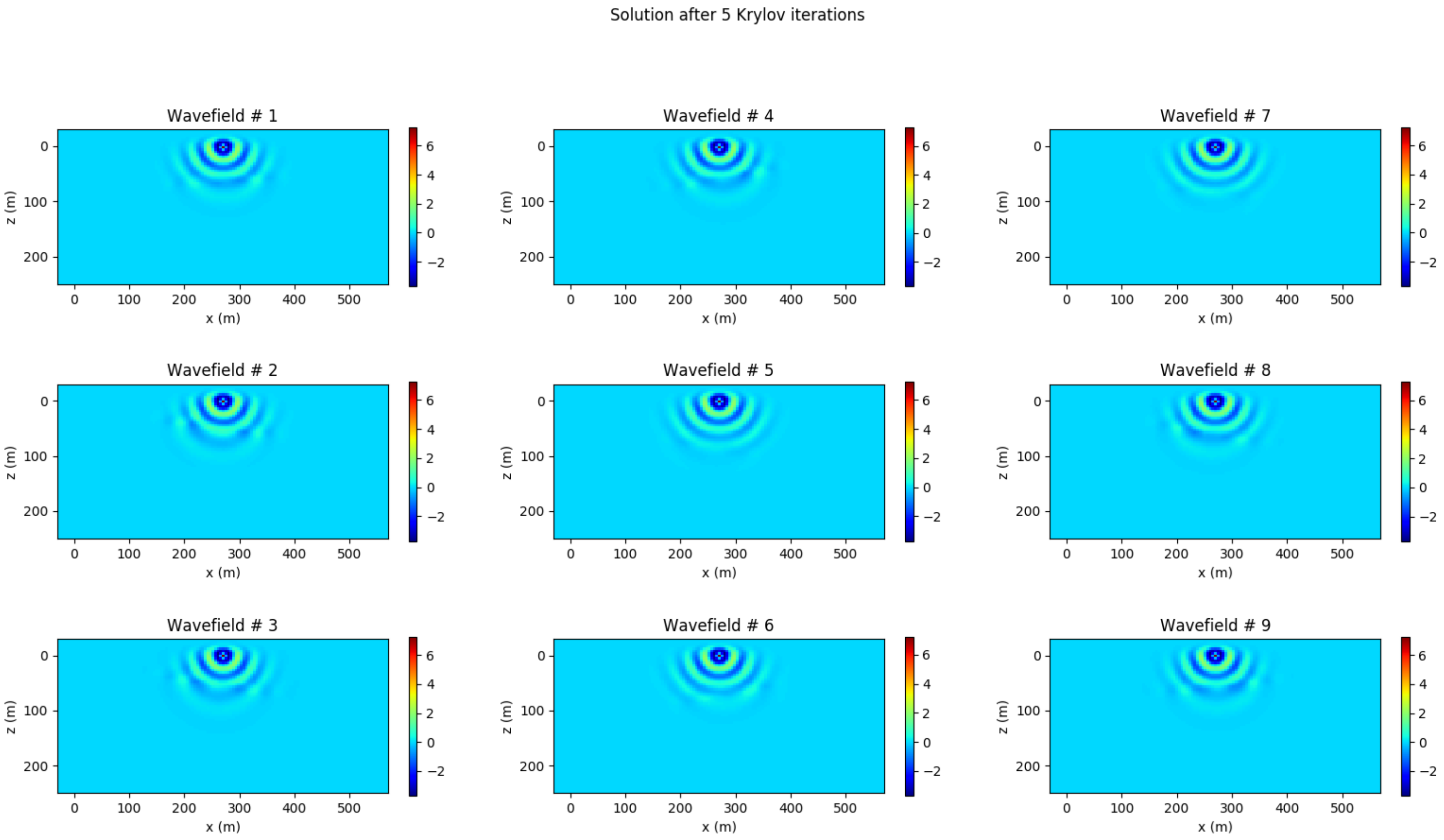
Example 1: layered model distribution (train size: 1024, test size: 16)



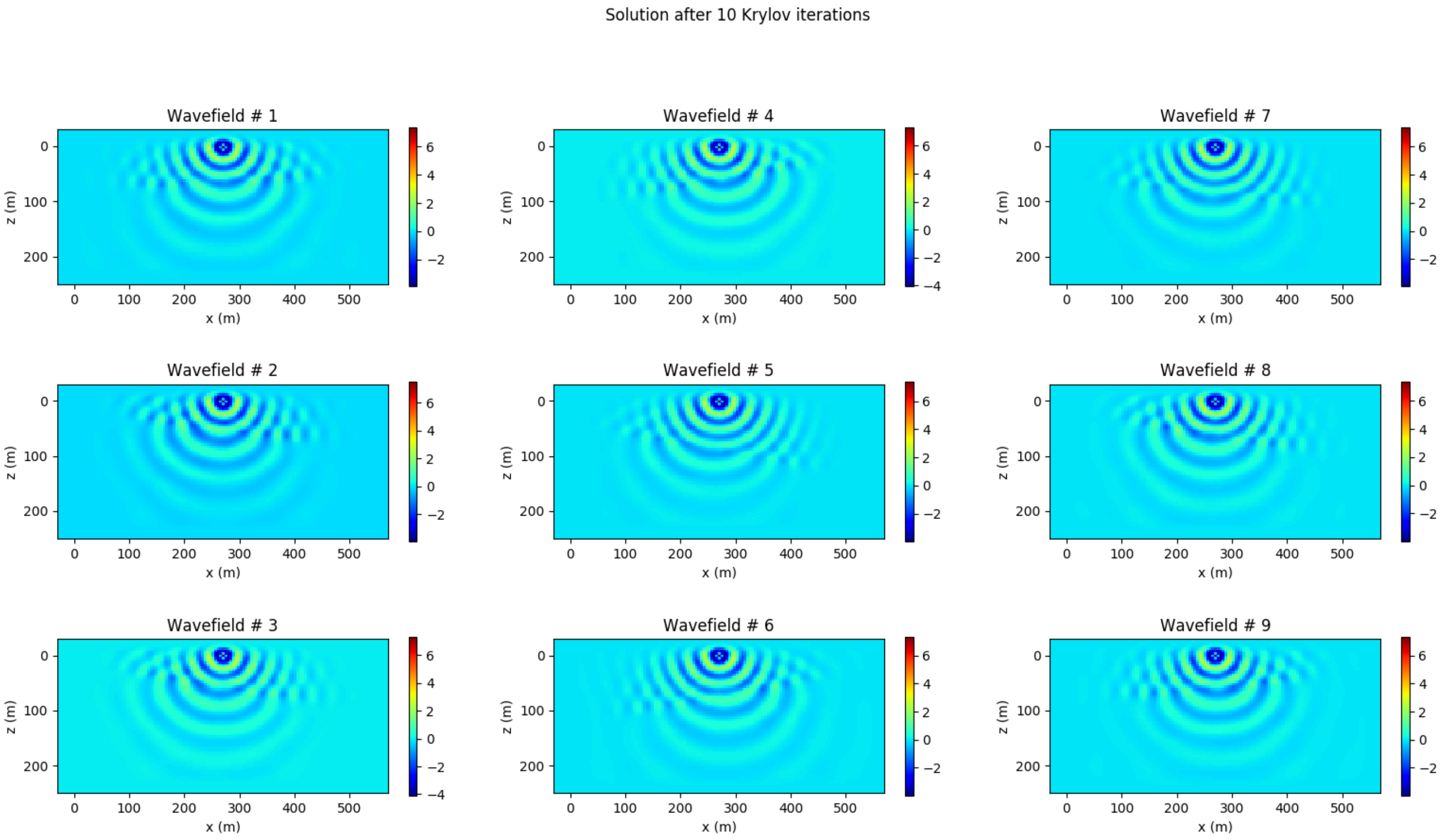
Example 1: solution distribution at 60 Hz (train size: 1024, test size: 16)



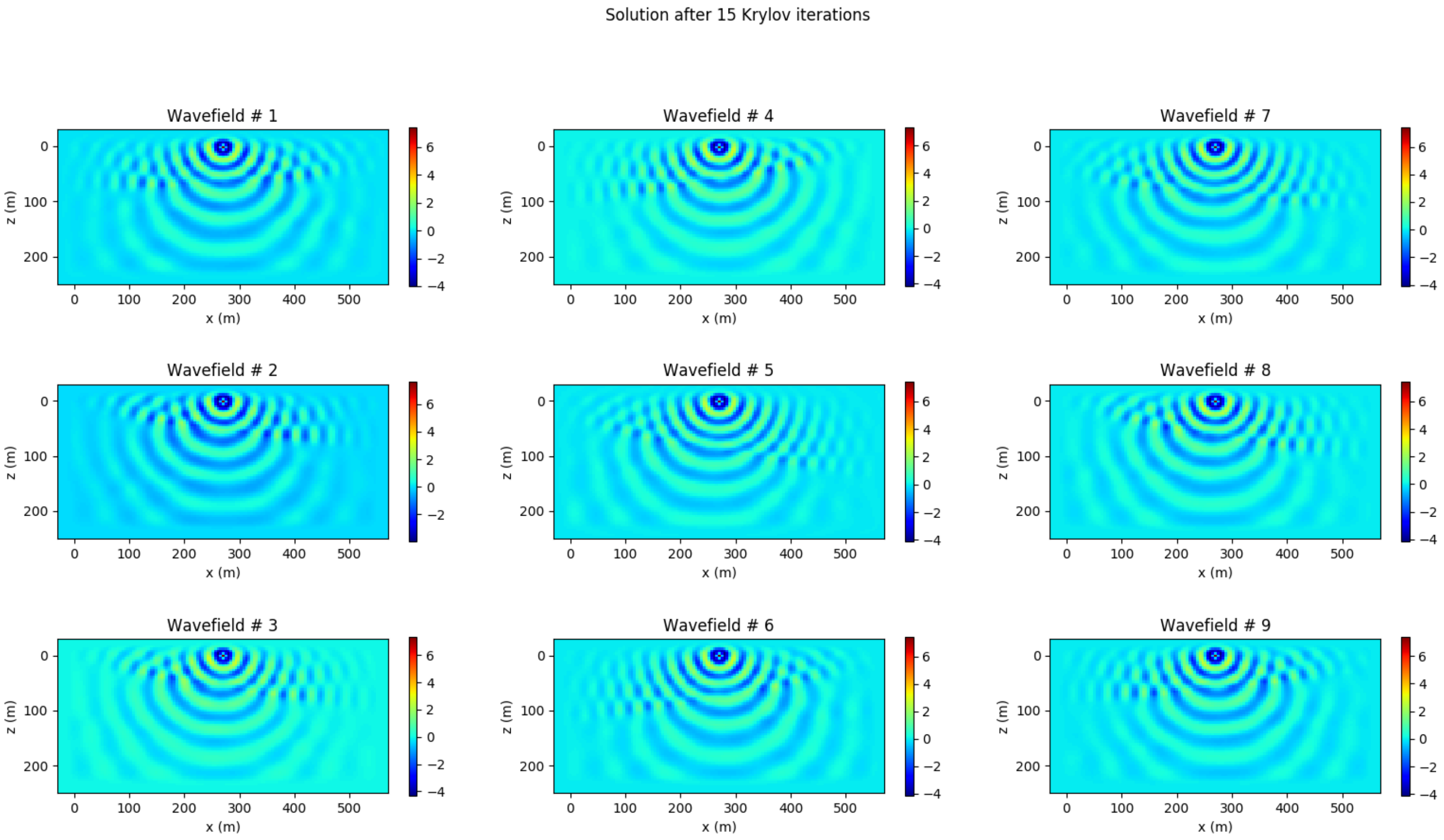
Example 1: approximated wavefield at 60 Hz (after 5 Krylov iterations)



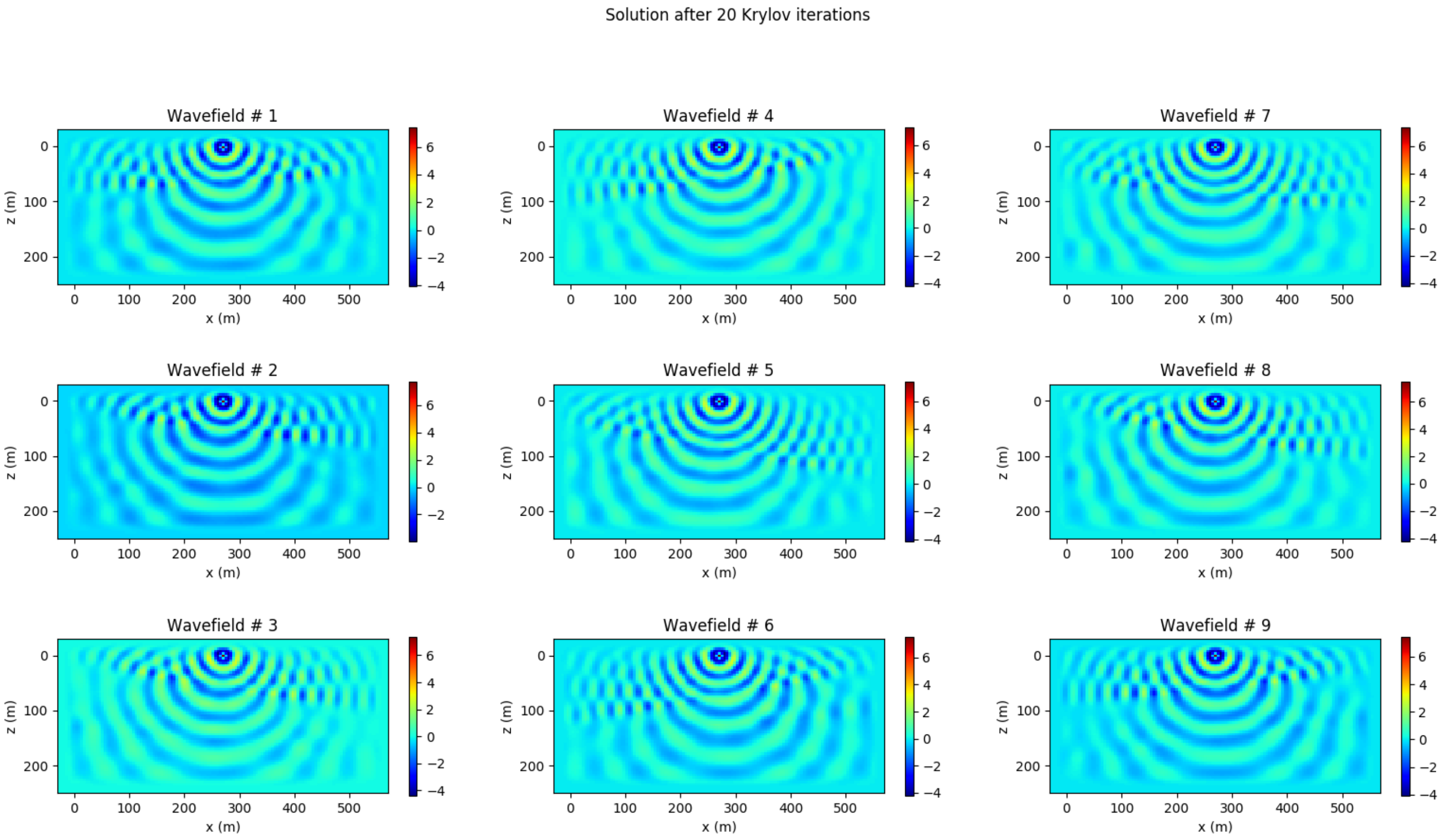
Example 1: approximated wavefield at 60 Hz (after 10 Krylov iterations)



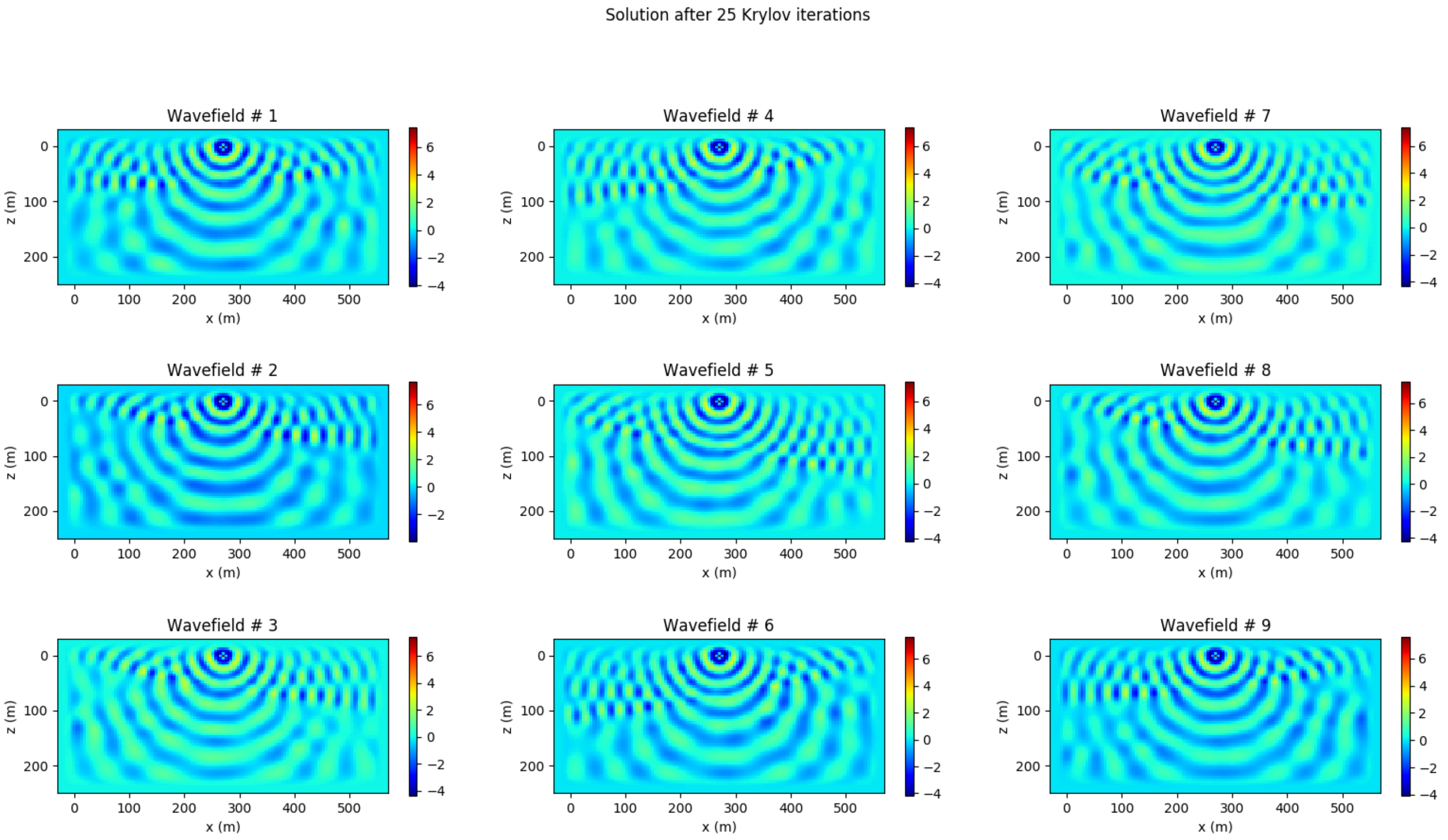
Example 1: approximated wavefield at 60 Hz (after 15 Krylov iterations)



Example 1: approximated wavefield at 60 Hz (after 20 Krylov iterations)



Example 1: approximated wavefield at 60 Hz (after 25 Krylov iterations)



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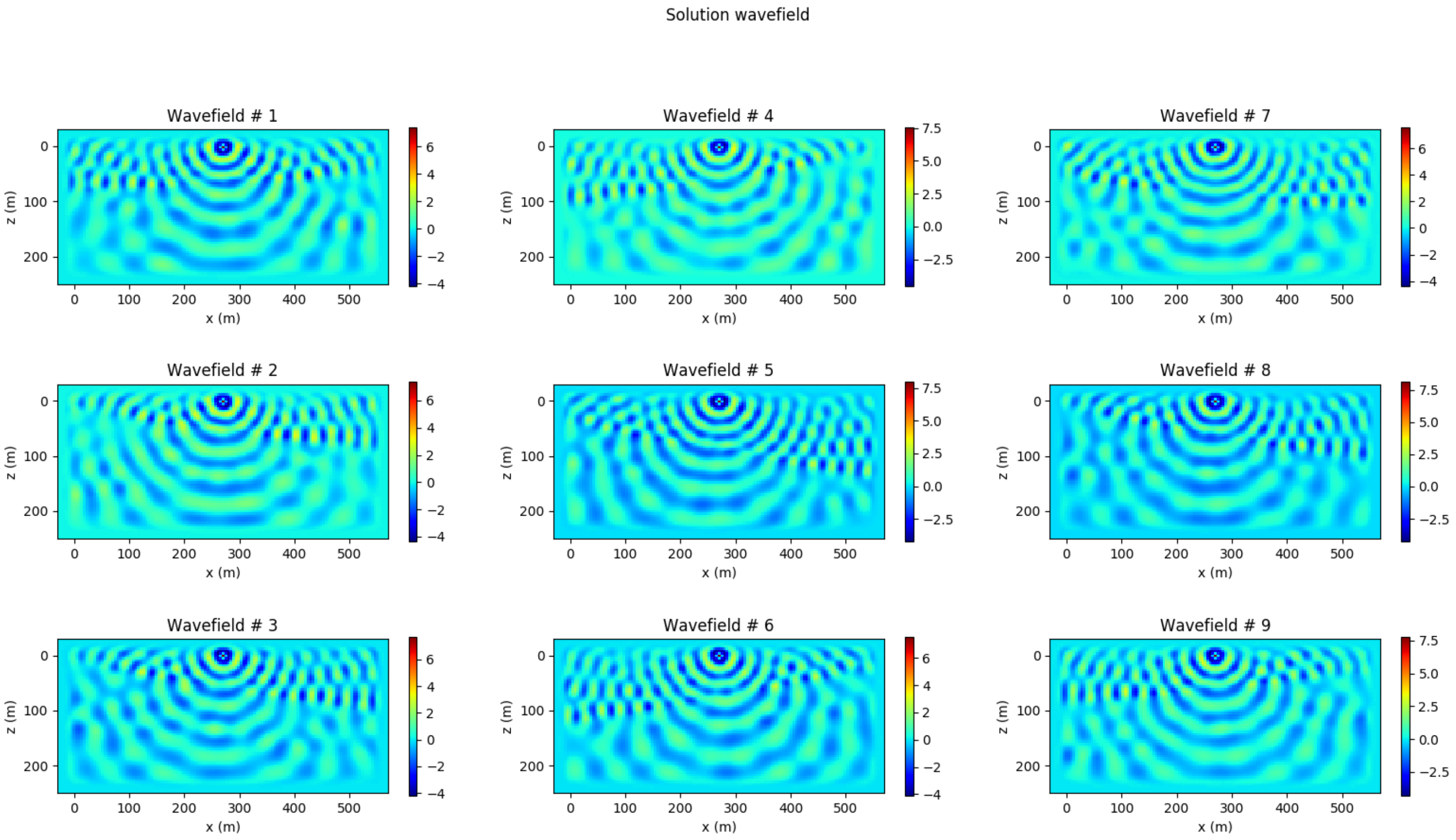
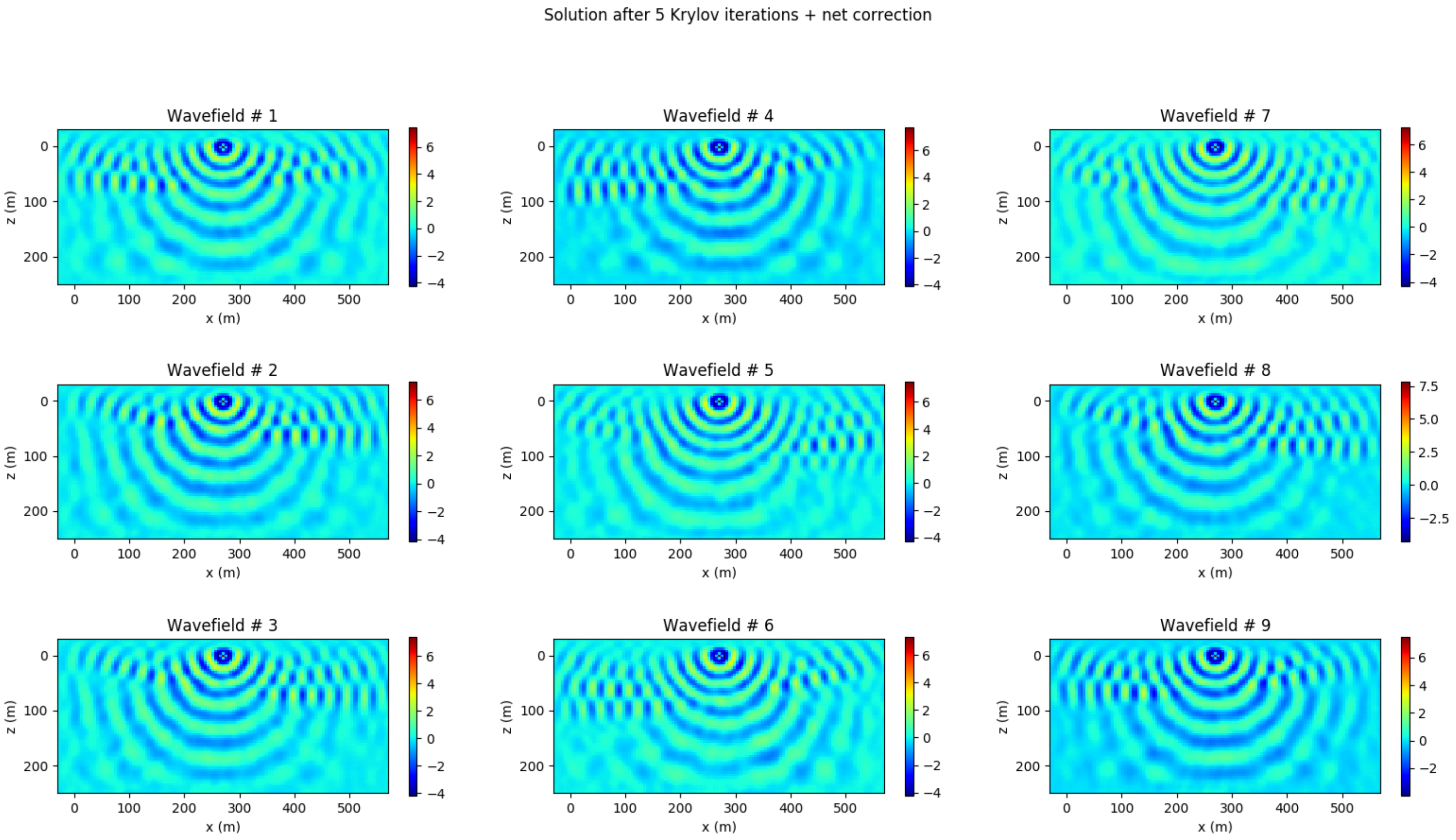
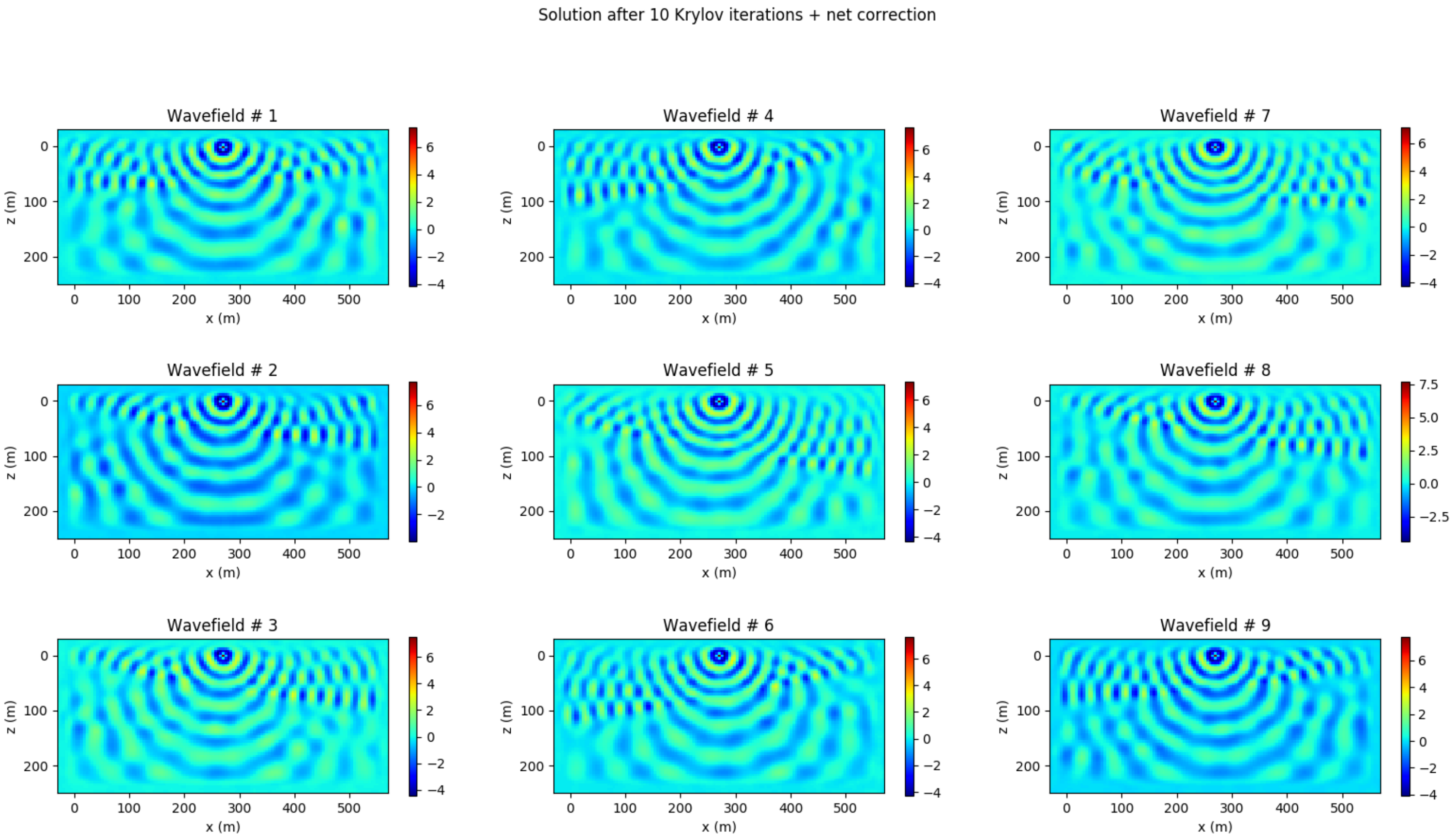


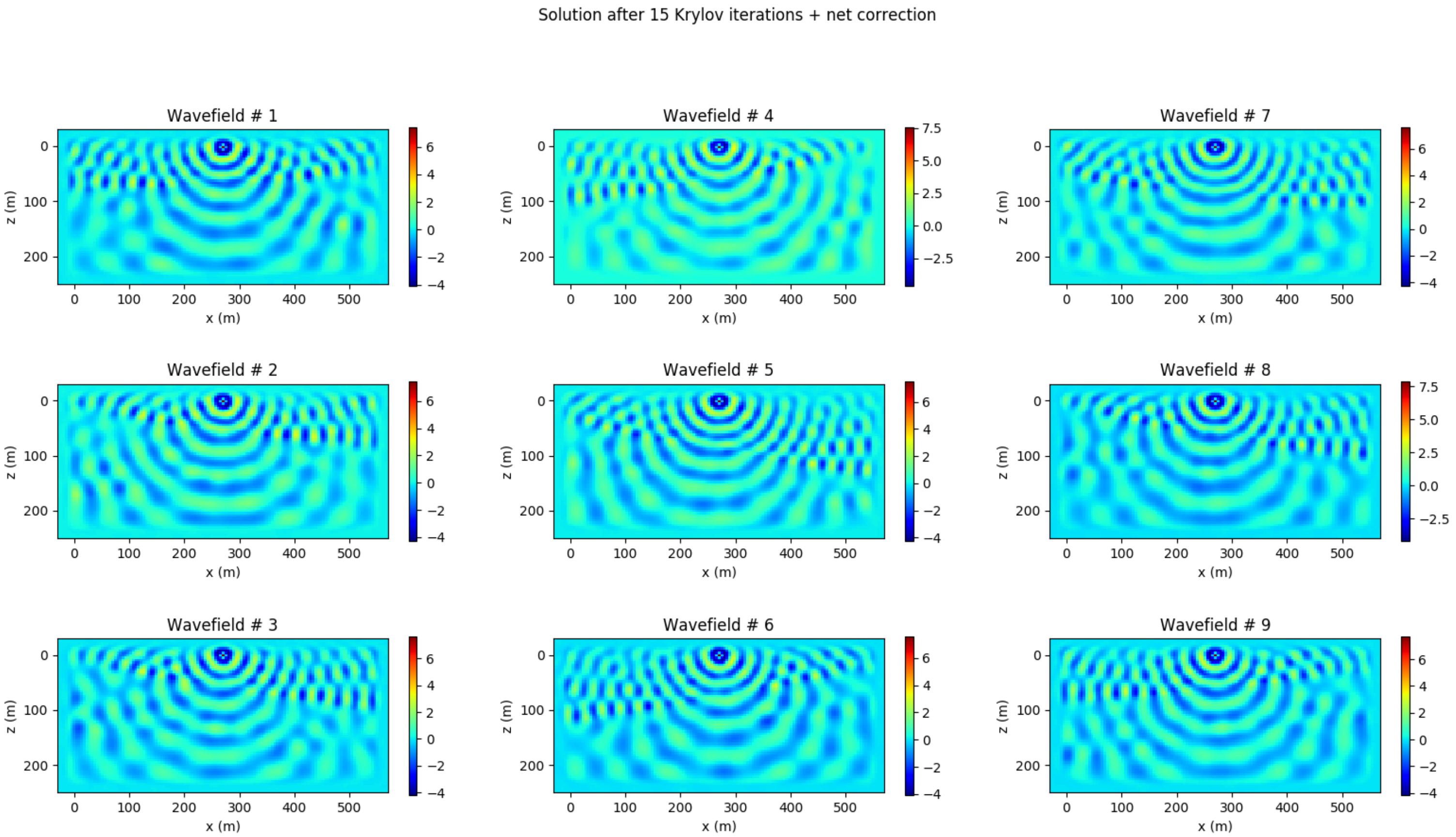
Example 1: approximated wavefield at 60 Hz (after 5 Krylov iterations + net)



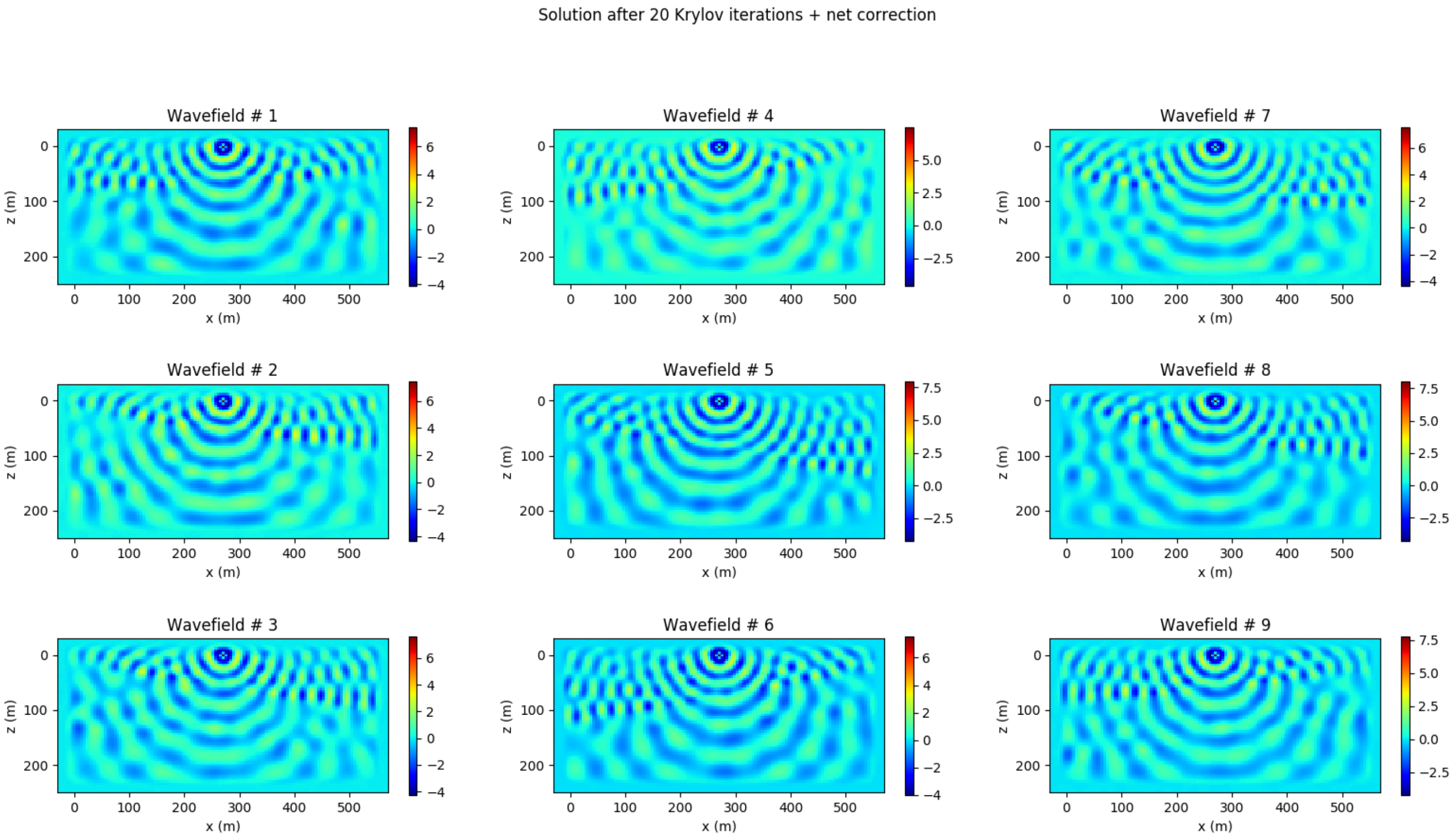
Example 1: approximated wavefield at 60 Hz (after 10 Krylov iterations + net)



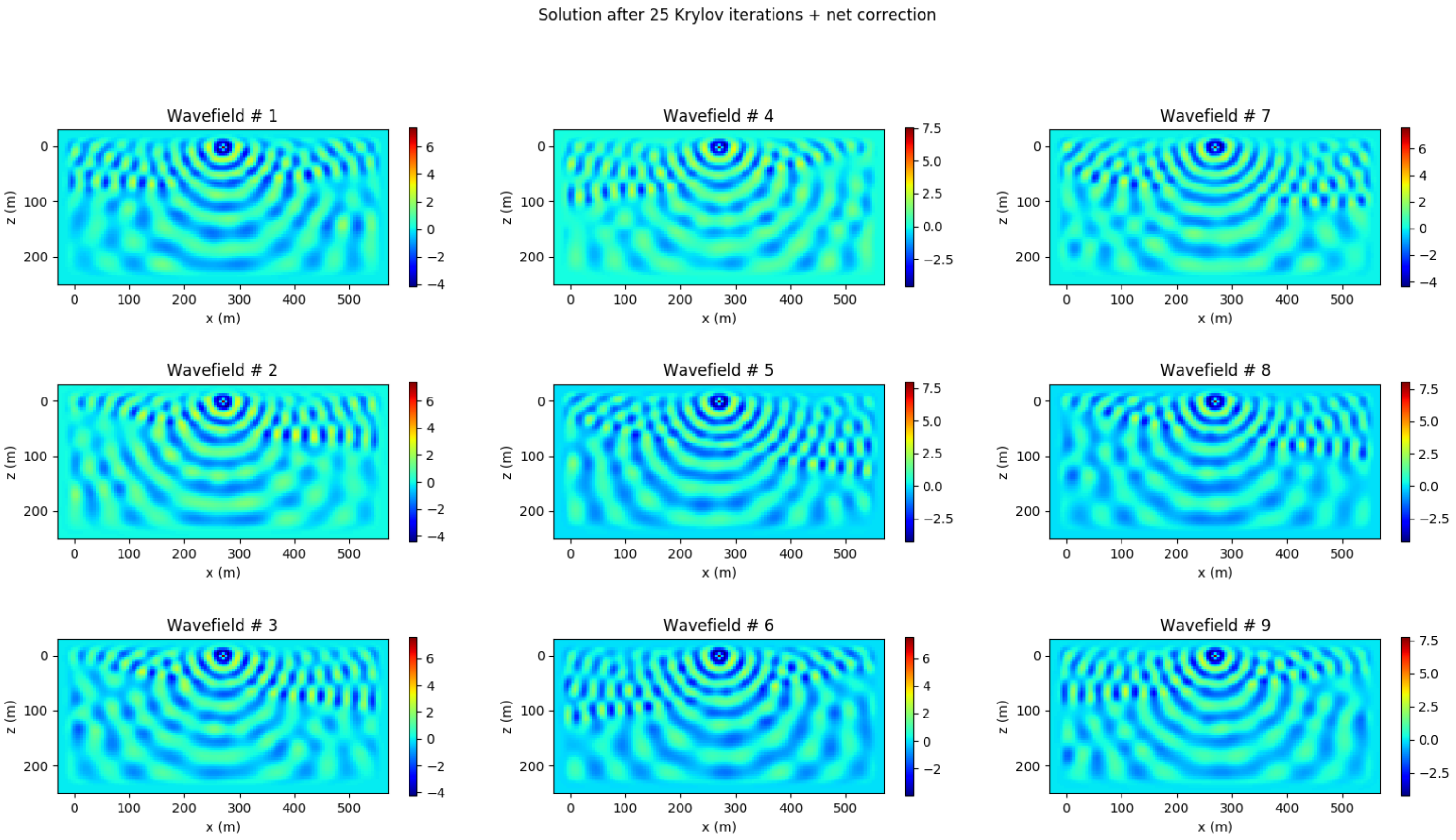
Example 1: approximated wavefield at 60 Hz (after 15 Krylov iterations + net)



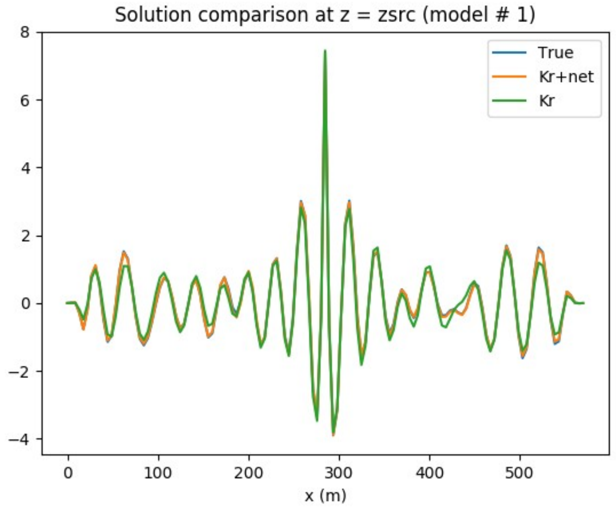
Example 1: approximated wavefield at 60 Hz (after 20 Krylov iterations + net)

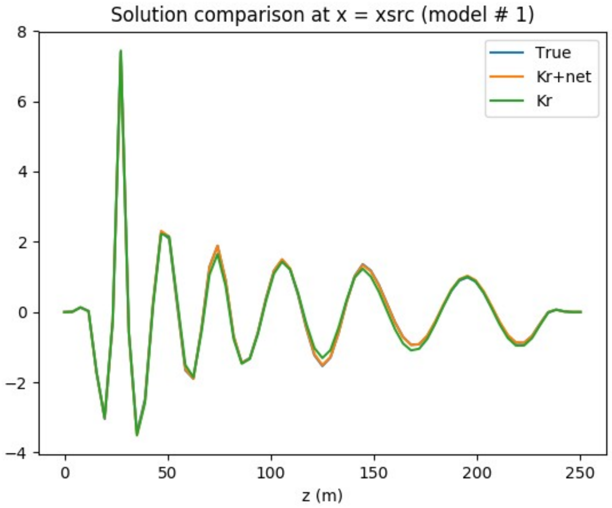


Example 1: approximated wavefield at 60 Hz (after 25 Krylov iterations **+ net**)

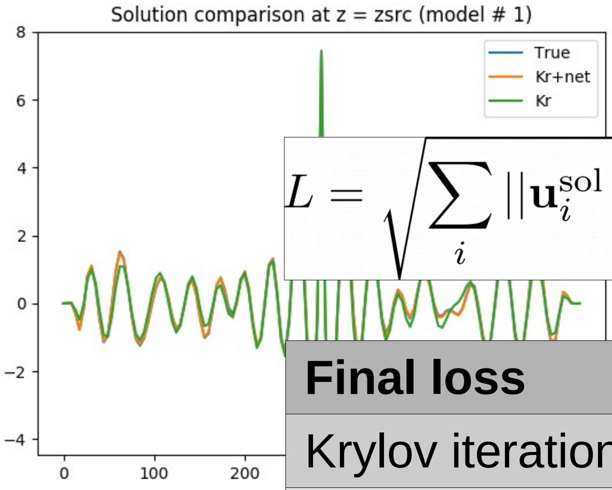


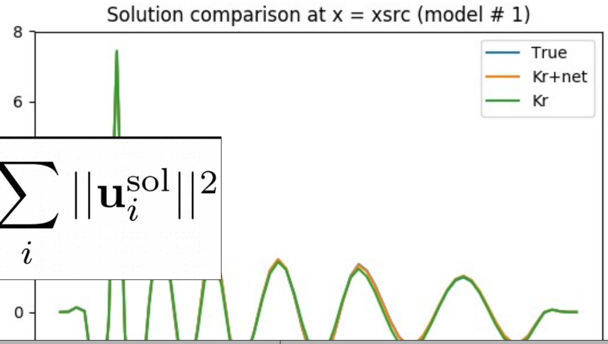
Example 1: solution trace comparison





Example 1: training/test errors

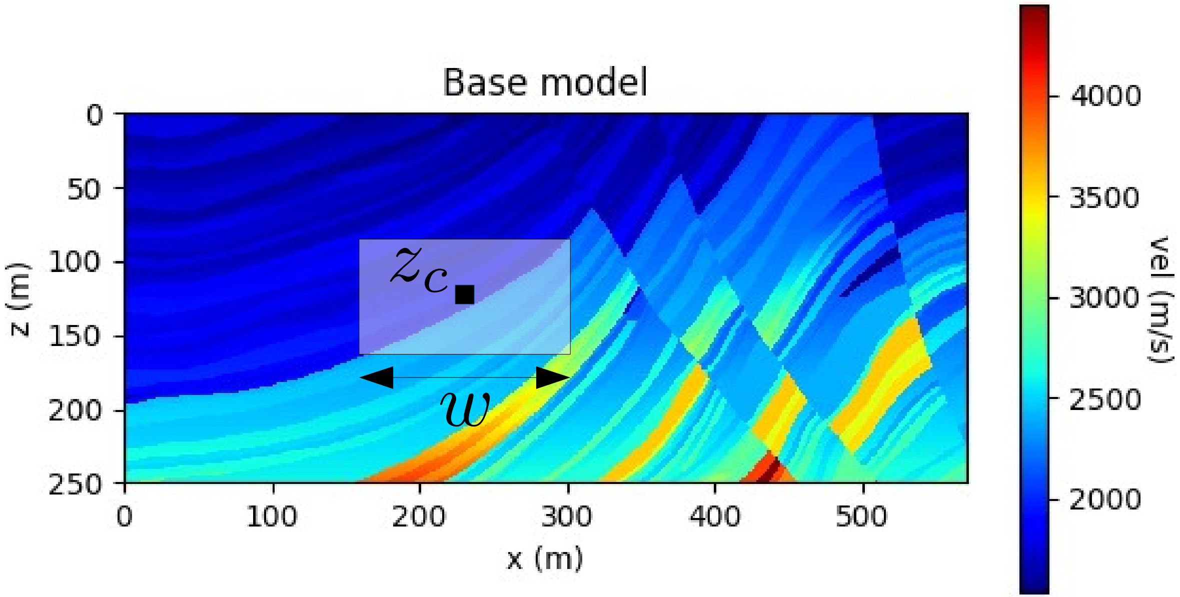




$$L = \sqrt{\sum_i ||\mathbf{u}_i^{\text{sol}} - \tilde{\mathbf{u}}_i||^2 / \sum_i ||\mathbf{u}_i^{\text{sol}}||^2}$$

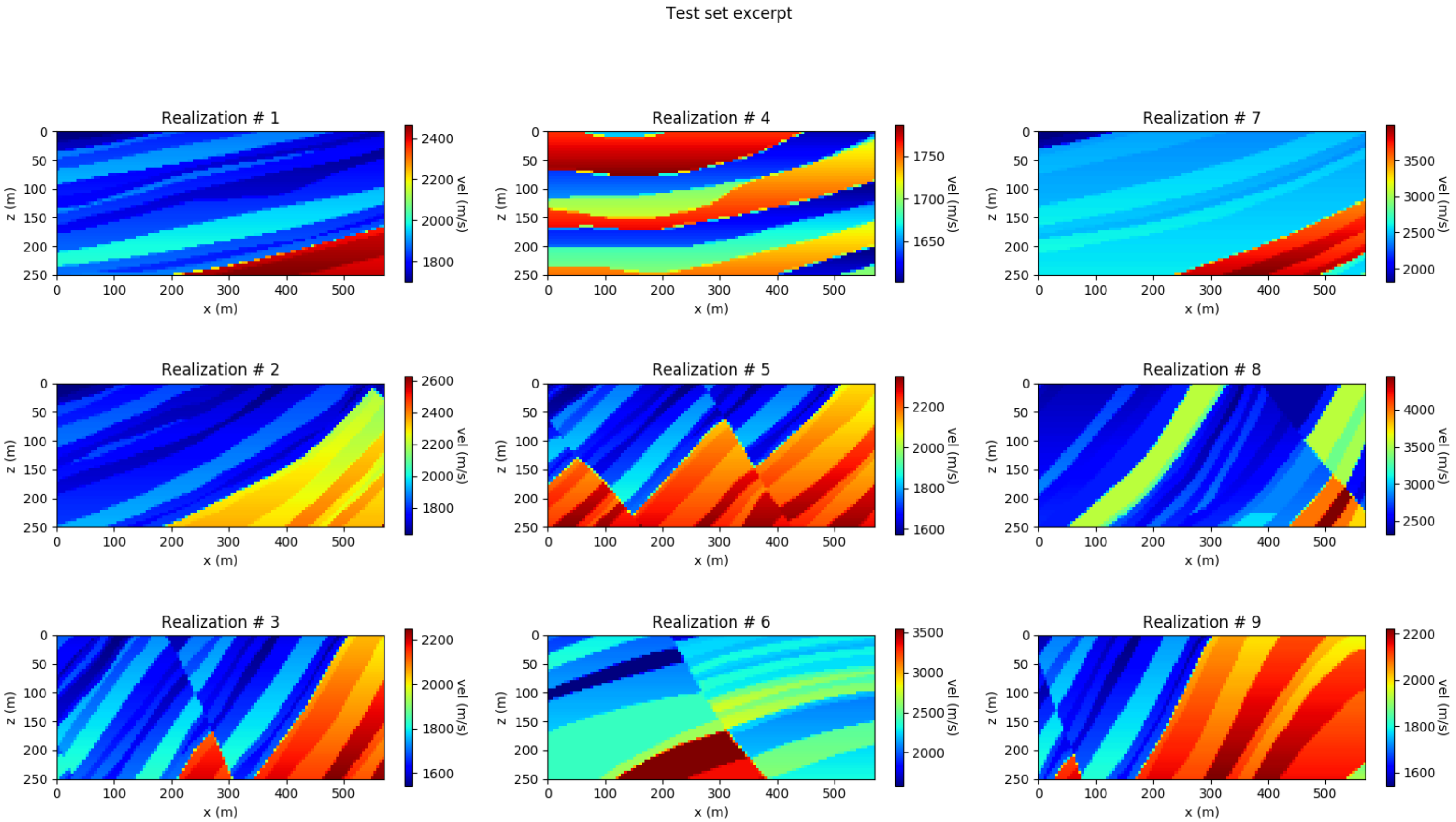
Final loss	Train error	Test error
Krylov iterations	23%	24%
Krylov net	3.9%	5.2%

Example 2: Marmousi-like distribution (fixed source and frequency)

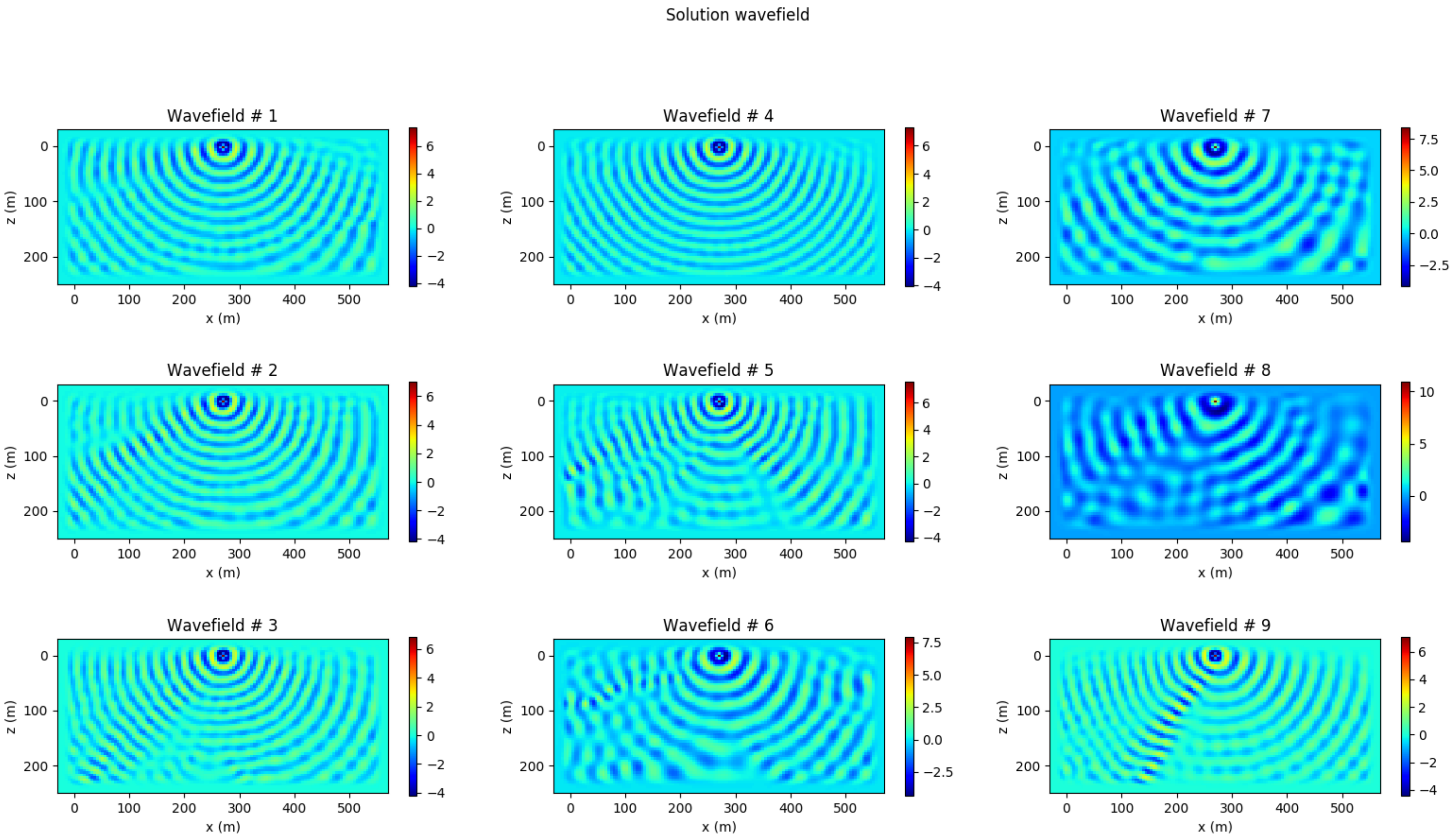


$z_c \sim U(z_0, z_{\text{end}})$ $\quad w \sim w_0 + U(-a, a)$

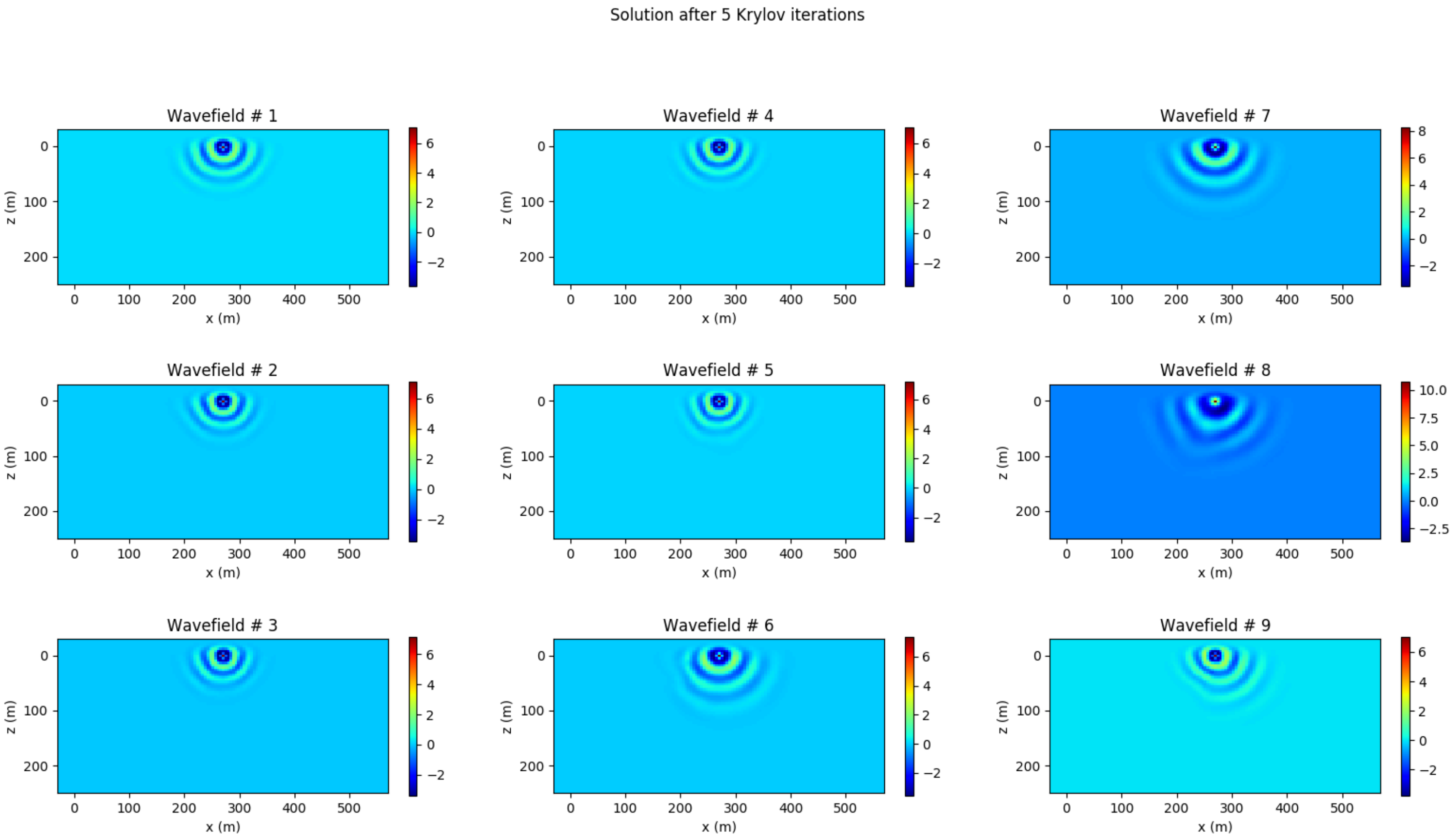
Example 2: Marmousi-like distribution (train size: 1024, test size: 16)



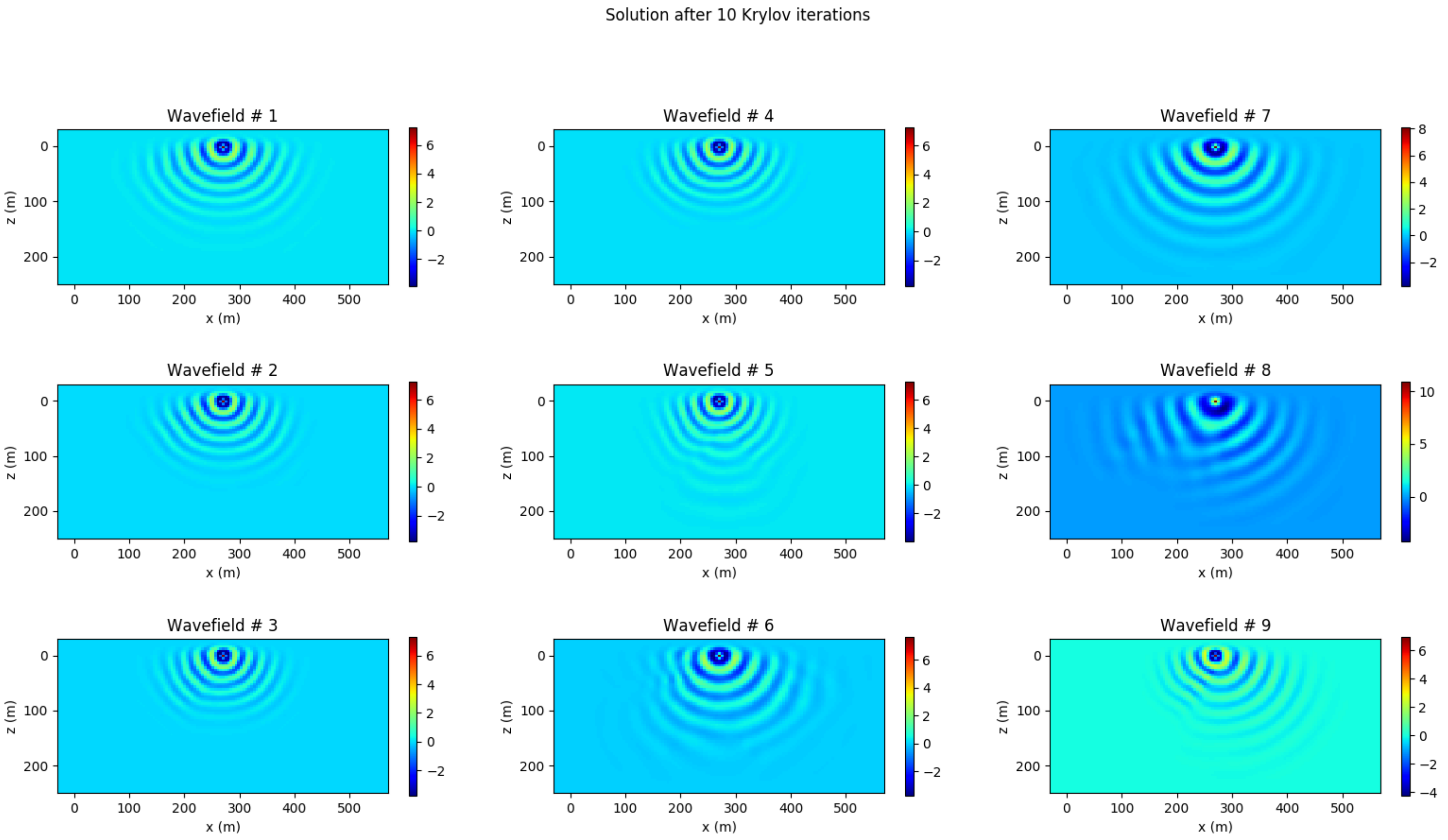
Example 2: solution distribution at 60 Hz (train size: 1024, test size: 16)



Example 2: solution wavefield at 60 Hz (after 5 Krylov iterations)



Example 2: solution wavefield at 60 Hz (after 10 Krylov iterations)



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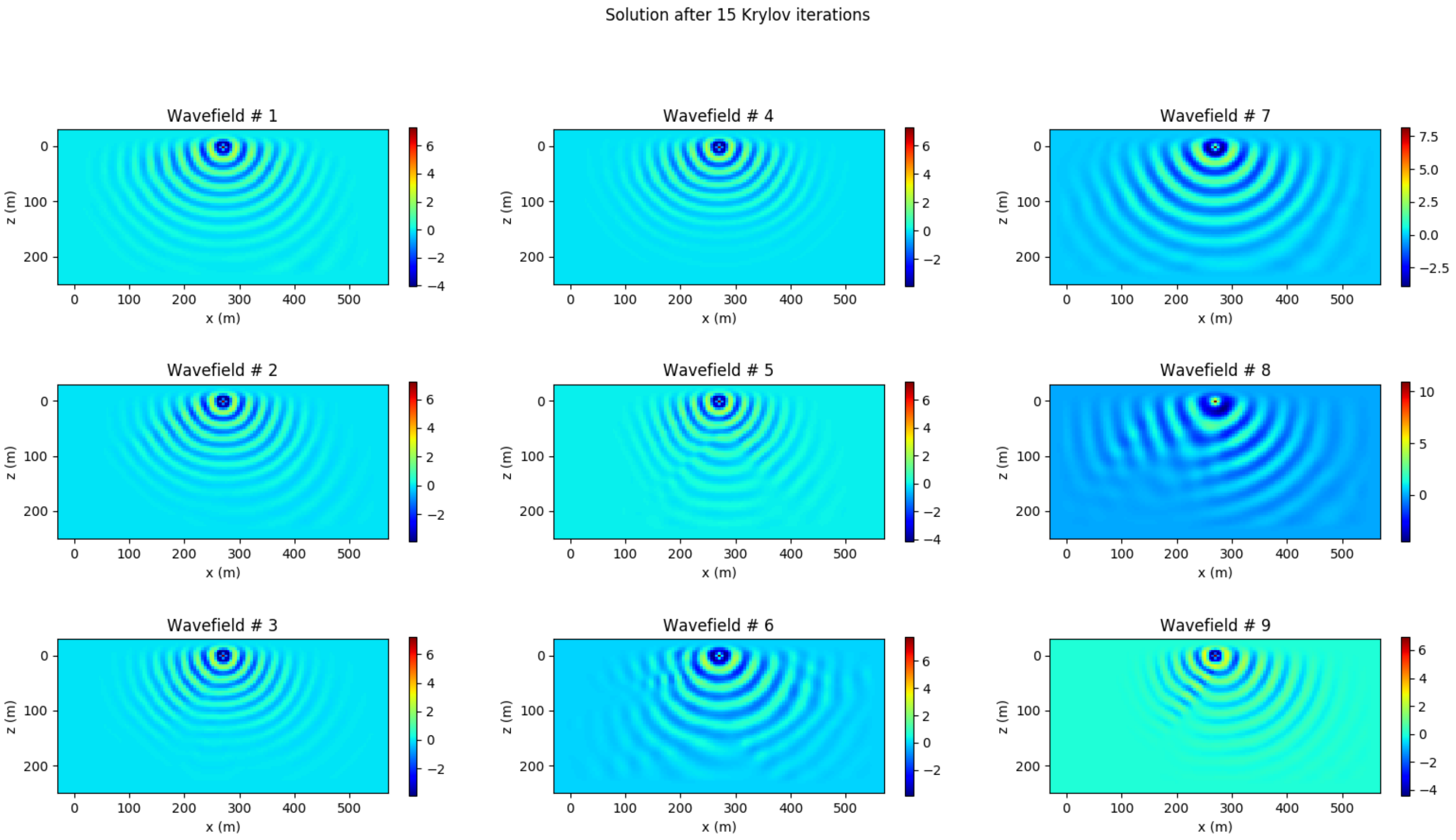
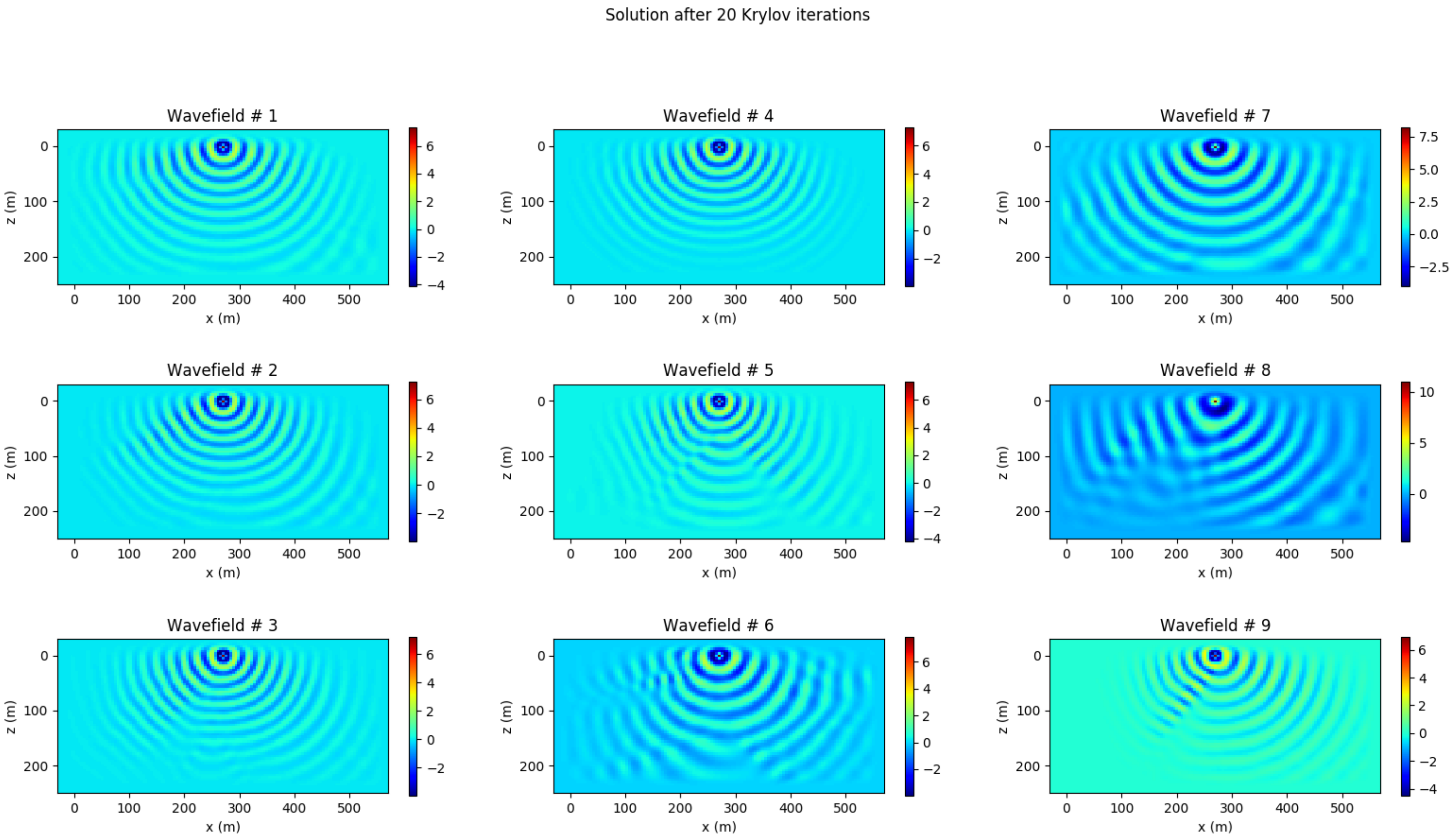


Example 2: solution wavefield at 60 Hz (after 20 Krylov iterations)



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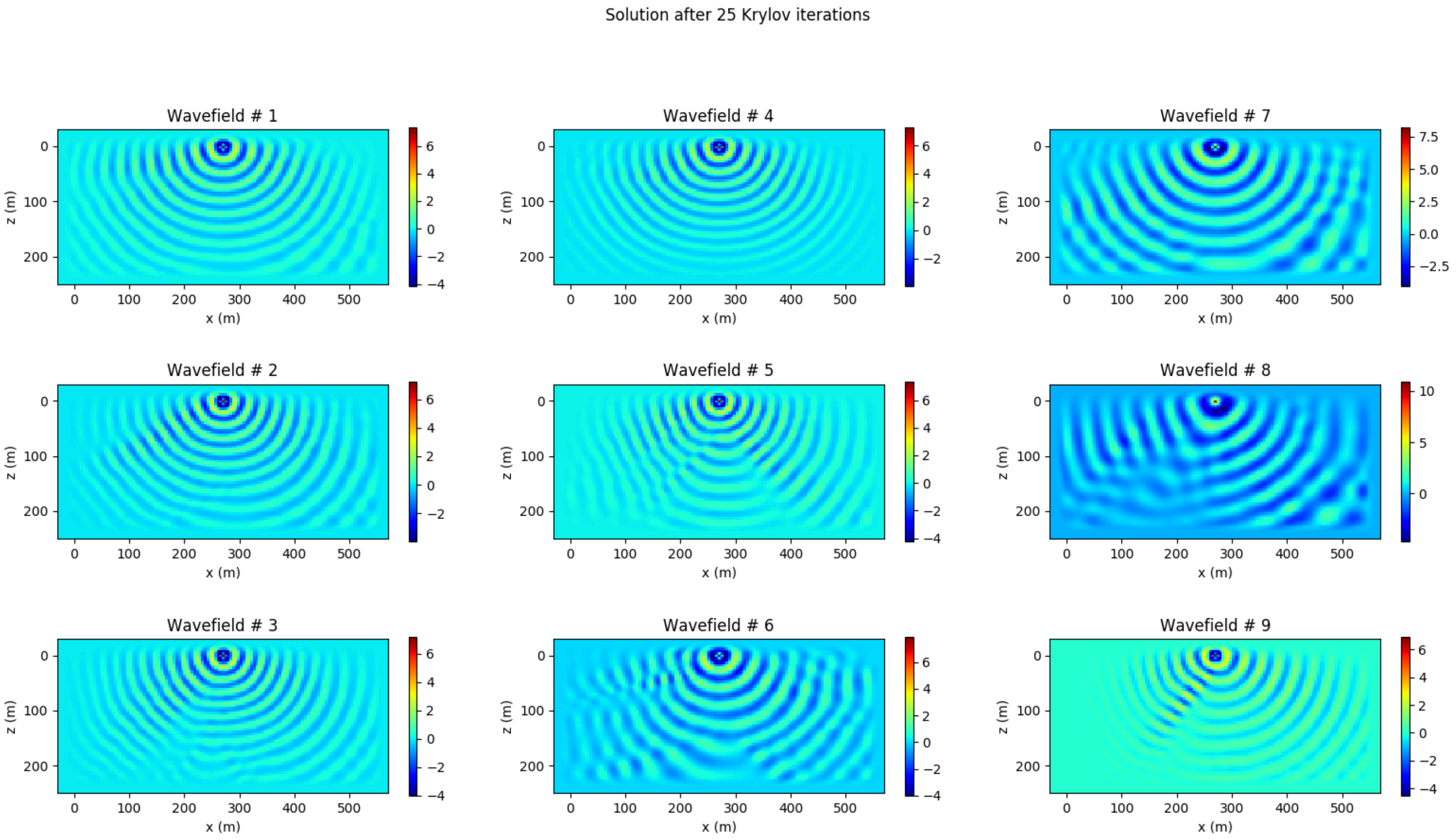
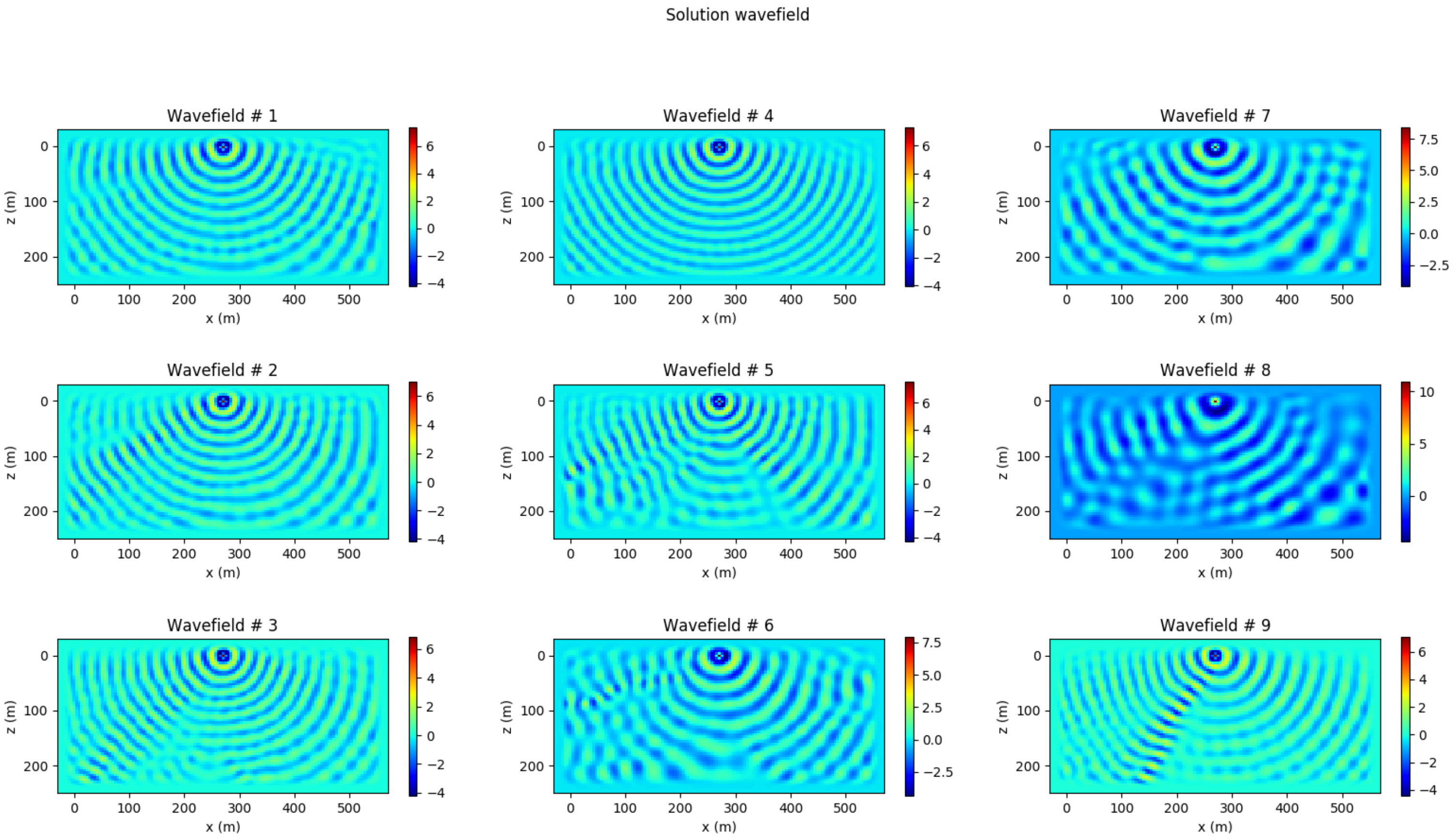
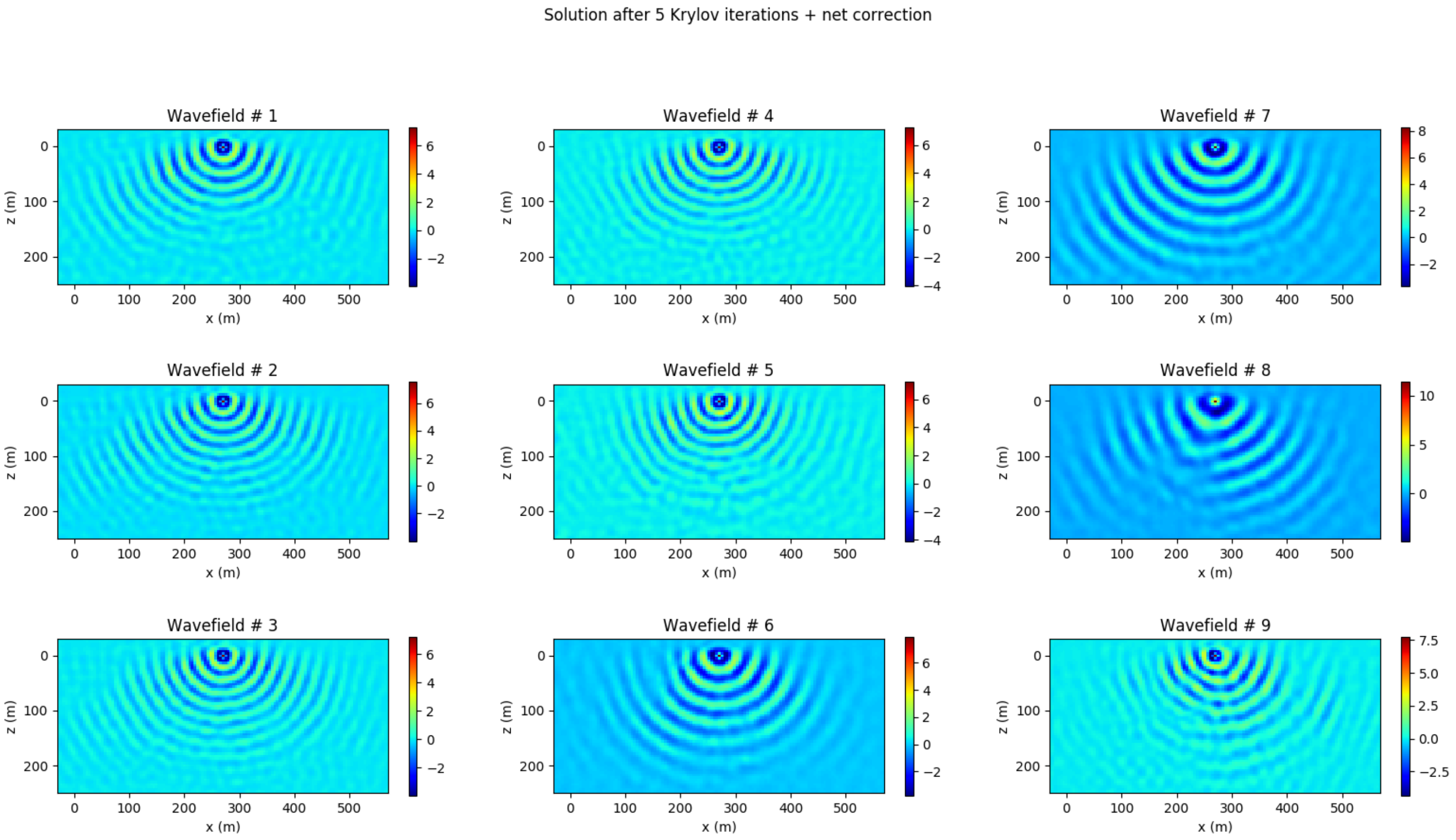


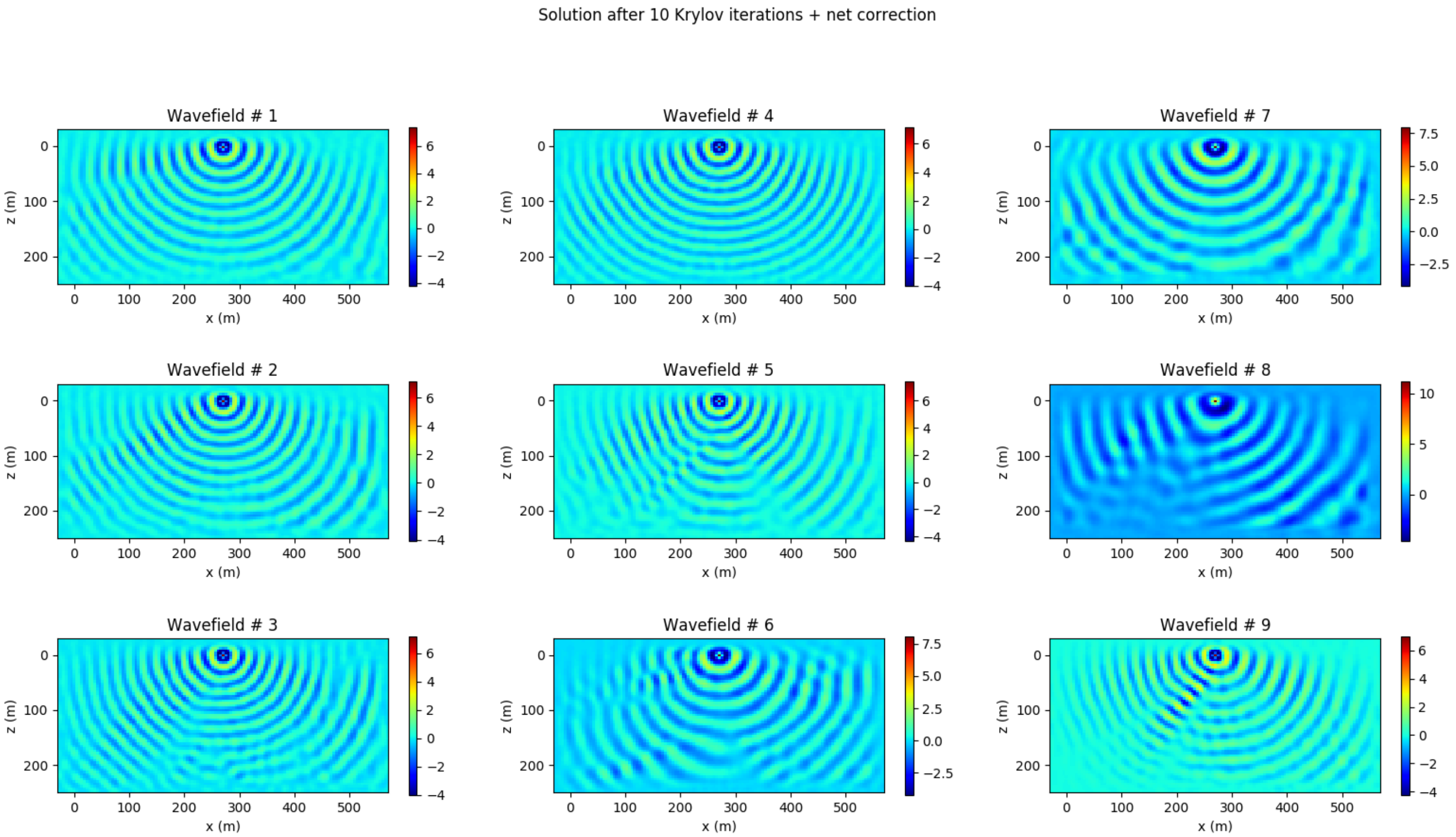
Example 2: solution distribution at 60 Hz (train size: 1024, test size: 16)



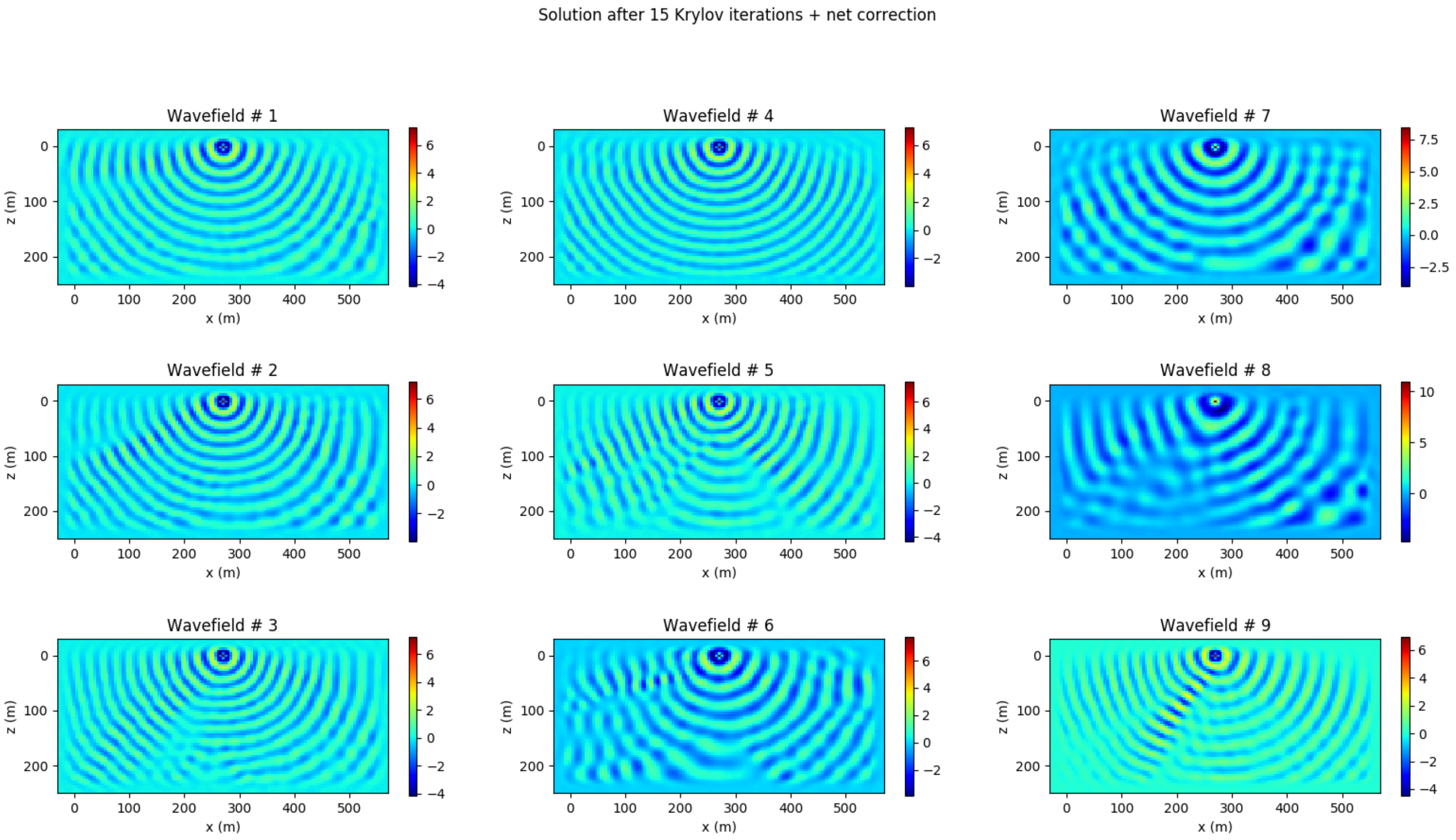
Example 2: solution wavefield at 60 Hz (after 5 Krylov iterations **+ net**)



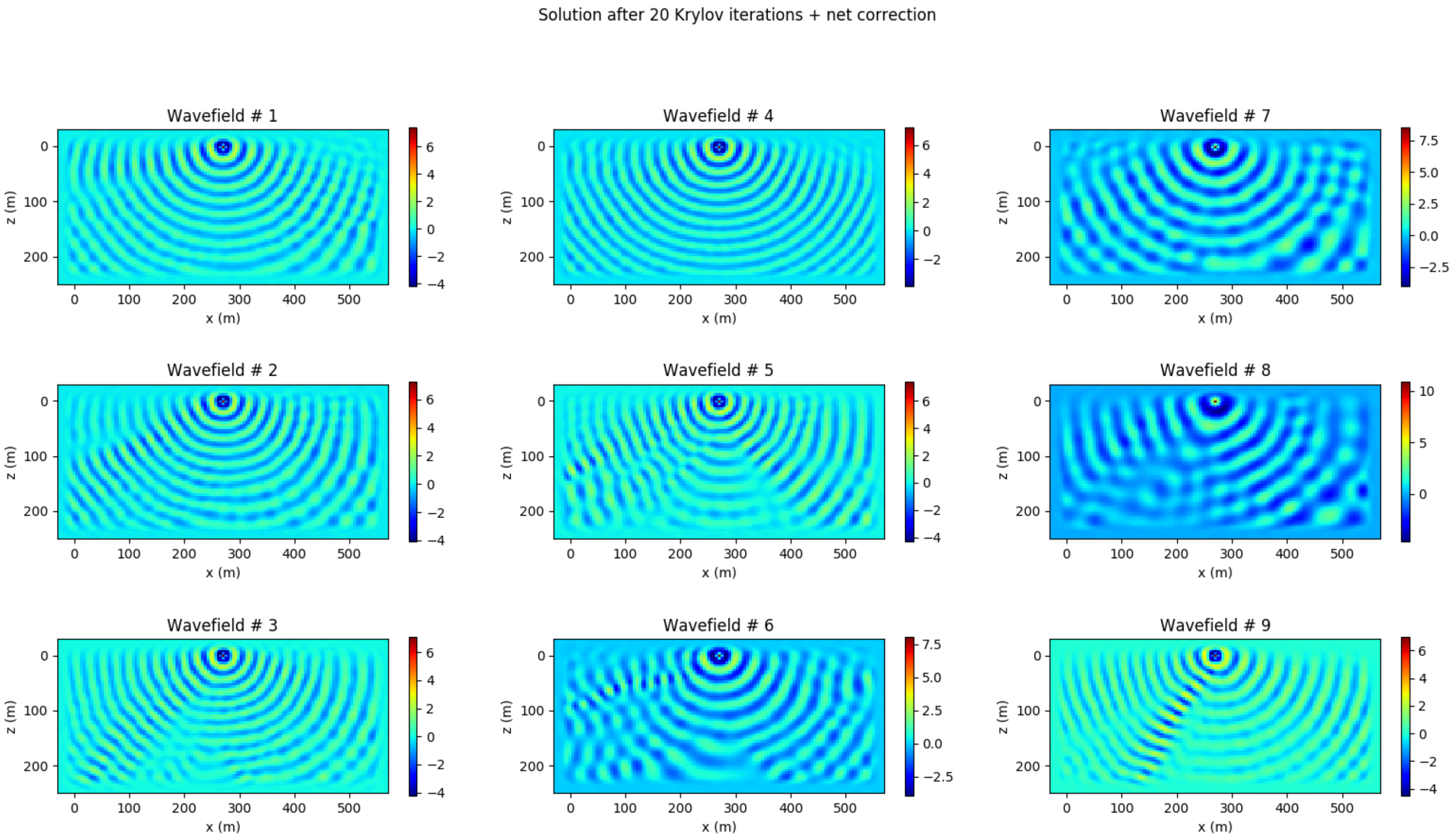
Example 2: solution wavefield at 60 Hz (after 10 Krylov iterations **+ net**)



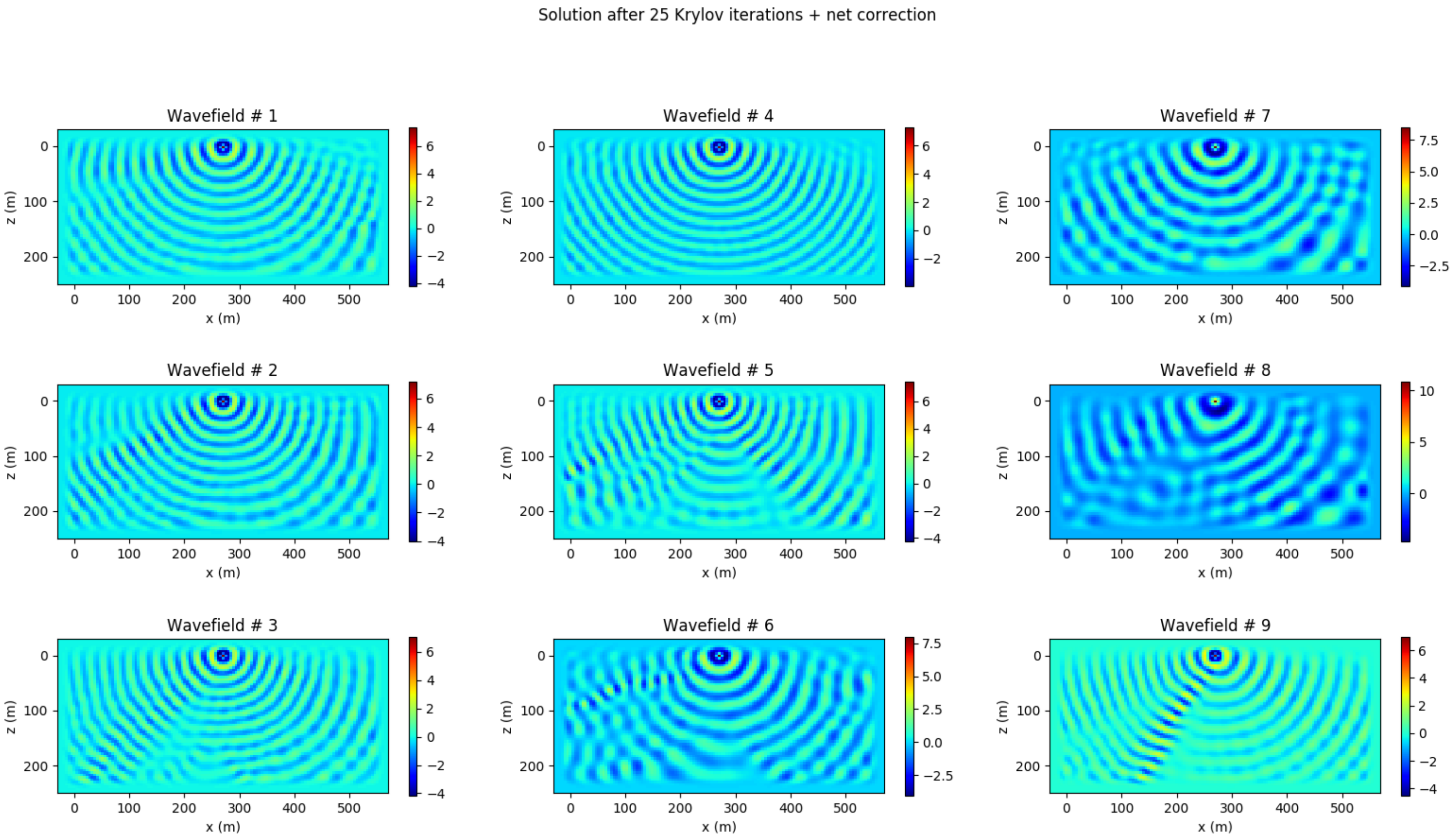
Example 2: solution wavefield at 60 Hz (after 15 Krylov iterations + net)



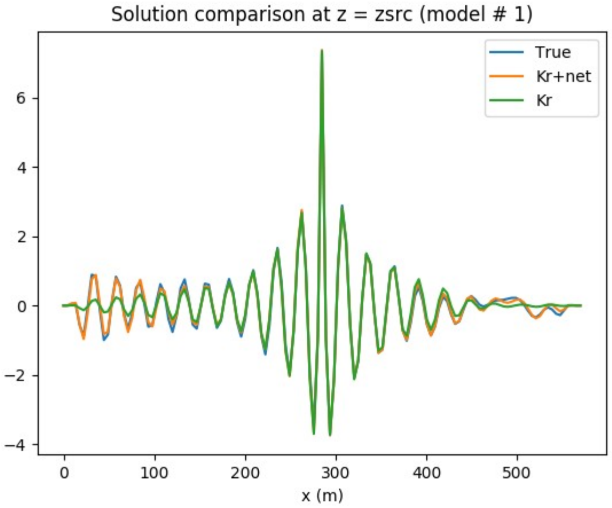
Example 2: solution wavefield at 60 Hz (after 20 Krylov iterations **+ net**)

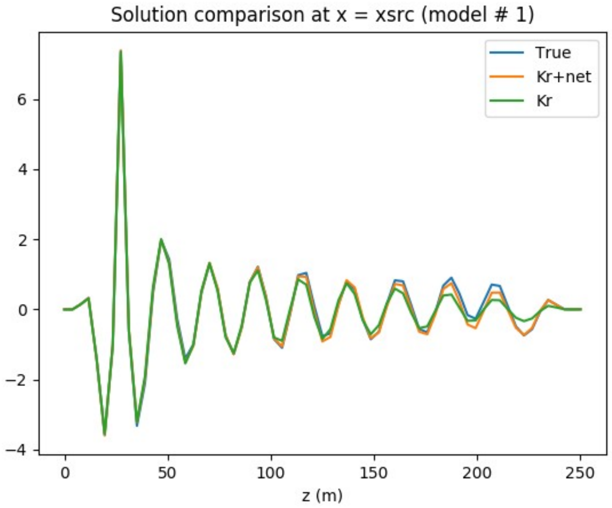


Example 2: solution wavefield at 60 Hz (after 25 Krylov iterations **+ net**)

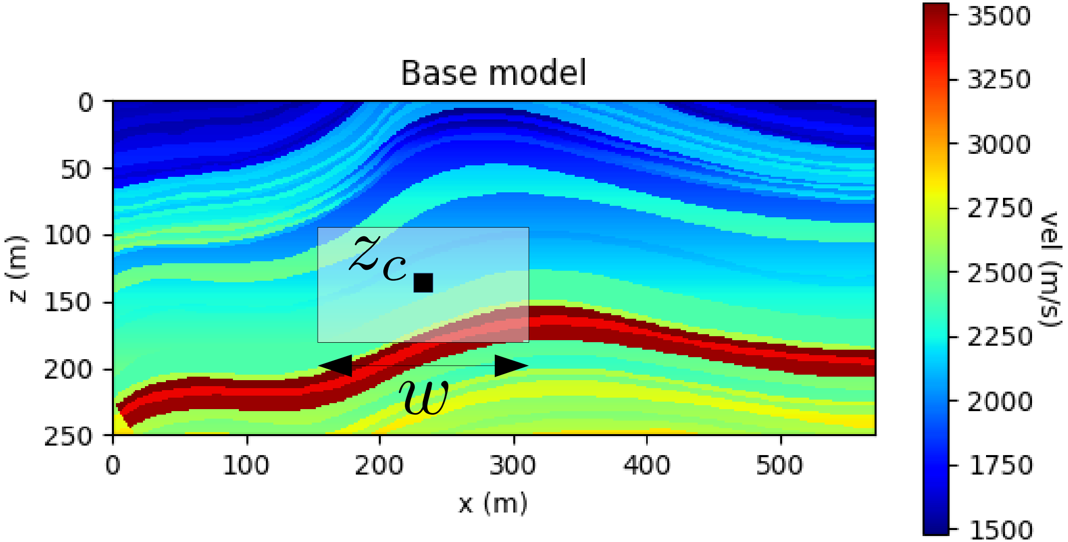


Example 2: solution trace comparison





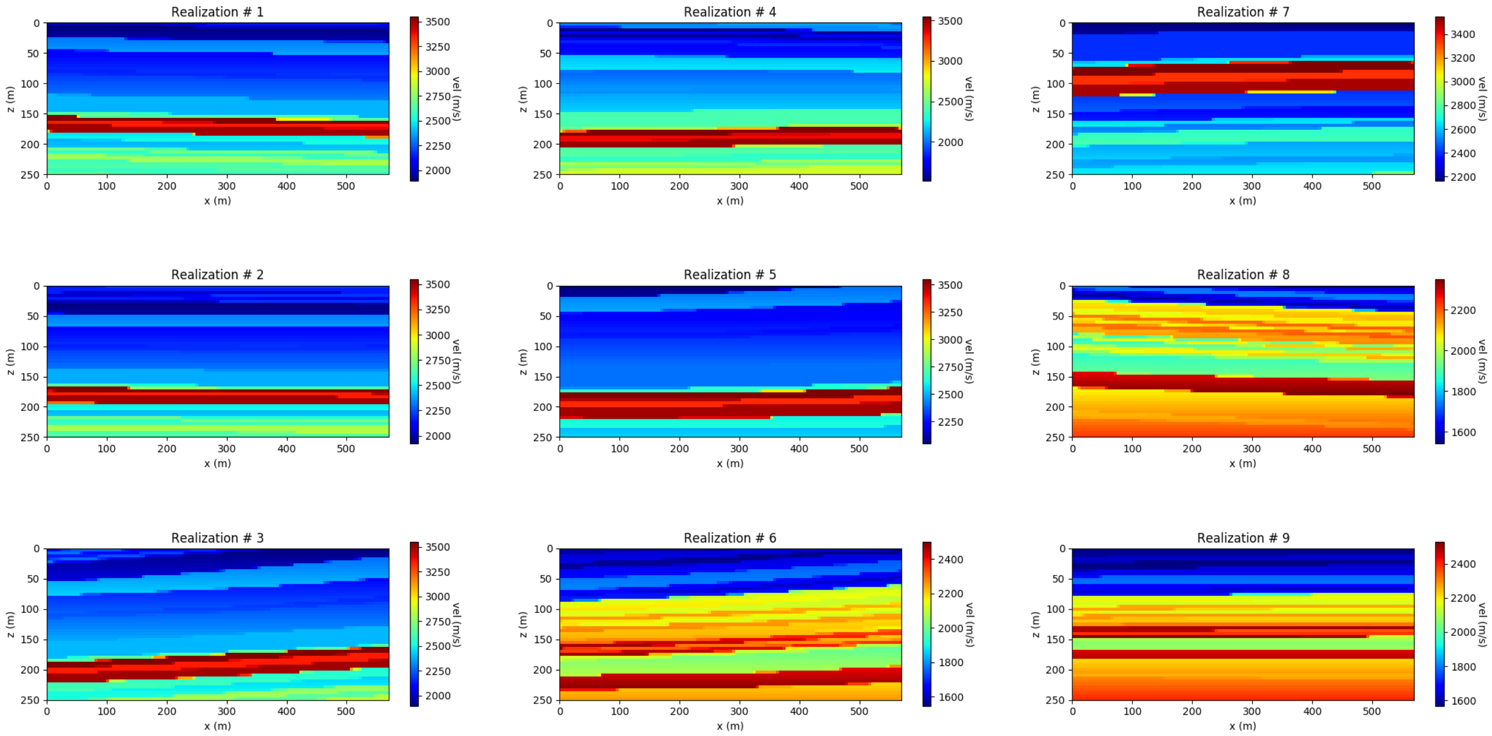
Example 2: testing generalization to different model distributions



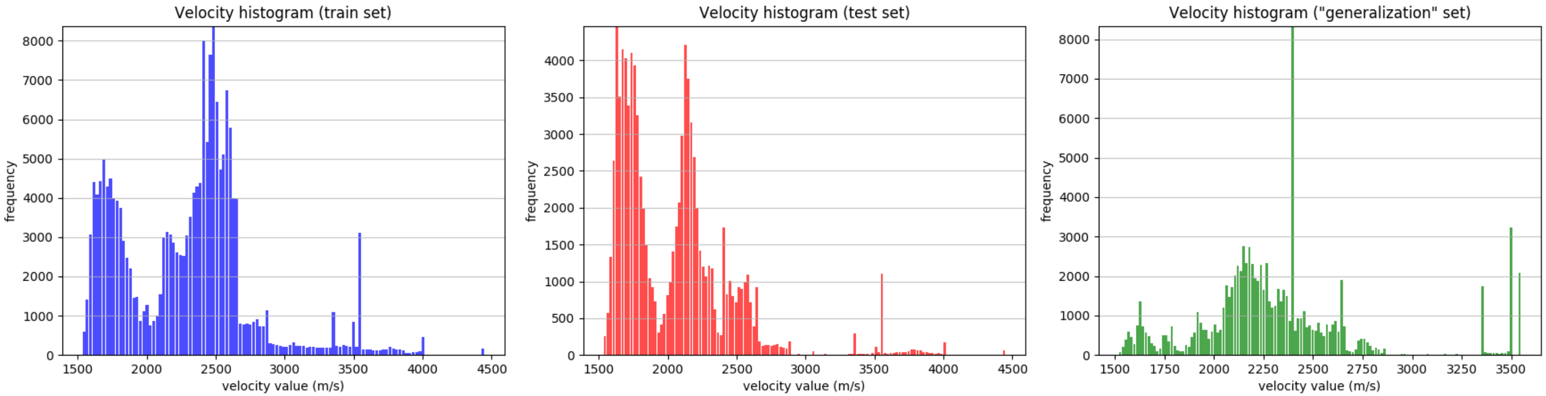
$$z_c \sim U(z_0, z_{\text{end}}) \qquad w \sim w_0 + U(-a, a)$$

Example 2: Marmousi-like distribution (generalization test size: 16)

Generalization test set excerpt



Example 2: Train/test errors



$$L = \sqrt{\sum_i ||\mathbf{u}_i^{\mathrm{sol}} - \tilde{\mathbf{u}}_i||^2 / \sum_i ||\mathbf{u}_i^{\mathrm{sol}}||^2}$$

Final loss	Train error	Test error	“Generalization” error
Krylov iterations	37.6%	40.5%	32.3%
Krylov net	12.1%	12.9%	17.2%

Conclusions/Future plans

Possible improvements:

- GANs

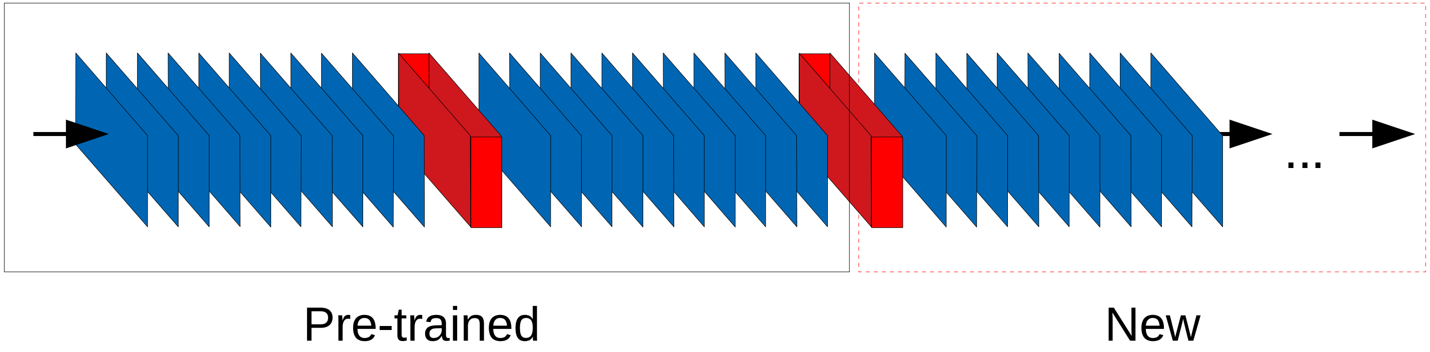
$D_\varphi : \mathcal{U} \to [0,1]$ discriminator

$$L(\theta,\varphi) = \mathbb{E}_{\mathbf{u}\sim p_U}(1 - D_\varphi(\mathbf{u}))^2 + \mathbb{E}_{\mathbf{m}\sim p_M}(D_\varphi \circ F_\theta(\mathbf{m}))^2 + \lambda \mathbb{E}_{\mathbf{m},\mathbf{u}\sim p_{M,U}} ||\mathbf{u} - F_\theta(\mathbf{m})||^2$$

Conclusions/Future plans

Possible improvements:

- GANs
- transfer learning: fine-tune net on a new model distribution



Conclusions/Future plans

Possible improvements:

- GANs
- transfer learning: fine-tune net on a new model distribution
- neural net architecture: inject linear operator residuals at each level and learn restriction/prolongation to beat indefiniteness

e.g., smoothing: $\mathbf{x}^h \leftarrow \mathbf{x}^h + N_\theta^h(\mathbf{r}^h)$

Conclusions/Future plans

Possible improvements:

- GANs
- transfer learning: fine-tune net on a new model distribution
- neural net architecture: inject linear operator residuals at each level and learn restriction/prolongation to beat indefiniteness
- multiscale loss function for unsupervised case

$$L = \sum_j ||R_h^{jh}(\mathbf{f} - H[\mathbf{m}]\, F_\theta(\mathbf{m}))||^2$$

Conclusions/Future plans

Possible improvements:

- GANs
- transfer learning: fine-tune net on a new model distribution
- neural net architecture: inject linear operator residuals at each level and learn restriction/prolongation to beat indefiniteness
- multiscale loss function for unsupervised case

Alternative applications/extensions:

- implicit time-stepping
- source-to-source / low-to-high frequency / acoustic-to-elastic transfer
- combination with learned reconstruction operators

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