

# Large-scale workflows for wave-equation based inversion in Julia

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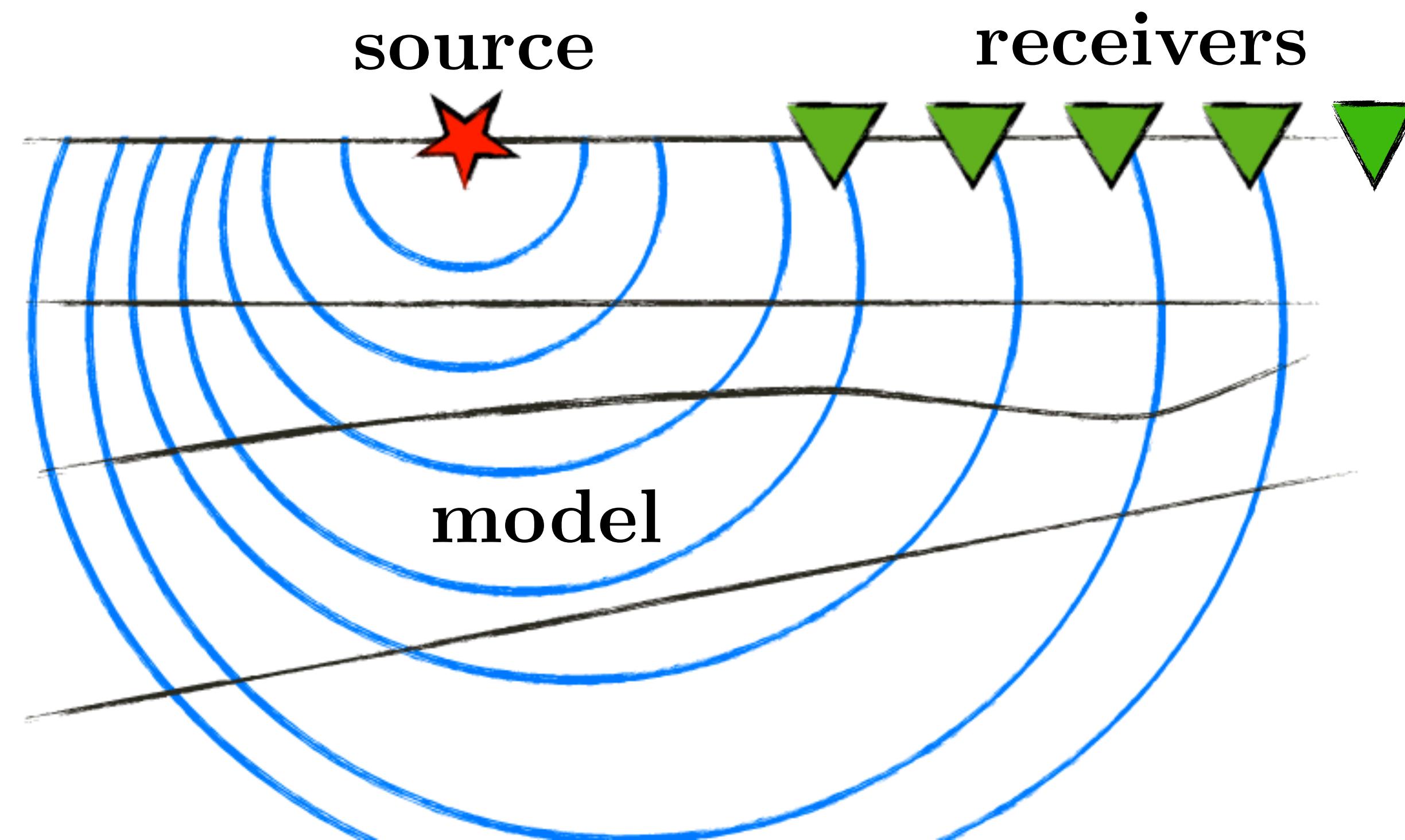


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# Motivation

Use Geophysics to understand the earth

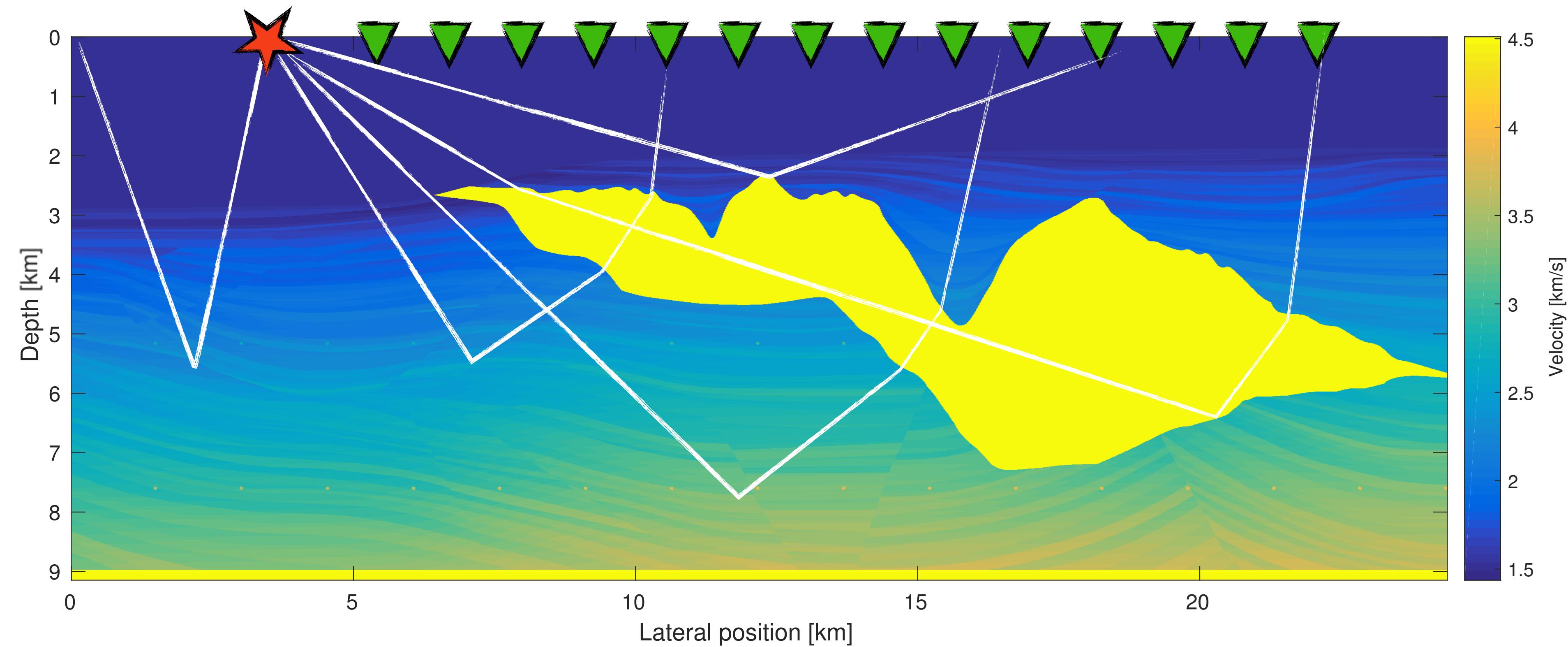
- ▶ obtain information about the earth from surface seismic experiments



# Motivation

Use Geophysics to understand the earth

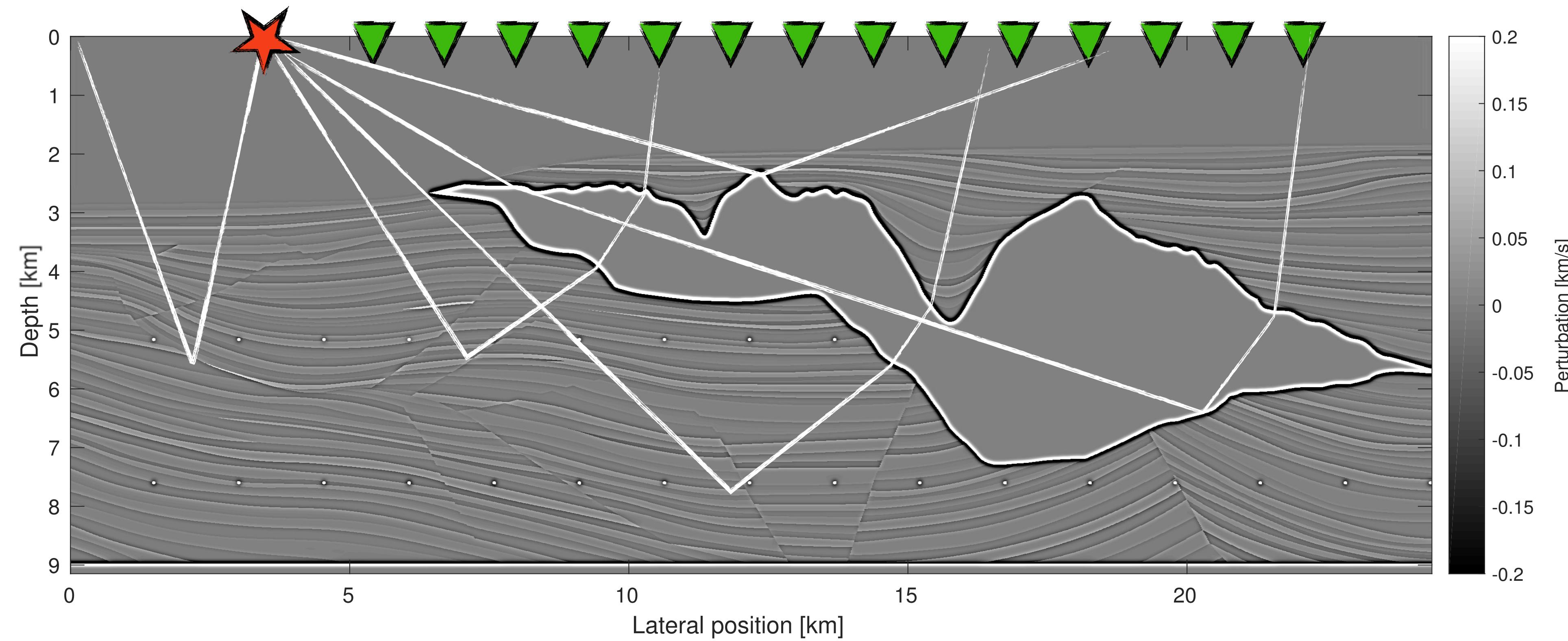
- ▶ invert for subsurface parameters, e.g. velocity, density, porosity



# Motivation

Use Geophysics to understand the earth

- ▶ image geological interfaces (perturbations of earth parameters)



# Motivation

Formulate inverse problems and use numerical optimization

- invert for velocity → nonlinear least squares optimization problem

$$\underset{\mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{A}(\mathbf{m}) \cdot \mathbf{q} - \mathbf{d}\|_2^2 \quad (\text{Virieux and Operto, 2009})$$

- image the subsurface → linear least squares optimization problem

$$\underset{\delta\mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{J} \cdot \delta\mathbf{m} - \delta\mathbf{d}\|_2^2 \quad (\text{Dong et al., 2012})$$

Need:

- access to objective function values and gradients
- matrices  $\mathbf{A}(\mathbf{m})$   $\mathbf{J}$ , or actions of these matrices on vectors

# Motivation

## Challenges:

- ▶ problem sizes are huge:
  - seismic surveys consist of tens of thousands of individual experiments
  - model wave propagation over thousands of time steps in large domains
  - typical size of modeling matrix  $\mathbf{A}(\mathbf{m}) \in \mathbb{R}^{n \times n}$ ,  $n = 1e16$
- ▶ model physical system → data is irregular, has coordinates and meta data
- ▶ inverse problems are difficult to solve (ill-posed, non-convex, non-unique)
- ▶ software to solve seismic inverse problems:
  - needs to be fast and handle large amounts of data
  - often tailored towards a specific application
  - difficult to maintain and modify, often slow adaptation of new concepts

# Motivation

Our goal:

- ▶ flexible framework for solving seismic inverse problems
- ▶ abstract matrices and vectors to easily formulate algorithms
- ▶ data containers for irregular seismic data
- ▶ robust parallel framework that scales on HPC environments/the cloud
- ▶ interface Devito (finite difference DSL) to solve PDEs
- ▶ framework that can handle actual 3D industry-sized problems
  - lower computational costs using stochastic optimization

## The forward problem

Solve (acoustic) wave equation for a given model

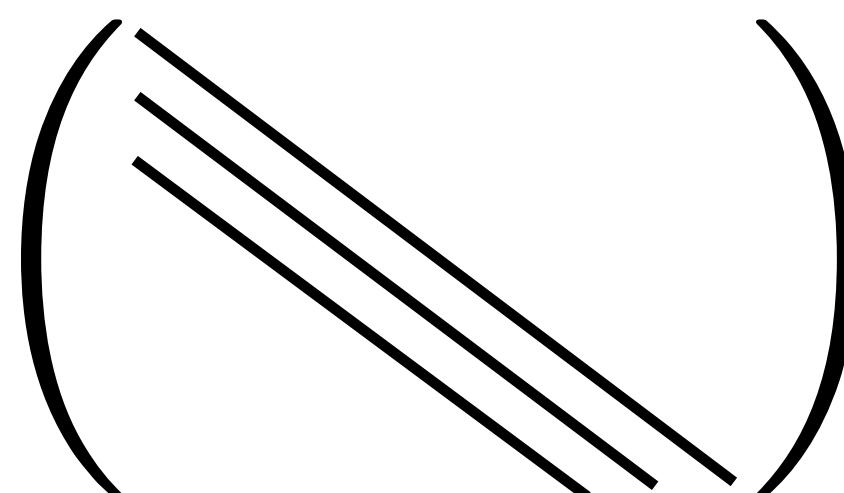
- ▶ continuous form

$$m \frac{\partial^2}{\partial t^2} u - \nabla^2 u = s$$

*m*: model parameters (slowness squared)  
*u*: wave fields  
*s*: source wave fields

- ▶ discretize and rewrite as linear system

$$\mathbf{A} \cdot \mathbf{u} = \mathbf{s}$$



$\mathbf{A}$  is lower triangular, solve with forward elimination

# The forward problem

Model surface recorded seismic data

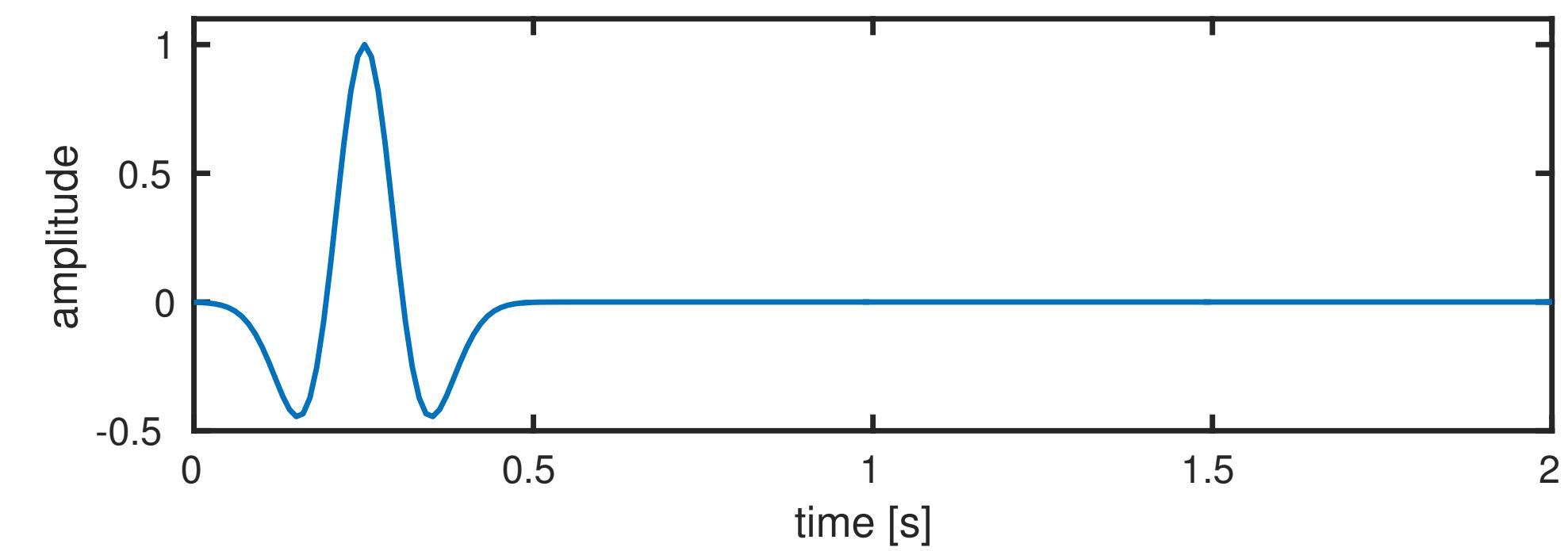
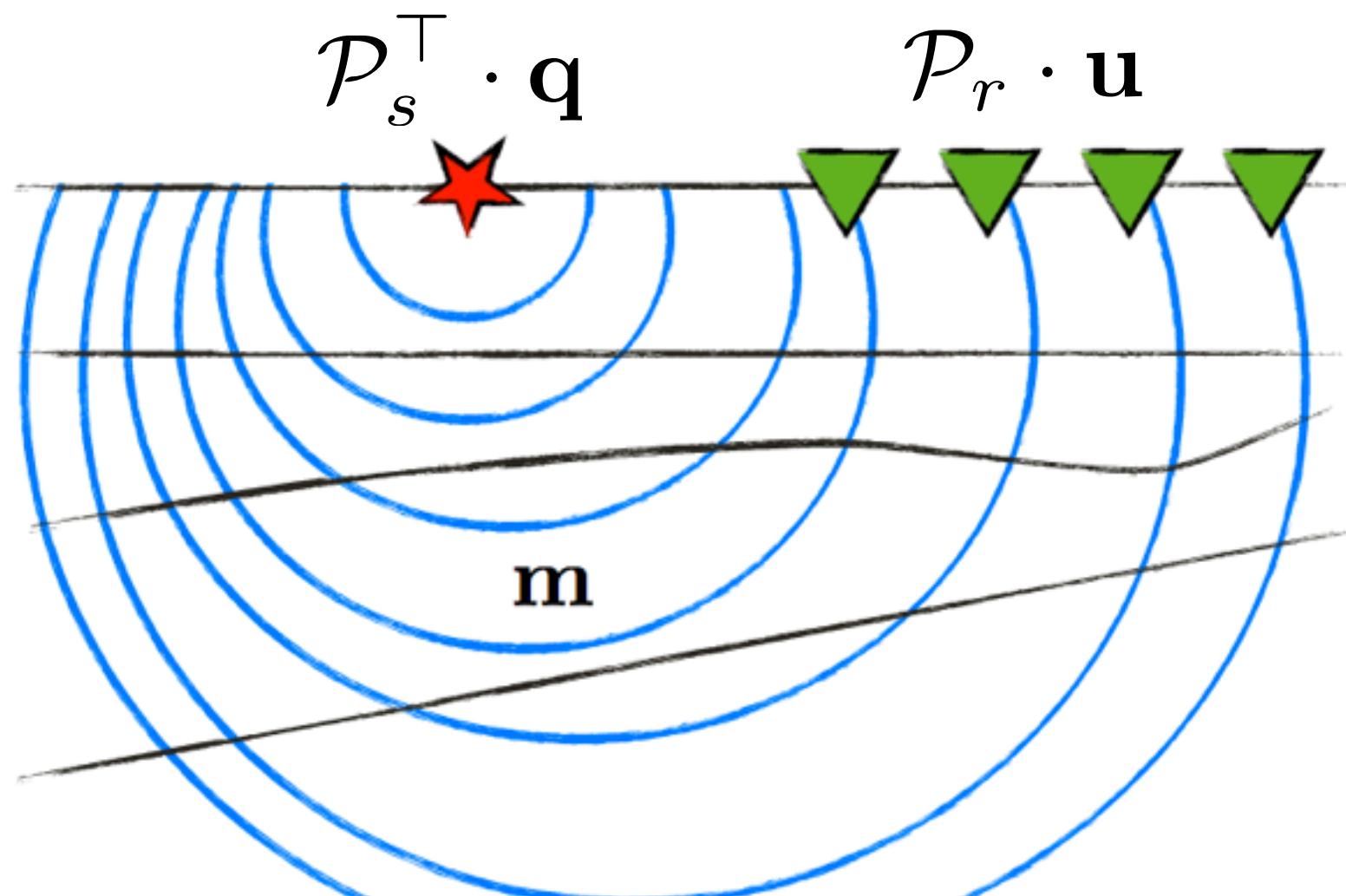
$$\mathbf{d} = \mathcal{P}_r \cdot \mathbf{F} \cdot \mathcal{P}_s^\top \cdot \mathbf{q}$$

$$\mathbf{F} := \mathbf{A}(\mathbf{m})^{-1}$$

$\mathcal{P}_r$ : receiver restriction

$\mathcal{P}_s^\top$ : source injection

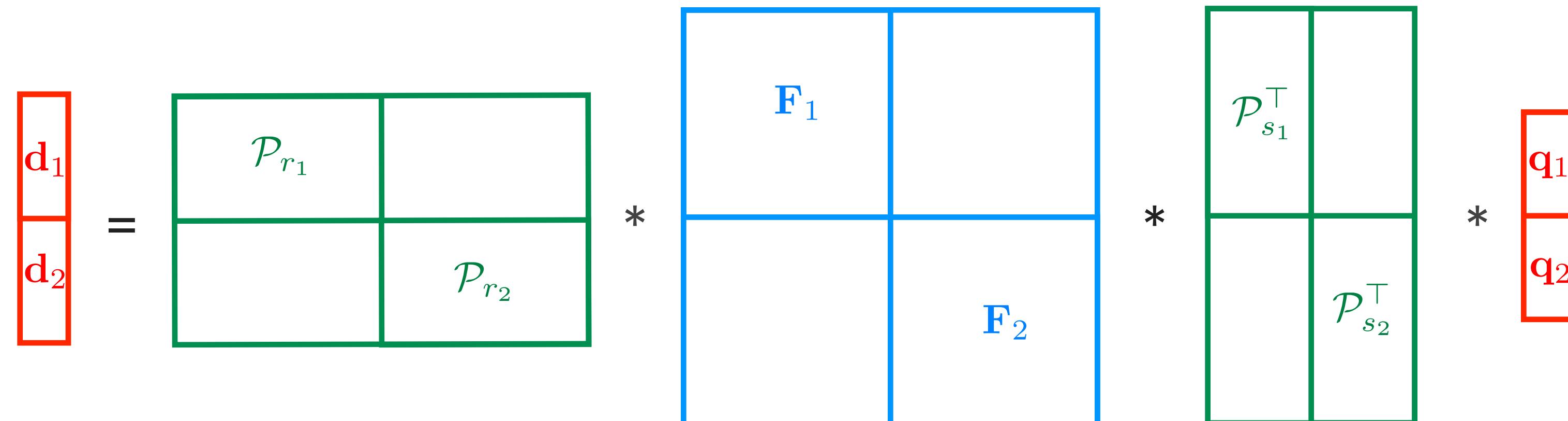
$\mathbf{q}$ : source wavelet



# The forward problem

Model surface recorded seismic data (2 experiments)

$$\mathbf{d} = \mathcal{P}_r \cdot \mathbf{F} \cdot \mathcal{P}_s^\top \cdot \mathbf{q}$$



- ▶ can barely store  $\mathbf{d}$  ( $1e11 \times 1$ )
- ▶ cannot store  $\mathcal{P}_s^\top \cdot \mathbf{q}$  ( $1e16 \times 1$ )
- ▶ cannot form  $\mathbf{F}, \mathcal{P}_r, \mathcal{P}_s$  explicitly ( $1e16 \times 1e16$ )

# The forward problem

Adapt idea of matrix-free linear operators

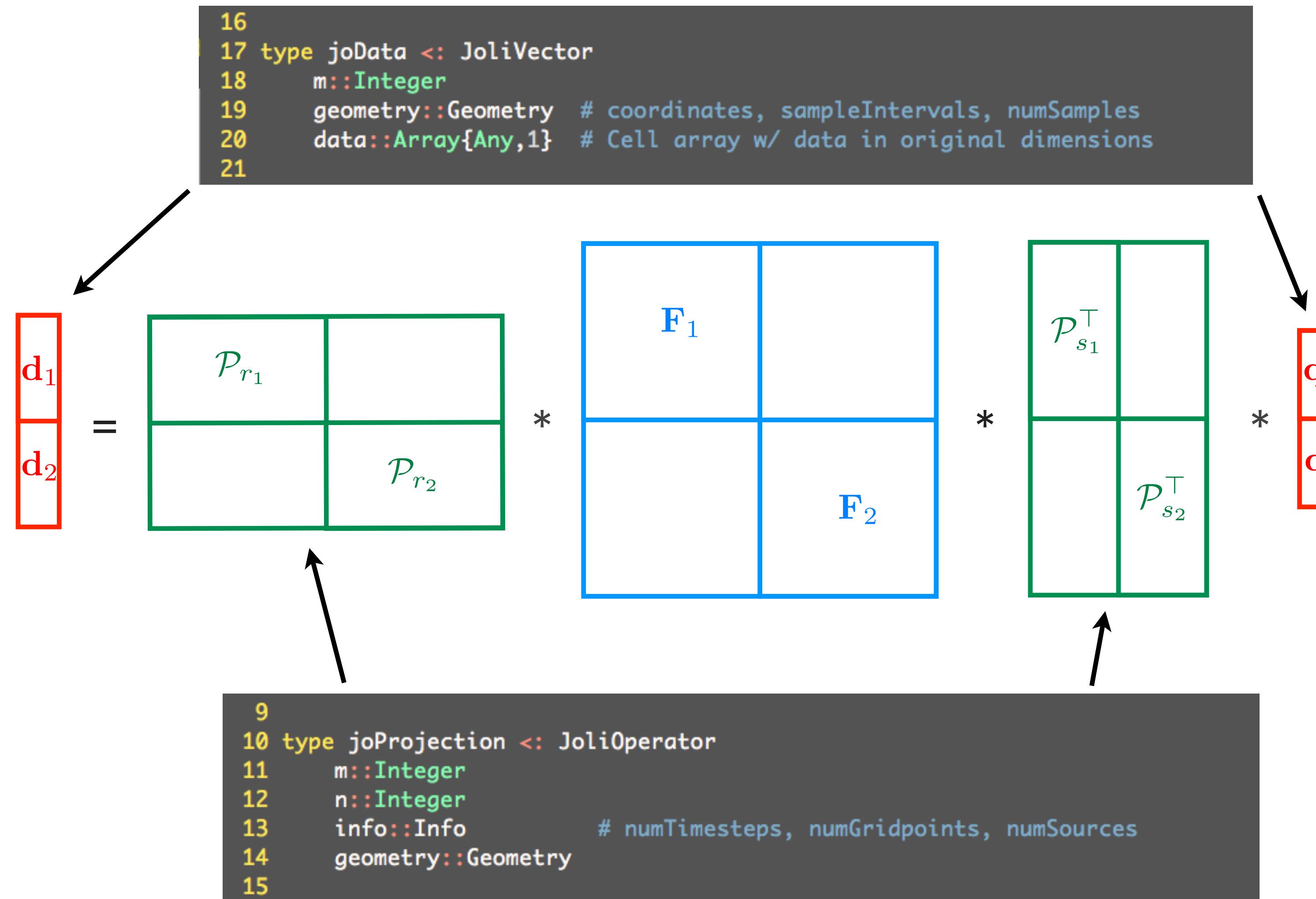
- ▶ SPOT - a linear operator toolbox in Matlab(van den Berg and Friedlander, 2012)
- ▶ operators look and behave like explicit matrices
- ▶ matrix “knows” how to apply itself to vectors
- ▶ forward, adjoint matrix-matrix, matrix-vector products etc.

```
>> n = 1e3;
>> % Set up operator
>> F = opDFT(n)
F =
    Spot operator: DFT(1000,1000)
        rows: 1000      complex: yes
        cols: 1000      type: DFT
>> % FFT
>> y = F*x;
>> % iFFT
>> z = F'*y;
```

# The forward problem

Implement abstract linear operators and vectors in Julia

- JOLI - Julia Operator Library



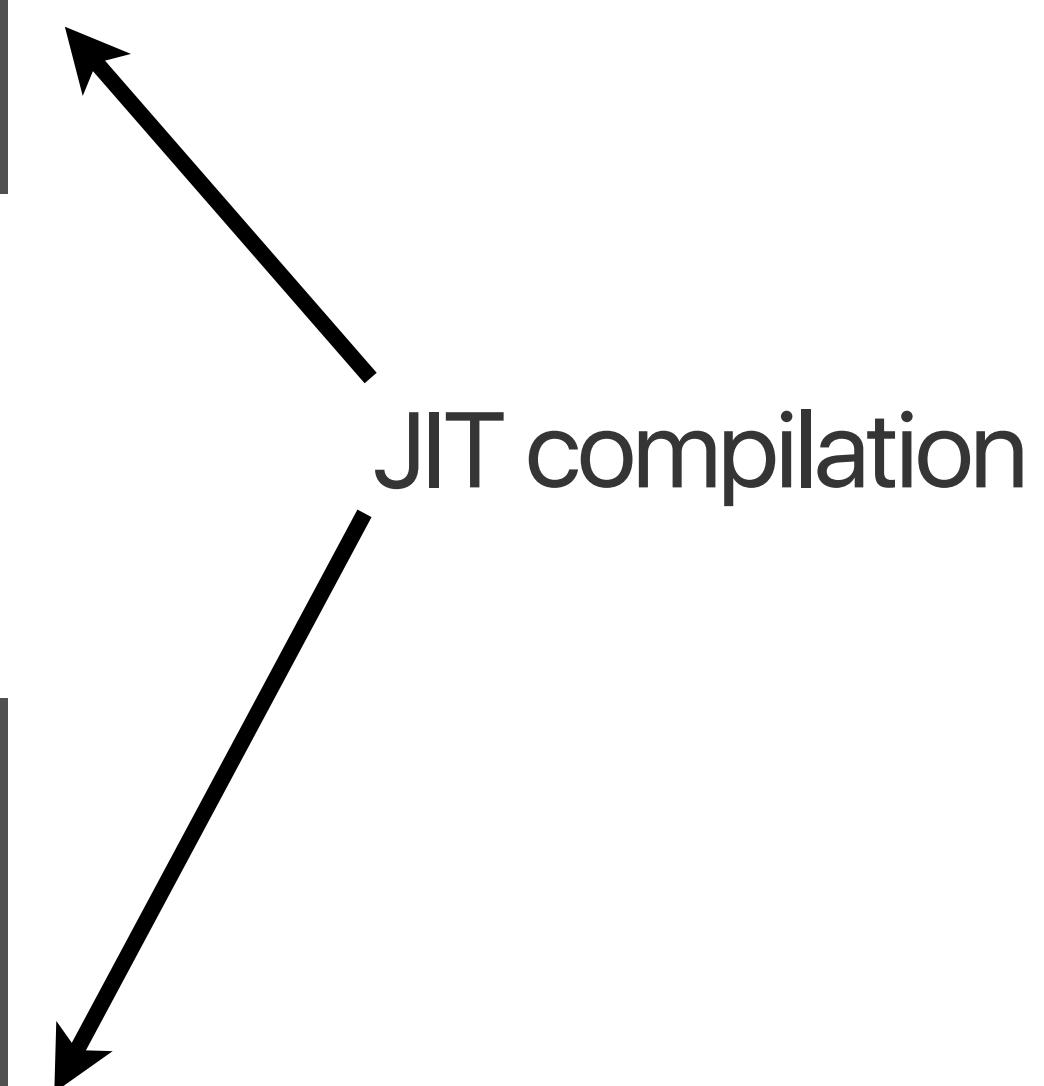
# The forward problem

Solve forward wave equation:

```
julia> d = Pr*F*Ps'*q
      From worker 5: Nonlinear forward modeling (source no. 2)
      From worker 4: Nonlinear forward modeling (source no. 3)
      From worker 3: Nonlinear forward modeling (source no. 4)
      From worker 2: Nonlinear forward modeling (source no. 1)
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/3443b8b1660866d91815a00df85b3a6cceed7ed9.c [0.20 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/83f4ea5a3ee3ebf1c51e1243816b457c431b50c7.c [0.22 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/415a7b8d0cf2663d3c552655b56bf924e343a30f.c [0.21 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/8ac99a871f7a68ef619460c7a5cdcfb1f2e58dd3.c [0.20 s]
(TimeModeling.joData{Float32}, "Julia seismic data container", 161555, 1)
```

Solve adjoint wave equation:

```
julia> q̂ = Ps*F'*Pr'*d
      From worker 4: Nonlinear adjoint modeling (source no. 4)
      From worker 3: Nonlinear adjoint modeling (source no. 3)
      From worker 2: Nonlinear adjoint modeling (source no. 2)
      From worker 5: Nonlinear adjoint modeling (source no. 1)
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/f43d668c3bca252a307acf2dbe0c51417a8a6f01.c [0.20 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/a0dbc0f7d088b2073dadeb15929a7347e244d417.c [0.21 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/87d901287ff2ce08855dde4c08fa9e825b5b1562.c [0.20 s]
CustomCompiler: compiled /tmp/pwittCT5MeP/devito-4080/3d1cb82e3ac510f999869dee3c5af806adedd5ab.c [0.21 s]
(TimeModeling.joData{Float32}, "Julia seismic data container", 1971, 1)
```



# Software design

What happens after executing the modeling command?

```
julia> d = Pr*F*Ps'*q
```

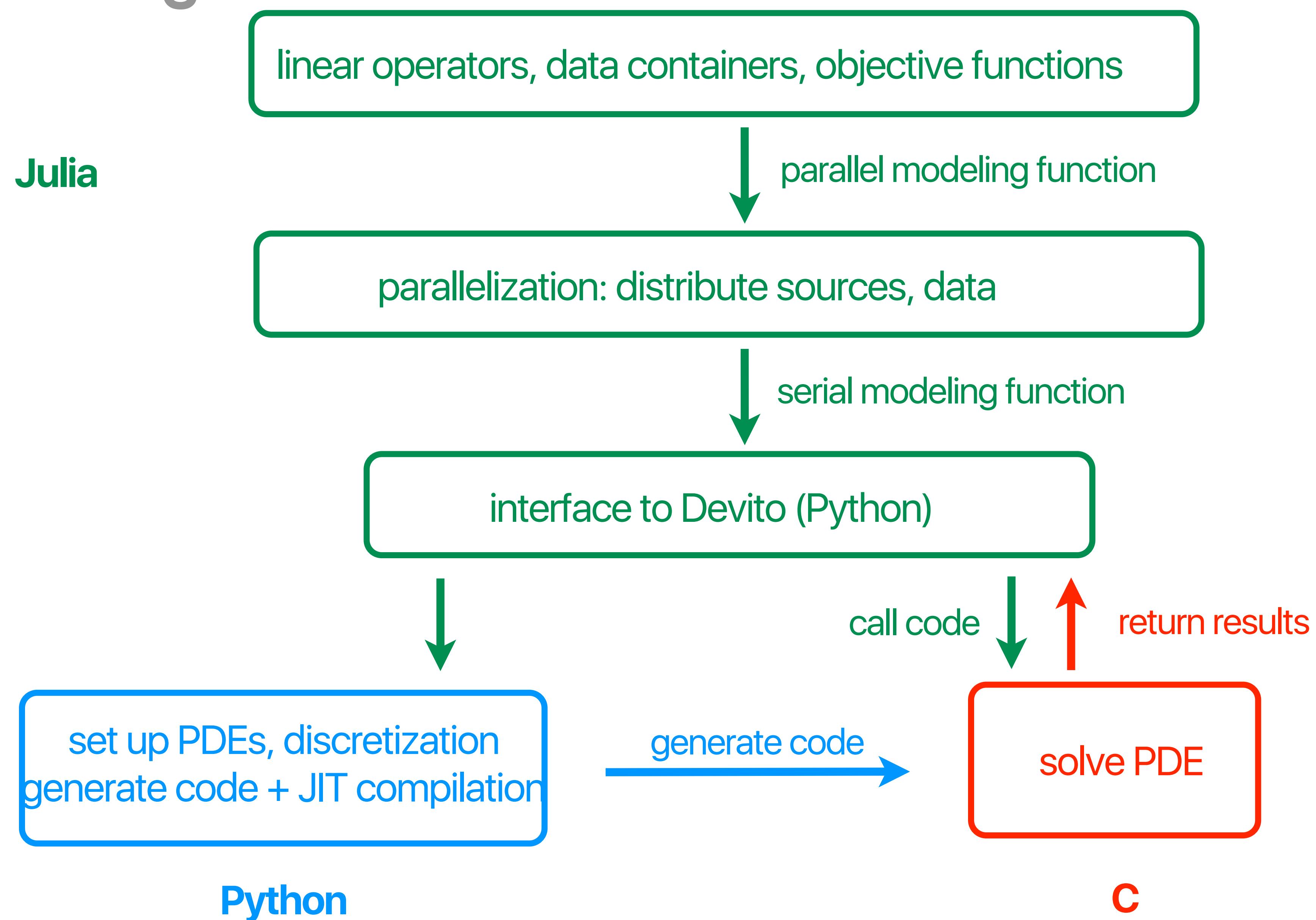


- ▶ check that dimensions are correct
- ▶ check that geometries match

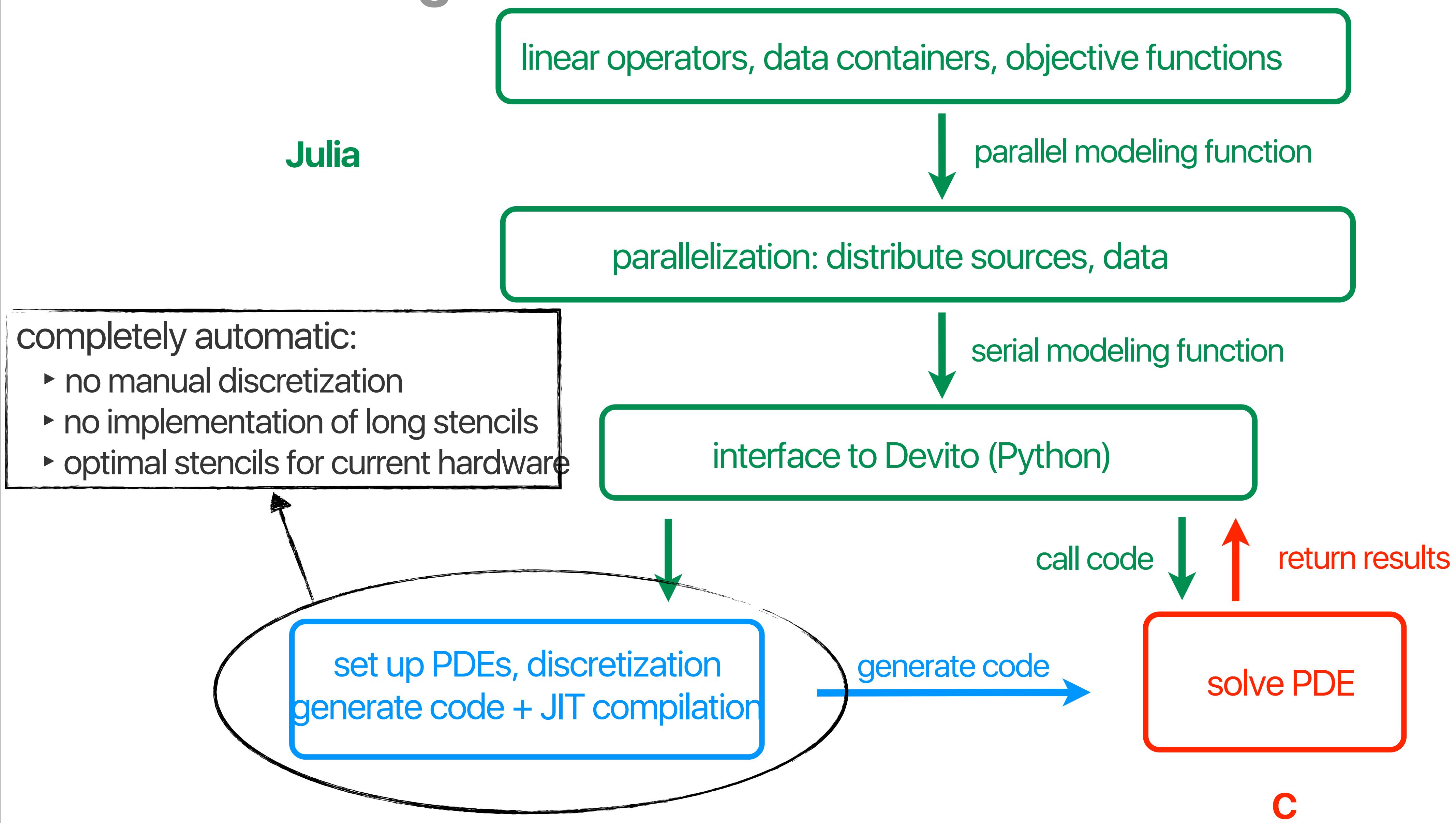
```
julia> time_modeling(model,srcGeometry,srcData,recGeometry,recData,'F',1)
```

- ▶ call serial/parallel modeling function
- ▶ set function arguments with parameters from linear operators

# Software design



# Software design



# The inverse problem

## Inverse problem

- ▶ invert model for given data
- ▶ how does a perturbation in the model relate to a perturbation in the wave field?

$$\mathbf{u} = \mathbf{A}(\mathbf{m})^{-1} \cdot \mathbf{q}$$

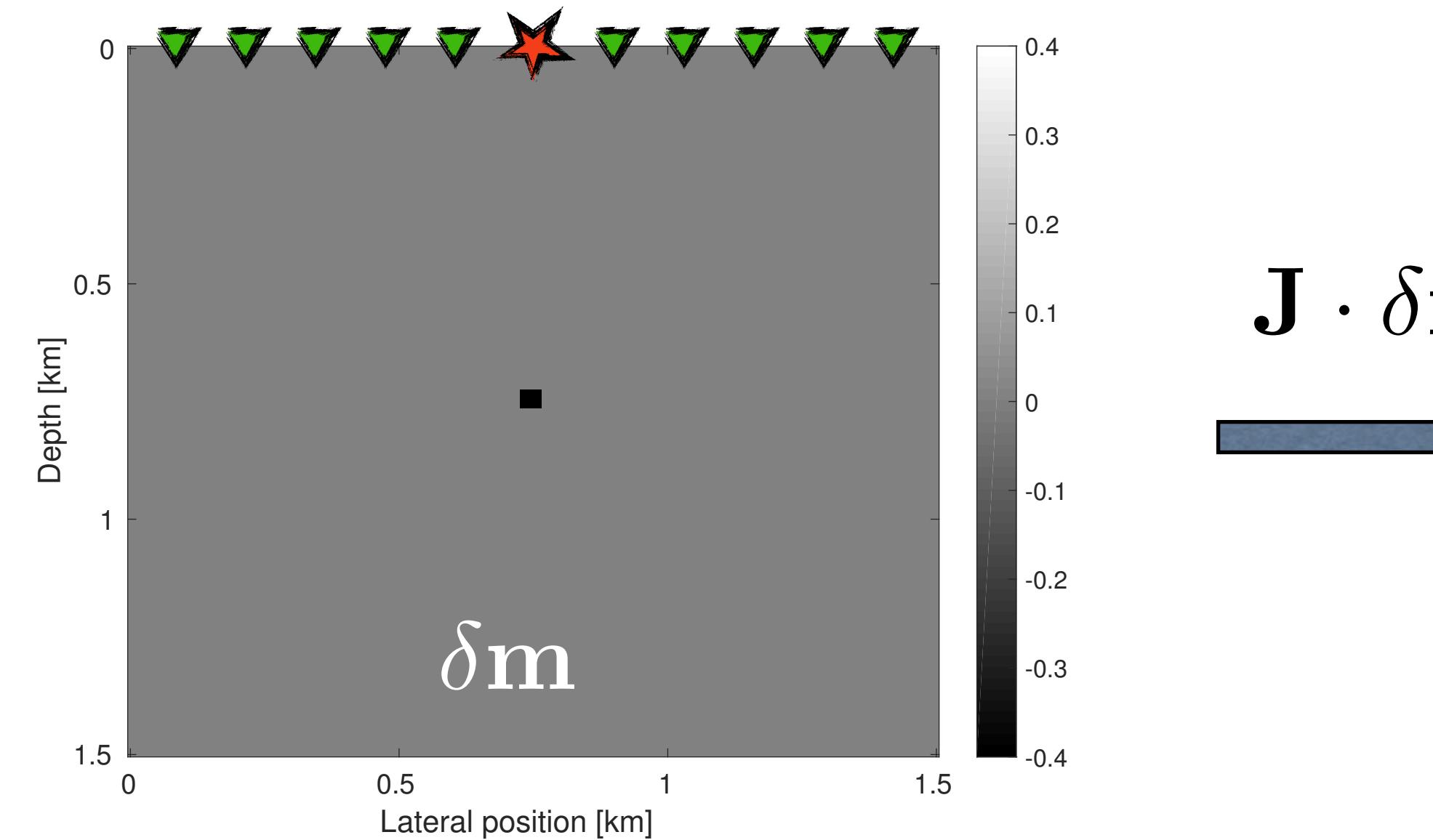
$$\frac{\partial \mathbf{u}}{\partial \mathbf{m}} = \frac{\partial}{\partial \mathbf{m}} \left( \mathbf{A}(\mathbf{m})^{-1} \cdot \mathbf{q} \right) := \mathbf{J} \quad (\text{Jacobian})$$

(Virieux and Operto, 2009)

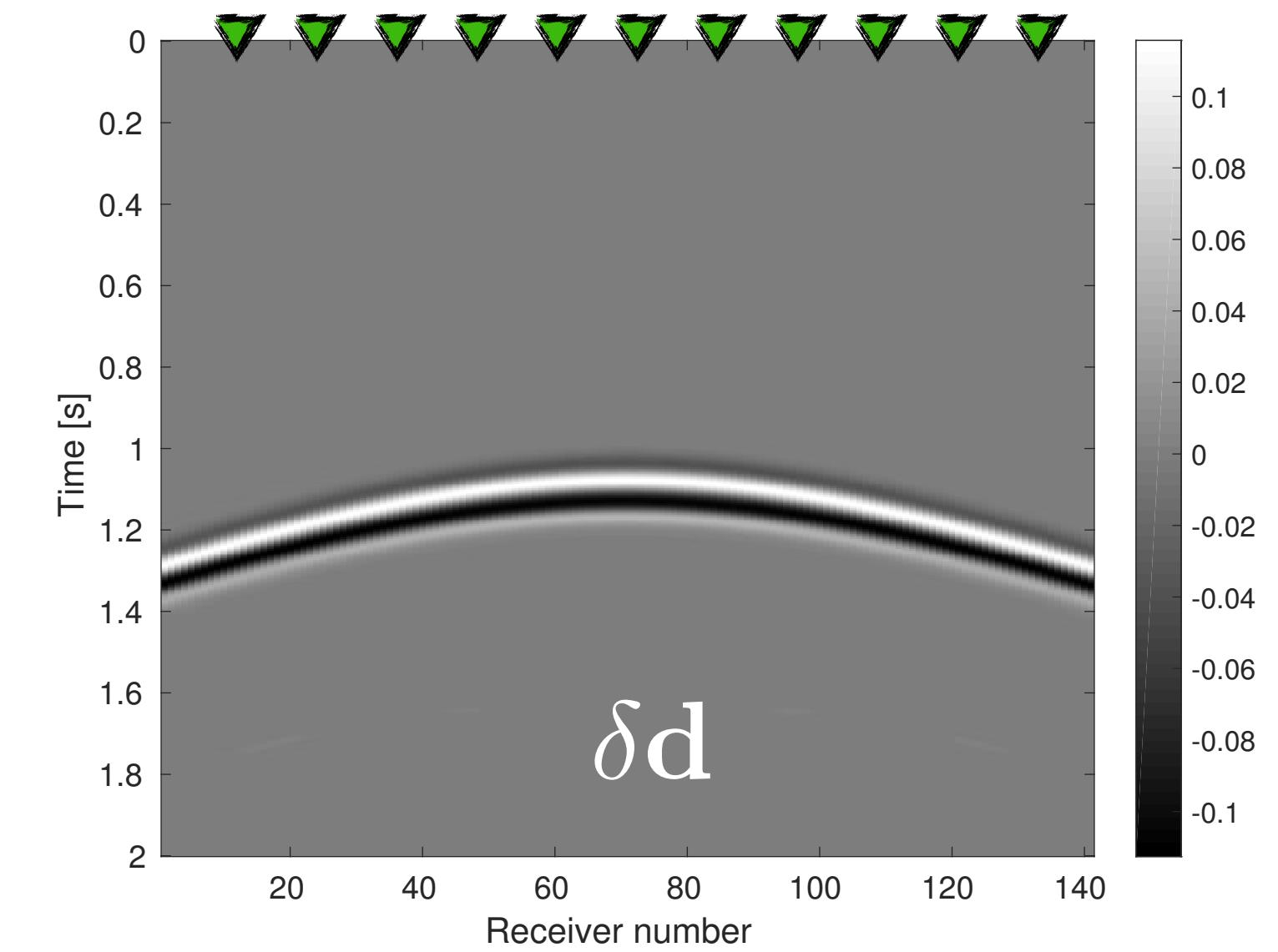
- ▶ including source/receiver projections:

$$\mathbf{J} = -\mathcal{P}_r \cdot \mathbf{A}(\mathbf{m})^{-1} \cdot \frac{\partial \mathbf{A}(\mathbf{m})}{\partial \mathbf{m}} \cdot \mathbf{A}(\mathbf{m})^{-1} \cdot \mathcal{P}_s^\top \cdot \mathbf{q}$$

# The inverse problem

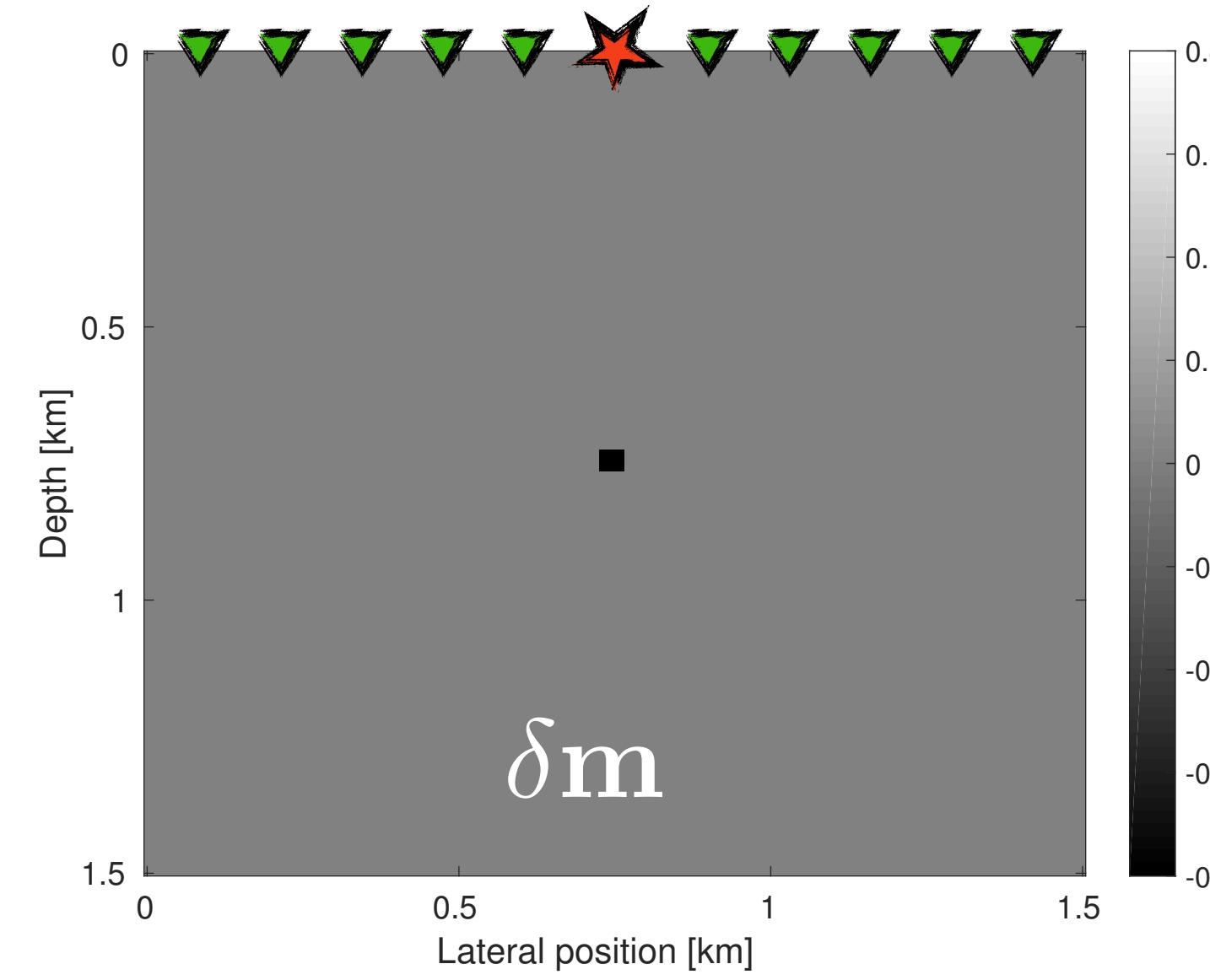


Perturbation w.r.t background model



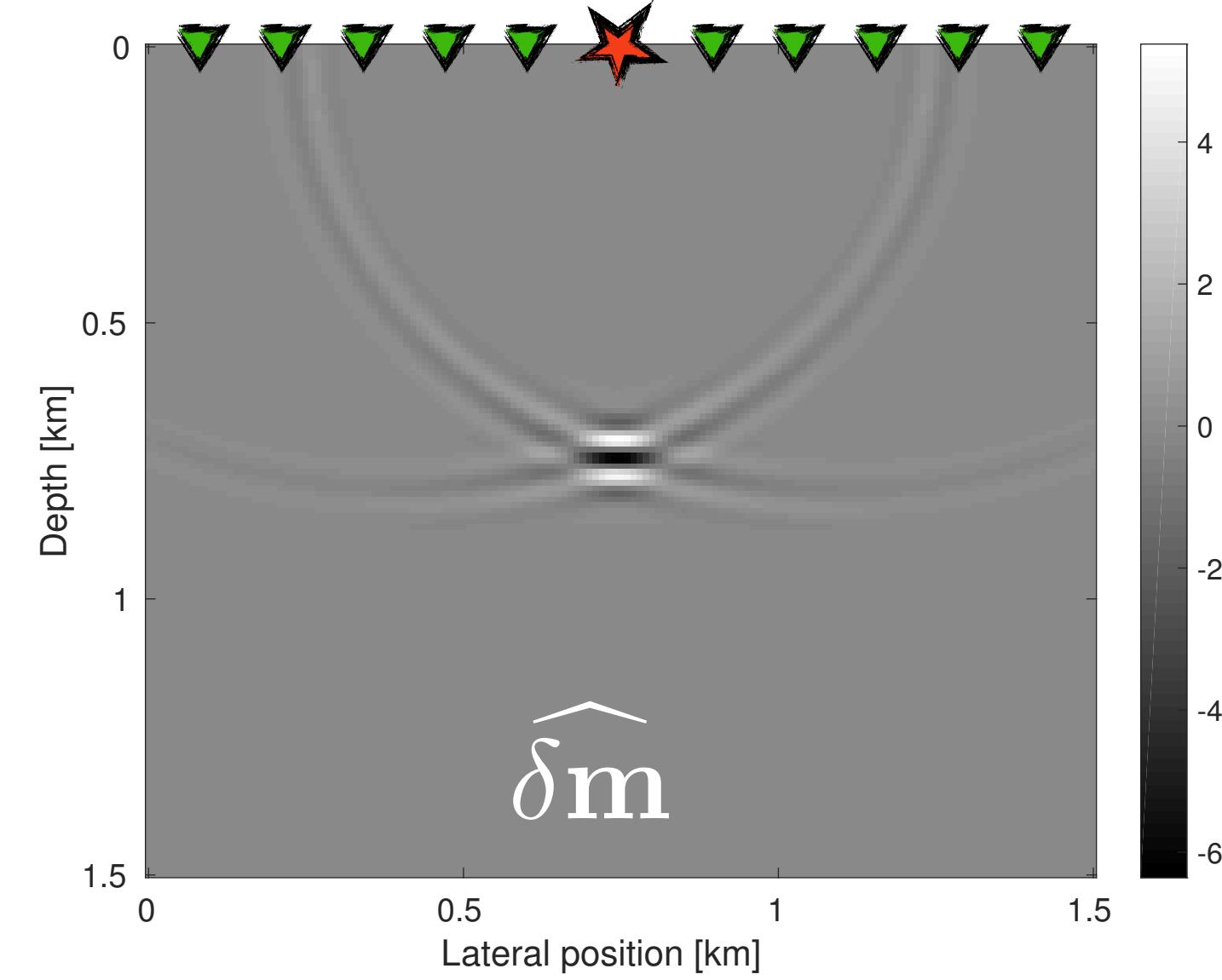
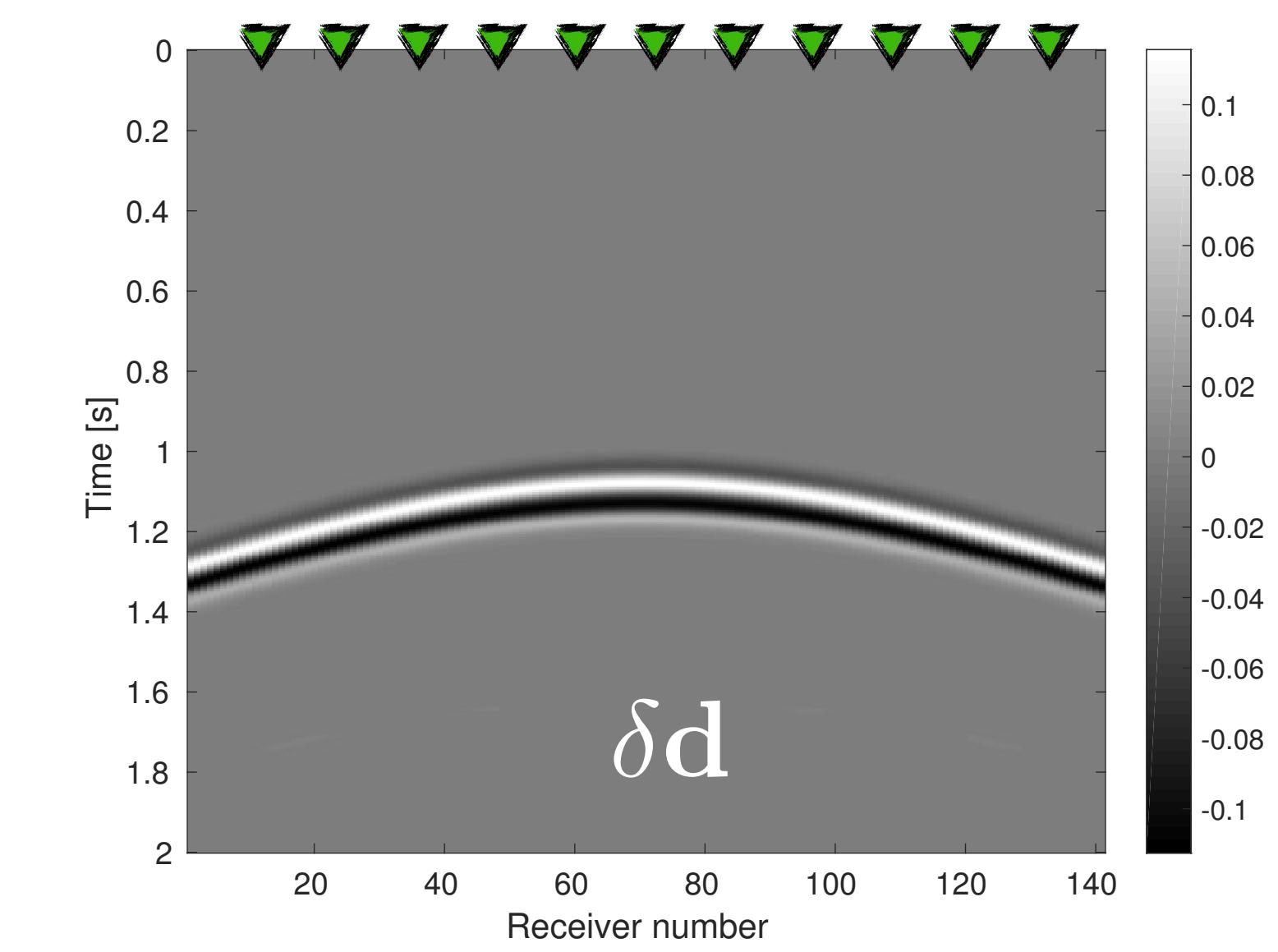
Surface recorded seismic data

# The inverse problem



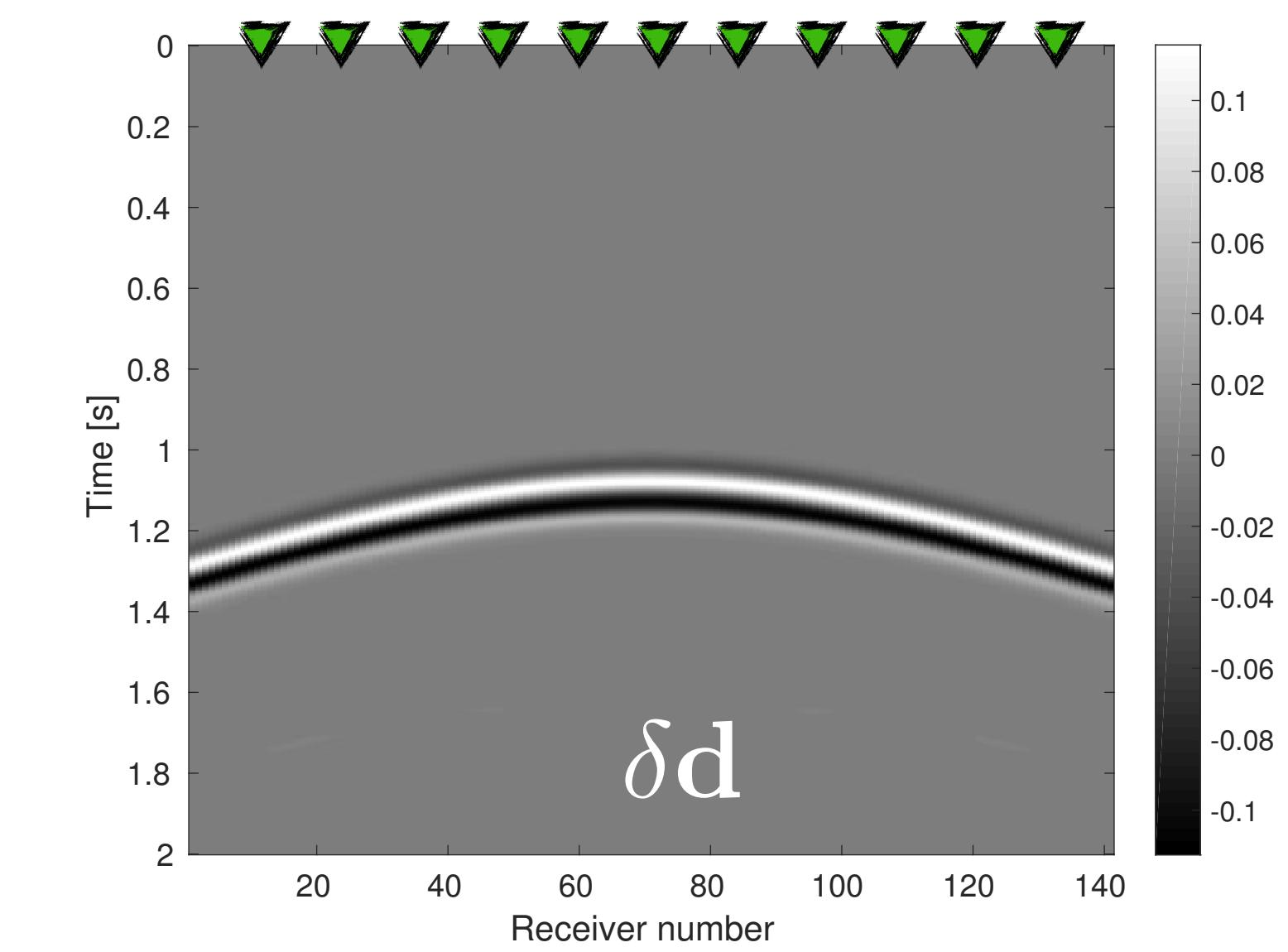
$\mathbf{J} \cdot \delta\mathbf{m}$

“modeling”



$\mathbf{J}^\top \cdot \delta\mathbf{d}$

“imaging”



# Linear inverse problems: seismic imaging

Seismic imaging as a linear least squares problem

(Dong et al., 2012)

- ▶ objective function:

$$\underset{\delta \mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{J} \cdot \delta \mathbf{m} - \delta \mathbf{d}\|_2^2 \quad (\mathbf{J} \in \mathbb{R}^{m \times n}, m > 1e11, n > 1e9)$$

- ▶ easy to implement a solver using JOLI operators:

```
2 # initialize solution
3 dm = zeros(n)
4
5 for j=1:k
6     # residual and gradient
7     r = J*dm - d
8     g = J'*r
9
10    # step size
11    t = norm(r)^2/norm(g)^2
12
13    # update x
14    dm -= t*g
15 end
```

# Seismic least squares imaging

## Seismic imaging as a linear least squares problem

- $\mathbf{J}$  is ill-conditioned and very large, can only afford 10s of iterations, need to ~~solve~~<sup>[7]</sup> ( $\sim$ TB)
- reduce computational cost using techniques from stochastic optimization  
(Yin, 2010)
- linearized Bregman method

$$\underset{\delta \mathbf{m}}{\text{minimize}} \quad \lambda \|\mathbf{x}\|_1 + \frac{1}{2} \|\mathbf{x}\|_2^2$$

$$\text{subject to: } \|\mathbf{A} \cdot \mathbf{x} - \mathbf{b}\|_2 \leq \sigma$$

$\lambda$ : thresholding parameter  
 $\sigma$ : noise level

$$\mathbf{A} \in \mathbb{R}^{m \times n}, m \ll n$$

- designed for compressive sensing problems with

$$\mathbf{A} \in \mathbb{R}^{m \times n} \quad (\text{Lorenz et al., 2014})$$

- related to sparse (block-) Kaczmarz solver for problems w/ any

# Seismic least squares imaging

Linearized Bregman method for least squares imaging:

$$\underset{\delta \mathbf{m}}{\text{minimize}} \quad \lambda \|\mathbf{C} \cdot \delta \mathbf{m}\|_1 + \frac{1}{2} \|\mathbf{C} \cdot \delta \mathbf{m}\|_2^2$$

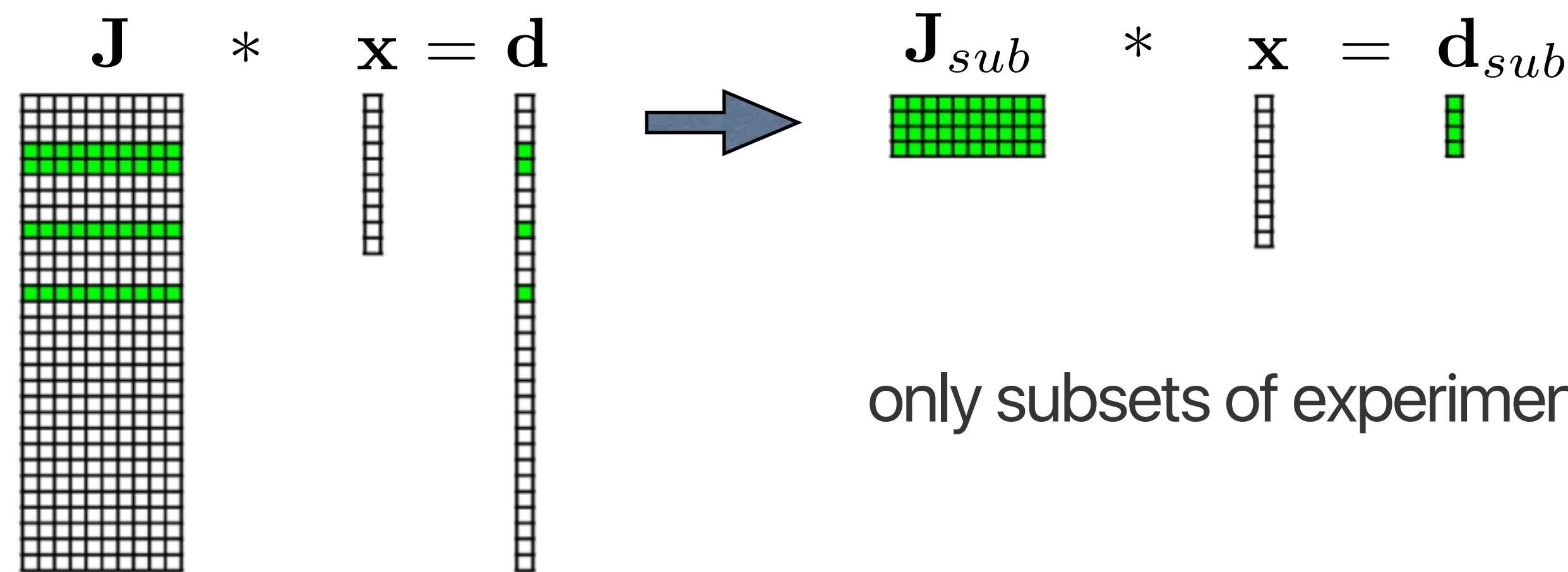
$$\text{subject to: } \|\mathbf{J} \cdot \delta \mathbf{m} - \delta \mathbf{d}\|_2 \leq \sigma$$

$\mathbf{C}$ : Curvelet transform

$\lambda$ : thresholding parameter

$\sigma$ : noise level

- in each iteration possible to work w/ subset of rows of  $\mathbf{J}$ ,  $\delta \mathbf{d}$



only subsets of experiments in each iteration

# Seismic least squares imaging

Linearized Bregman method for least squares imaging:

- ▶ Algorithm (Lorenz et al. , 2014)

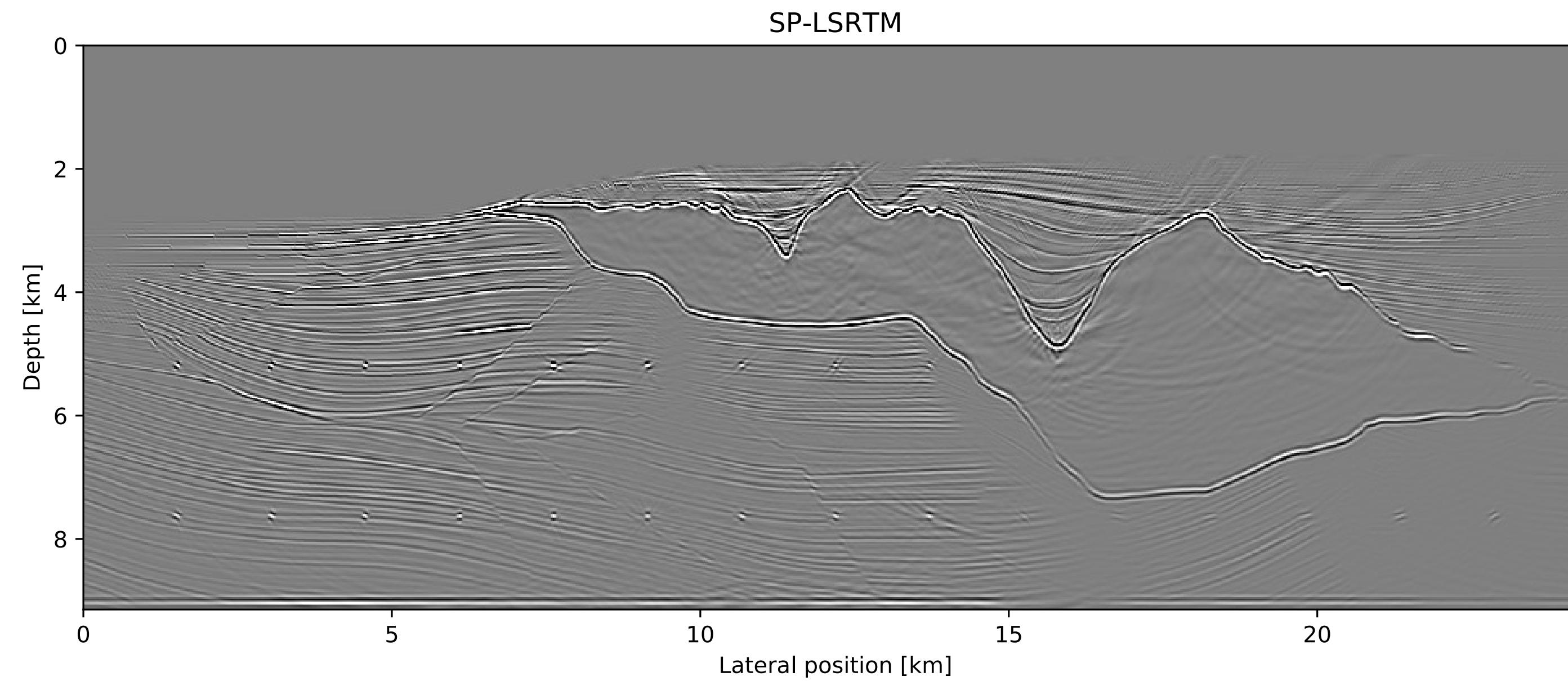
```
1.   for  $k = 0, 1, \dots$ 
2.    $\mathbf{z}_{k+1} = \mathbf{z}_k - t_k \mathbf{J}_{r(k)}^\top (\mathbf{J}_{r(k)} \mathbf{x}_k - \delta \mathbf{d}_{r(k)}) \cdot \max(0, 1 - \frac{\sigma}{\|\hat{\mathbf{J}}_{r(k)} \mathbf{x}_k - \mathbf{b}_{r(k)}\|_2})$ 
3.    $\mathbf{x}_{k+1} = \mathbf{C}^* S_\lambda(\mathbf{C} \mathbf{z}_{k+1})$ 
4. end for
```

- ▶  $r(k)$  is sequence of subsampled experiments (cyclic or random)
- ▶ instead of “touching” full data set in each iteration, only touch every data sample one or twice
- ▶ calculate gradients on a few large nodes (TB RAM) rather than many small ones

# Seismic least squares imaging

Example with model from the introduction:

- ▶ large 2D model ( $4e6$  grid points)
- ▶ 1000 surface seismic experiments ( $5e9$  data points)
- ▶ 20 iterations w/ 100 experiments per iteration (4000 PDE solves)



# Nonlinear inverse problems

## Objective functions for nonlinear inverse problems

- ▶ functions that spin off function values and gradients
- ▶ can be passed to black-box optimization libraries (e.g. NLOpt, JuMP)

## Example: invert for velocity model (full waveform inversion)

- ▶ nonlinear least squares problem

$$\underset{\mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \|\mathcal{P}_r \cdot \mathbf{A}(\mathbf{m}) \cdot \mathcal{P}_s^\top \cdot \mathbf{q} - \mathbf{d}\|_2^2$$

- ▶ gradient given by

$$\mathbf{g} = \mathbf{J}^\top \cdot \left( \mathcal{P}_r \cdot \mathbf{A}(\mathbf{m})^{-1} \cdot \mathcal{P}_s^\top \cdot \mathbf{q} - \mathbf{d} \right) \longrightarrow$$

```
3 # fwi function value and gradient
4 f,g = fwi_objective(m,dobs,q)
```

# Nonlinear inverse problems

Some final words about scaling:

- ▶ so far only large 2D example ( $4e6$  model parameters,  $2.5e9$  data points)
- ▶ large 3D problems have ( $2e8$  model parameters,  $1e12$  data points (or more))

For large-scale 3D inverse problems:

- ▶ bounded by RAM, need to store the forward wavefields for all experiments
- ▶ with stochastic optimization methods (linearized Bregman etc.), reduce number of experiments per iteration

# Conclusions

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## Julia framework for seismic modeling and inversion

- ▶ modular software structure
- ▶ matrix-free linear operators and seismic data containers
- ▶ efficient and fast PDE solves through Devito
- ▶ scales to very large and realistic problem sizes
- ▶ parallel framework, resilience to hardware failures
- ▶ easy to formulate algorithms, objective functions + gradients, etc.
- ▶ easy to interface optimization libraries

# Outlook

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In the future we plan to:

- ▶ test our framework in the cloud
- ▶ add IO functions for seismic data (automatic set up of data containers + geometry)
- ▶ application to 3D seismic field data sets (requires nodes with ~ TB RAM)

## Acknowledgements

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