

A large-scale time-domain modeling and inversion workflow in Julia

Philipp A. Witte and Felix J. Herrmann

Why Julia?

dynamically typed languages

- interpreted languages:
 - ▶ Matlab
 - ▶ Python
 - ▶ Perl
 - ▶ Ruby etc.
- easy to write Code (no type declarations)

statically typed languages

- compiled languages:
 - ▶ C, C++, C#
 - ▶ Fortran
 - ▶ Java, etc.
- types declared at compilation time
- higher performance

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Scientists

statically typed languages

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Programmers

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Julia

statically typed languages

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Why Julia?

Main features of Julia:

- flexible dynamic language
- optional typing and just-in-time compilation (JIT)
- multiple dispatch (function overloading)
- performance in range of statically typed languages like C
- easy to write parallel programs (parallel loops, shared arrays)
- easy interaction with other languages
- free and open source
- large community with people from scientific computing and applied maths
- many packages for linear algebra, optimization etc.

Why Julia?

	Fortran	Julia	Python	R	Matlab	Octave	Mathe- matica	JavaScript	Go	LuaJIT	Java
	gcc 5.1.1	0.4.0	3.4.3	3.2.2	R2015b	4.0.0	10.2.0	V8 3.28.71.19	go1.5	gsl-shell 2.3.1	1.8.0_45
fib	0.70	2.11	77.76	533.52	26.89	9324.35	118.53	3.36	1.86	1.71	1.21
parse_int	5.05	1.45	17.02	45.73	802.52	9581.44	15.02	6.06	1.20	5.77	3.35
quicksort	1.31	1.15	32.89	264.54	4.92	1866.01	43.23	2.70	1.29	2.03	2.60
mandel	0.81	0.79	15.32	53.16	7.58	451.81	5.13	0.66	1.11	0.67	1.35
pi_sum	1.00	1.00	21.99	9.56	1.00	299.31	1.69	1.01	1.00	1.00	1.00
rand_mat_stat	1.45	1.66	17.93	14.56	14.52	30.93	5.95	2.30	2.96	3.27	3.92
rand_mat_mul	3.48	1.02	1.14	1.57	1.12	1.12	1.30	15.07	1.42	1.16	2.36

(<http://julialang.org/>)

Why Julia?

SLIM's first steps towards Julia:

- workflow for wave-equation based inversion (LSRTM, FWI)
- Devito toolbox as wave-equation solver
- higher level abstractions for optimization
- linear operators, function-handles for black-box optimization packages



coding close to mathematical formulations + high performance

Recap of Devito

Optimized FD schemes from symbolic PDEs

Automated code generation and Just-In-Time (JIT) compilation from symbolic Python expressions

Code design

- Level 1: Set up problem geometry
(-> PyObject for forward, adjoint, born modeling)
- Level 2: Once a specific operation is called (e.g. forward solve), set up symbolic PDE and generate FD scheme
- Level 3: Generate C code with optimized FD scheme and compile it
- Level 4: Solve wave equation

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Python

C

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Julia

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Julia

Python

C

Intermediate code design

Code design

Level 1: set up problem geometry (user level)

Julia

```
14
15 # Grid points, spacing and origin
16 n = (80, 80, 80)
17 d = (10., 10., 10.)
18 o = (0.,0.,0.)
19
20 # Velocity model
21 v = ones(n) + .4
22 v[:, :, Int(round(n[3]/2)):end] = 4.
23 v0 = smooth10(v,n)
24
25 # Slowness squared
26 m = (1./v).^2.
27 m0 = (1./v0).^2.
28 dm = m - m0
29
30 # Set source function (ricker wavelet)
31 f0 = 0.010 # source peak frequency [kHz]
32 tmax = 1000. # modeling time end [ms]
33 dt = calculate_dt(n,d,o,v)
34 q = source(tmax,dt,f0)
35
36 # Source coordinates [m]
37 srcnum = 1
38 xsrc = 200
39 ysrc = 400
40 zsrc = 40
41
42 # Setup receiver grid [m]
43 nxrec = 21
44 nyrec = 101
45 xrec = linspace(50,750,nxrec) # 21 receivers in x direction ranging from 50 to 950 meters
46 yrec = linspace(50,750,nyrec) # 101 receivers in y direction
47 zrec = 100 # the same depth for all receivers
48
49 # Set up model structure
50 model = Model(n,d,o,tmax,xsrc,ysrc,zsrc,xrec,yrec,zrec)
51
52 # Nonlinear forward modeling
53 data = time_modeling(model,srcnum,q,m,[],'F',1);
54
```

Code design

```
106
107 function time_modeling(model::TimeDomainInversion.Model, srcnum::Int64, q::Array{Float64,1}, m::Array{Float64,3}, x, op::Char, mode::Int64)
108 # Setup time-domain linear or nonlinear forward and adjoint modeling using OPESCI/devito
109
110 # Set up model structure
111 modelPy = ct.IGrid()
112 modelPy[:shape] = model.n
113 modelPy[:create_model](model.o, model.d, sqrt(1./m))
114 dt = modelPy[:get_critical_dt]()
115 h = modelPy[:get_spacing]()
116 nt = Int(round(1 + model.tmax / dt))
117 if mode==-1 && length(size(x))==3 ; x = squeeze(x,3); end
118
119 # Set up sources
120 src = ct.IShot()
121 source_coords = [model.xsrc model.ysrc model.zsrc]
122
123 src[:set_receiver_pos](source_coords)
124 src[:set_shape](nt,1)
125 src[:set_traces](reshape(q,length(q),1))
126
127 # Set up receiver grid
128 data = ct.IShot()
129 receiver_coords = setup_receiver_grid(model)
130 data[:set_receiver_pos](receiver_coords)
131 data[:set_shape](nt,size(receiver_coords,1))
132
133 # Initiate acoustic modeling object
134 Acoustic = ac.Acoustic_cg(modelPy, data, src, auto_tune=false)
135
136 # Modeling
137 if op=='F'
138     if mode==1
139         println("Nonlinear forward modeling")
140         (argout1, argout2) = Acoustic[:Forward]()
141     end
end
```

Set up Python objects

Julia

Call forward modeling

Code design

- **Level 2:** Set up symbolic PDE upon function call and generate stencil

```
139
140     println("Nonlinear forward modeling")
141     (argout1, argout2) = Acoustic[:Forward]()
142
```



```
155
156     # Derive stencil from symbolic equation
157     eqn = m / rho * u.dt2 - Lap + damp * u.dt
158     s, h = symbols('s h')
159     stencil = 1.0 / (2.0 * m / rho + s * damp) * \
160         (4.0 * m / rho * u + (s * damp - 2.0 * m / rho) *
161         u.backward + 2.0 * s**2 * Lap)
162     # Add substitutions for spacing (temporal and spatial)
163     subs = {s: dt, h: model.get_spacing()}
164     super(ForwardOperator, self).__init__(nt, m.shape,
165         stencils=Eq(u.forward, stencil),
166         subs=subs,
167         spc_border=spc_order/2,
168         time_order=time_order,
169         forward=True,
170         dtype=m.dtype,
171         **kwargs)
172
```

Python

- Define derivative operators
- Insert source/receivers terms
- ...

Code design

- **Level 3:** Generate C code and compile it upon calling apply() function

```
62
63 def Forward(self, save=False, cache_blocking=None, use_at_blocks=False, cse=True):
64     fw = ForwardOperator(self.model, self.src, self.damp, self.data,
65                          time_order=self.t_order, spc_order=self.s_order,
66                          save=save, cache_blocking=cache_blocking, cse=cse)
67     if use_at_blocks:
68         self.at = AutoTuner(fw)
69         fw.propagator.cache_blocking = self.at.block_size
70
71     u, rec = fw.apply()
72     return rec.data, u
73
```

Python

- **Level 4:** Run loop over time steps and run compiled C code

Parallel computing in Julia

Devito solves wave equation for 1 source

- build parallel Julia framework on top

For time-domain modeling/inversion:

- Parallelization over sources (easy, no communication within modeling functions, reduction or collection after function calls)
- Domain decomposition (difficult, communications within time loop)

For source parallelization: asynchronous (non-blocking) function calls

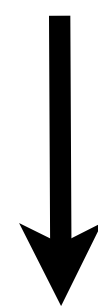
Parallel computing in Julia

Julia's parallel environment differs from MPI

- One-sided communication (manage only master process)

Higher level function calls instead of send/receive operations

- Remote calls: call function on remote process
- Remote references: object on remote process, can be used by any other process



Call modeling/gradient function on remote workers + pull result whenever needed

Source parallelization in Julia

Function overloading helps to structure code

```
36 # Source coordinates [m]
37 srcnum = 1
38 xsrc = 200
39 ysrc = 400
40 zsrc = 40
41
42 # Set up model structure
43 model = Model(n,d,o,tmax,xsrc,ysrc,zsrc,xrec,yrec,zrec)
44
45 # Nonlinear forward modeling
46 data = time_modeling(model,srcnum,q,m,□,'F',1);
47
```

1 source



serial modeling function

```
36 # Source coordinates [m]
37 srcnum = 1:3
38 xsrc = [200, 500, 700]
39 ysrc = [400, 500, 600]
40 zsrc = [40, 45, 50]
41
42 # Set up model structure
43 model = Model(n,d,o,tmax,xsrc,ysrc,zsrc,xrec,yrec,zrec)
44
45 # Nonlinear forward modeling
46 data = time_modeling(model,srcnum,q,m,□,'F',1);
47
```

3 sources



parallelization over sources



Linear operators

Linear operator package for matrix-free operations

- SPOT-like toolbox
- define operators from functions

Linear operators for non-linearized and linearized (Born) modeling

```
52
53 # Nonlinear modeling
54 F = opF(model,srcnum,q,m)
55
56 d_obs = F*q
57 q_adj = F'*d_obs
58
59
60 # Linearized born modeling
61 J = opJ(model,srcnum,q,m0)
62
63 dD = J*dm
64 image = J'*dD
65
```

(independent of number of sources)

Linear operators

Linear operators can be used to easily implement algorithms

- e.g. sparsity promoting least squares migration

```
51
52 # Nonlinear modeling
53 J = opJ(model,srcnum,q,m0)
54
55 # Observed reflection data
56 y = J*dm
57
58 # Sparsity promoting LSRTM
59 x = zeros(prod(n))
60 z = zeros(prod(n))
61 lambda = 1
62 numIterations = 10
63
64 for j=1:numIterations
65
66     # Step size
67     t = norm(J*x - y)^2/norm(J'*(J*x-y))^2
68
69     # Update variables
70     z = z - t*J'*(J*x - y)
71     x = softThresholding(z,lambda)
72
73 end
74
```

Linear operators

Linear operators can be used to easily implement algorithms

- e.g. gradient for full-waveform-inversion

```
52
53 # Set up operators
54 F = opF(model,srcnum,q,m0)
55 J = opJ(model,srcnum,q,m0)
56
57 # FWI gradient
58 d_pred = F*q
59
60 misfit = .5*norm(d_pred - d_obs)^2.
61
62 gradient = J'*(d_pred - d_obs)
63
```

Optimization

Objective functions that spin off gradient and function values for black-box optimization routines

```
55
56 # Nonlinear forward modeling
57 D = F*q
58
59 # Linearized forward modeling
60 dD = J*dm
61
62 # FWI
63 fval1, grad1 = pde_objective(model, srcnum, q, m0, □, D, "fwi")
64
65 # LSRTM
66 image = zeros(model.n)
67 fval2, grad2 = pde_objective(model, srcnum, q, m0, image, dD, "lsrtm")
68
```

Optimization

Objective function can be passed to one of the many available Julia optimization packages

- Optim.jl - standard optimization algorithms for unconstrained and box-constrained optimization (BFGS, Nelder-Mead, CG)
- JuMP - linear, quadratic and non-linear constrained optimization
- LsqFit.jl - least-squares non-linear curve fitting
- NLOpt.jl - interface to the NLOpt library for (un-)constrained optimization
- and others

Optimization

E.g. FWI with L-BFGS and bound constraints

$$\underset{\mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \|\mathbf{d}_{obs} - \mathbf{PA}(\mathbf{m})^{-1} \mathbf{q}\|_2^2$$

$$\text{subject to: } \mathbf{m} > \mathbf{m}_{min}$$
$$\mathbf{m} < \mathbf{m}_{max}$$

```
58
59 # Set up spot operator
60 F = opF(model,srcnum,q,m)
61
62 # Generate observed data
63 D = F*q
64
65 # Function for NLopt
66 count = 0
67 function f!(x,grad)
68     fval, grad[1:end] = pde_objective(model,srcnum,q,x,[],D,"fwi")
69     global count
70     count += 1
71     println(count)
72     return fval
73 end
74
75 # LBFGS with bound constraints
76 opt = Opt(:LD_LBFGS, prod(n))
77 lower_bounds!(opt, mmin)
78 upper_bounds!(opt, mmax)
79 min_objective!(opt, f!)
80 maxeval!(opt, 20)
81 (minf, minx, ret) = optimize(opt, vec(m0))
82
```


Unit testing

Adjoint tests for \mathbf{F} and \mathbf{J}

$$\hat{\mathbf{d}} = \mathbf{F}\mathbf{q}$$

$$\hat{\mathbf{q}} = \mathbf{F}^T \mathbf{d}$$

$$|\mathbf{d}^T \hat{\mathbf{d}} - \mathbf{q}^T \hat{\mathbf{q}}| \leq \epsilon$$

```

51
52 # Setup spot operator
53 F = opF(model,srcnum,q,m)
54
55 # Test
56 d_hat = F*q
57 d = rand(size(d_hat))
58 q_hat = F'*d
59
60 # Result
61 println("Residual: ", abs(d'*d_hat - q'*q_hat))
62

```

$$\delta \hat{\mathbf{d}} = \mathbf{J} \delta \mathbf{m}$$

$$\delta \hat{\mathbf{m}} = \mathbf{J}^T \delta \mathbf{d}$$

$$|\delta \mathbf{d}^T \delta \hat{\mathbf{d}} - \delta \mathbf{m}^T \delta \hat{\mathbf{m}}| \leq \epsilon$$

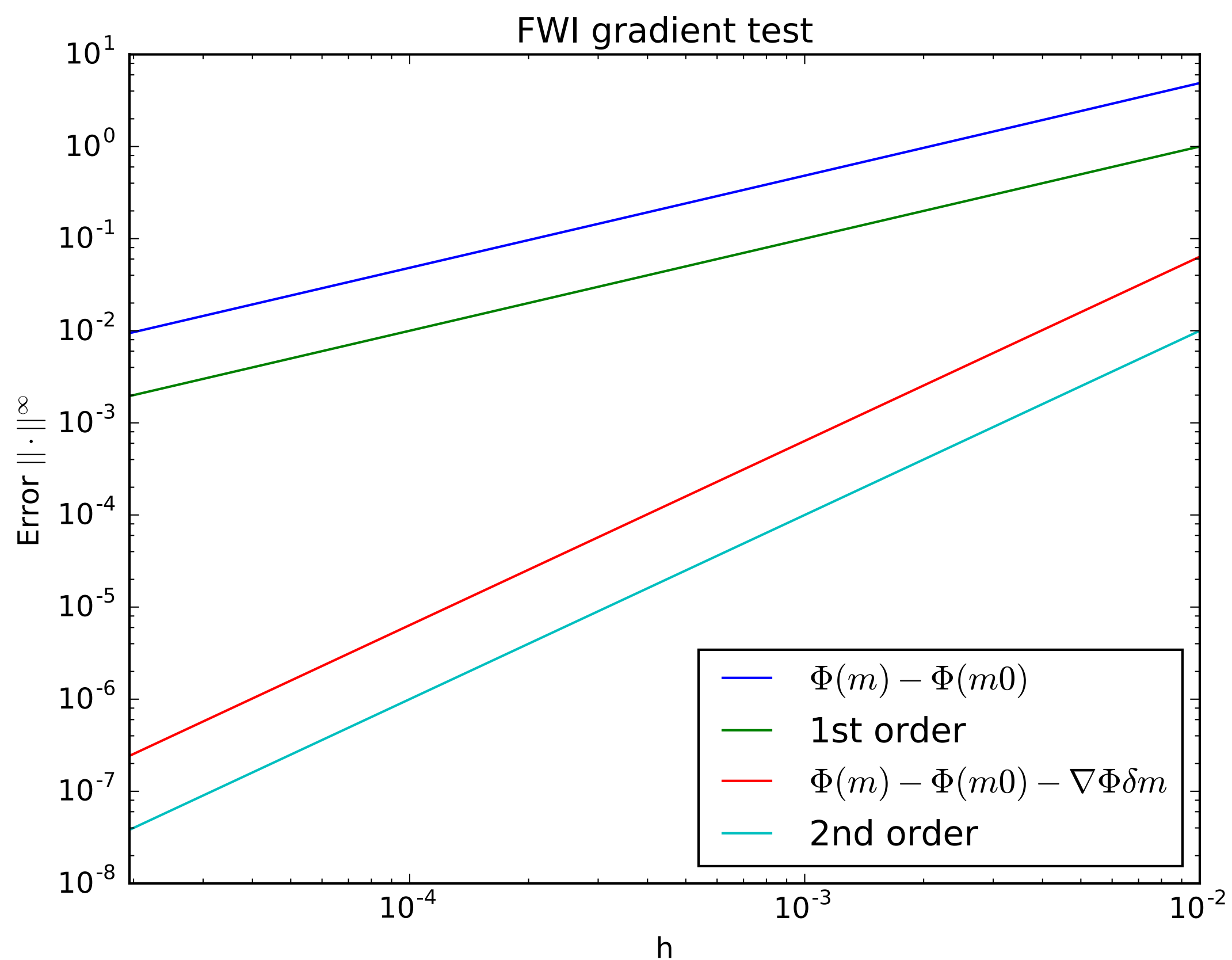
```

65
66 # Setup spot operator
67 J = opJ(model,srcnum,q,m0)
68
69 # Test
70 dD_hat = J*dm
71 dD = rand(size(dD_hat))
72 dm_hat = J'*dD
73
74 # Result
75 println("Residual: ", abs(dD'*dD_hat - dm'*dm_hat))
76

```

Unit testing

Check correct gradient implementation of FWI objective: $\Phi(\mathbf{m}) = \frac{1}{2} \|\mathbf{d}_{obs} - \mathbf{PA}(\mathbf{m})^{-1} \mathbf{q}\|_2^2$

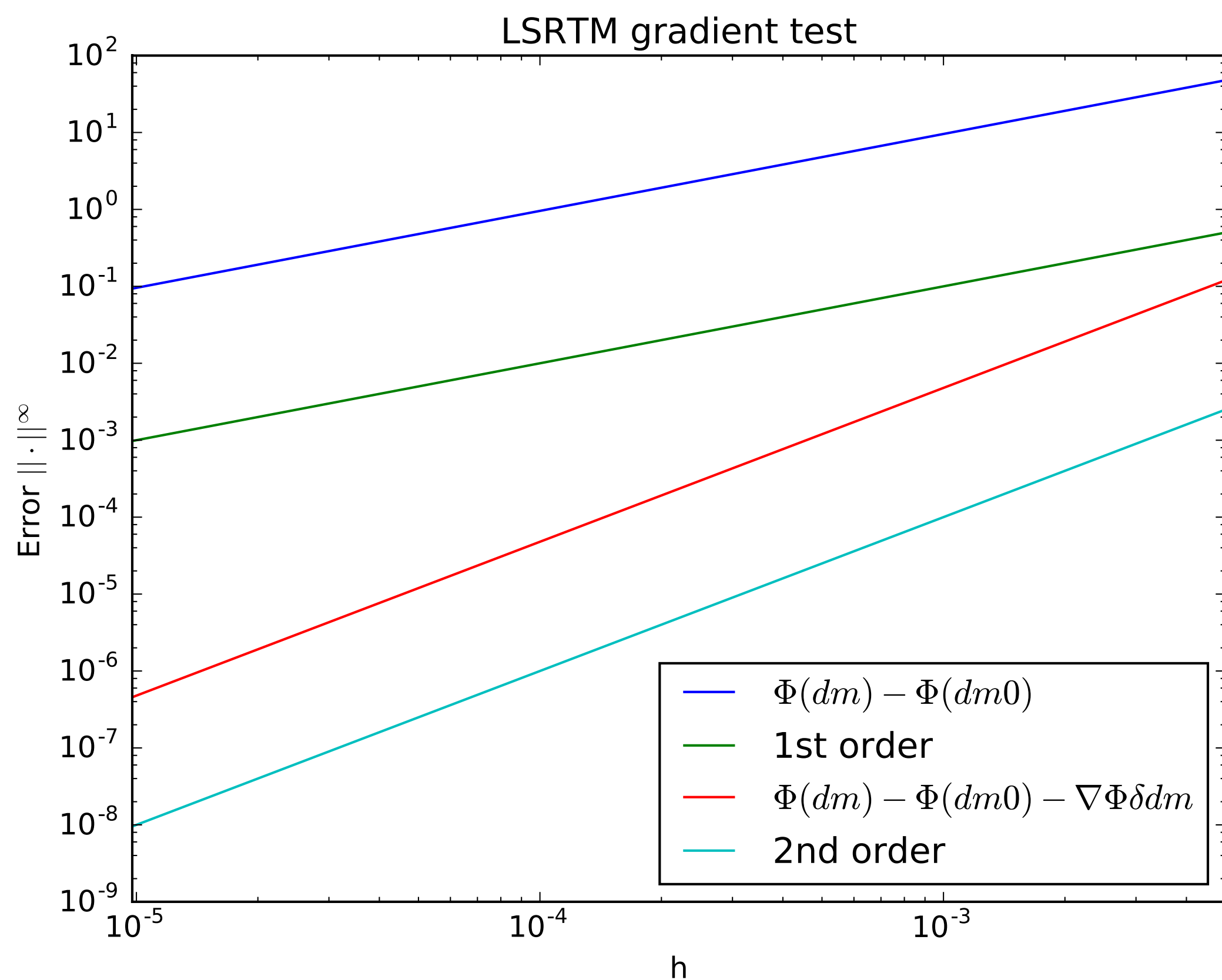


← $\Phi(\mathbf{m}_0 + h \cdot \delta\mathbf{m}) - \Phi(\mathbf{m}_0)$

← $\Phi(\mathbf{m}_0 + h \cdot \delta\mathbf{m}) - \left(\Phi(\mathbf{m}_0) - h \cdot \nabla_m \Phi(\mathbf{m}_0)^T \delta\mathbf{m} \right)$

Unit testing

Check correct gradient implementation of LSRTM objective: $\Phi(\delta\mathbf{m}) = \frac{1}{2} \|\delta\mathbf{d}_{obs} - \mathbf{J}\delta\mathbf{m}\|_2^2$



← $\Phi(\delta\mathbf{m}_0 + h \cdot \Delta\delta\mathbf{m}) - \Phi(\delta\mathbf{m}_0)$

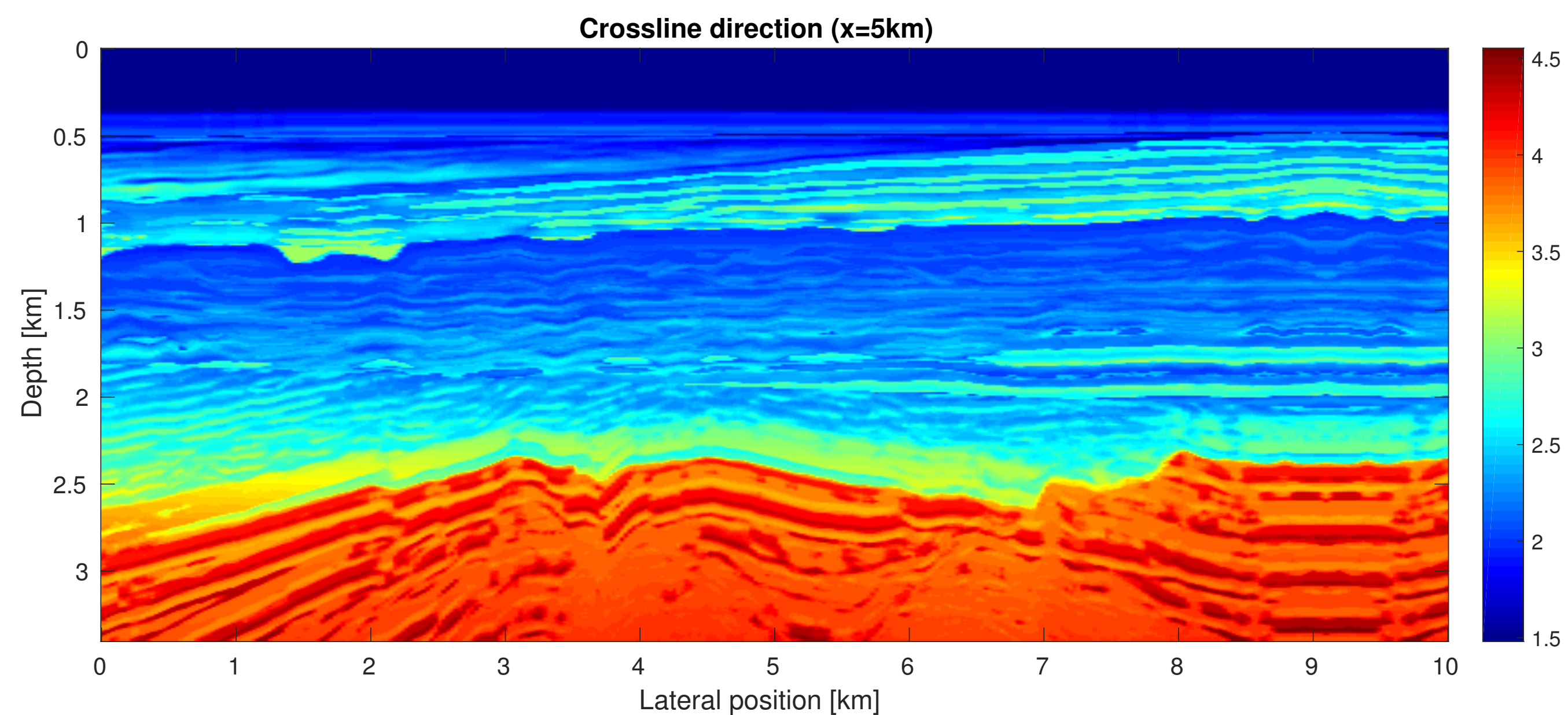
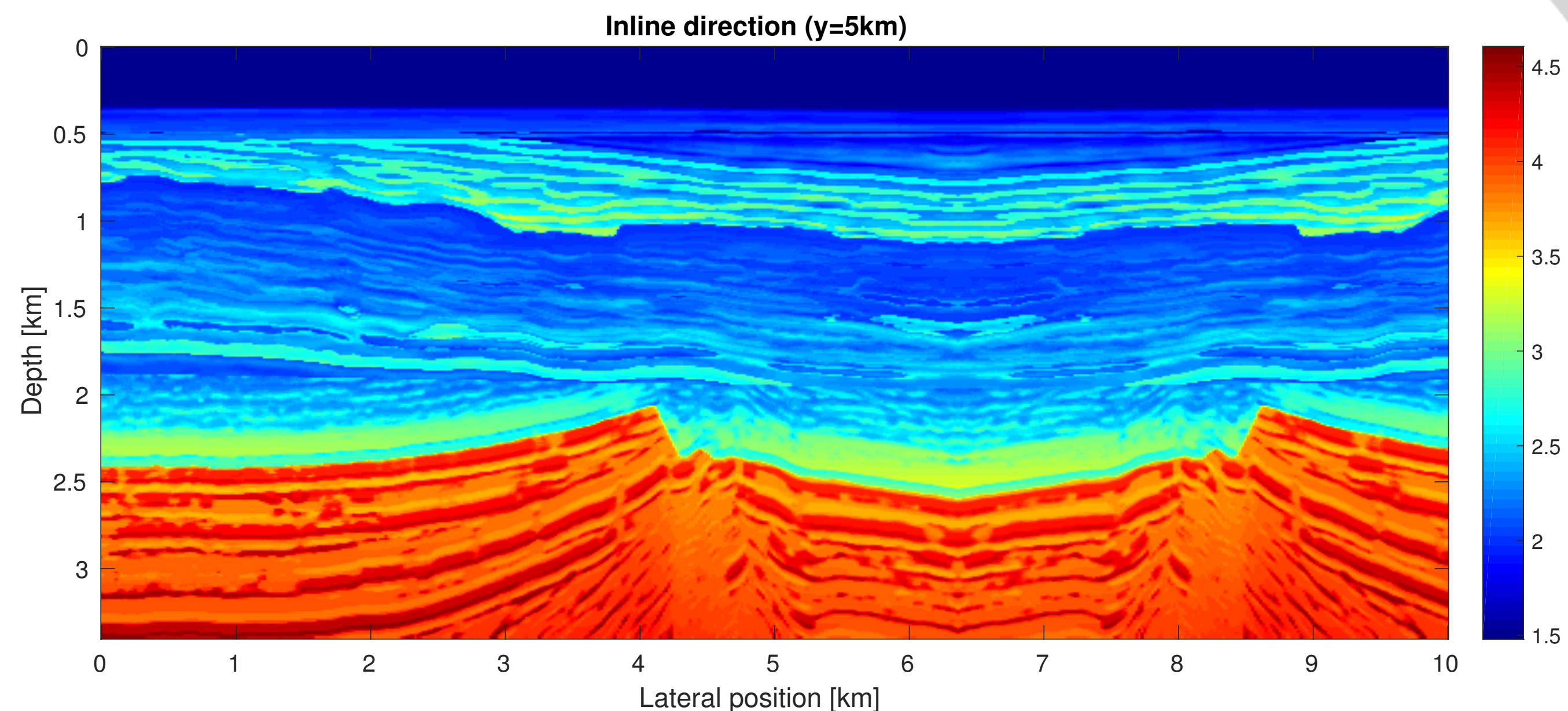
← $\Phi(\delta\mathbf{m}_0 + h \cdot \Delta\delta\mathbf{m}) -$
 $\left(\Phi(\delta\mathbf{m}_0) - h \cdot \nabla_m \Phi(\mathbf{m}_0)^T \Delta\delta\mathbf{m} \right)$

Modeling example

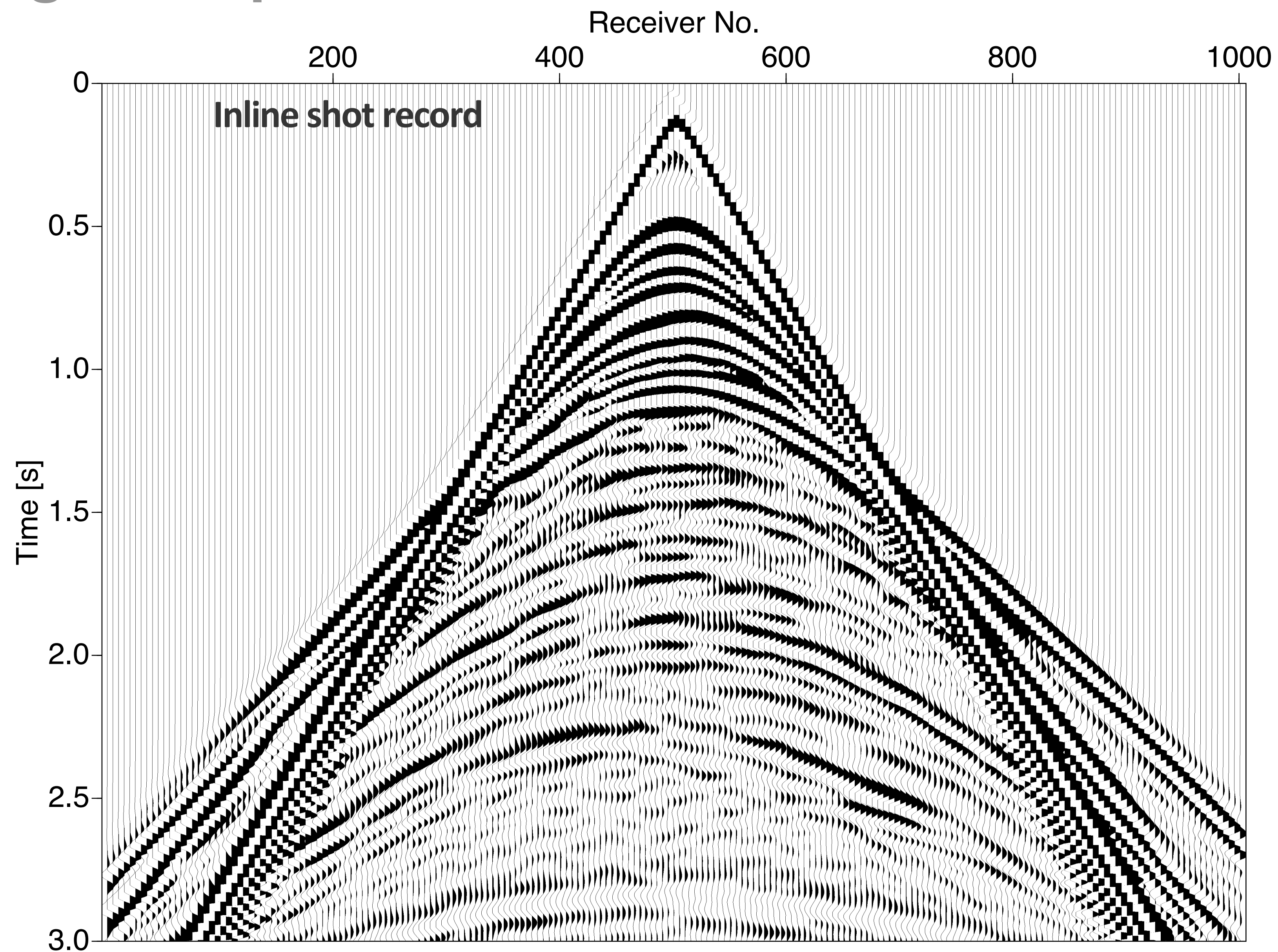
Model shot record on the 3D BG model:

- 10 x 10 x 3.4 km
- 1000 x 1000 x 340 grid points
- 3 s recording time (3700 time steps)
- 1001 inline receivers
- 201 crossline receivers
- source in model center (10 Hz Ricker wavelet)

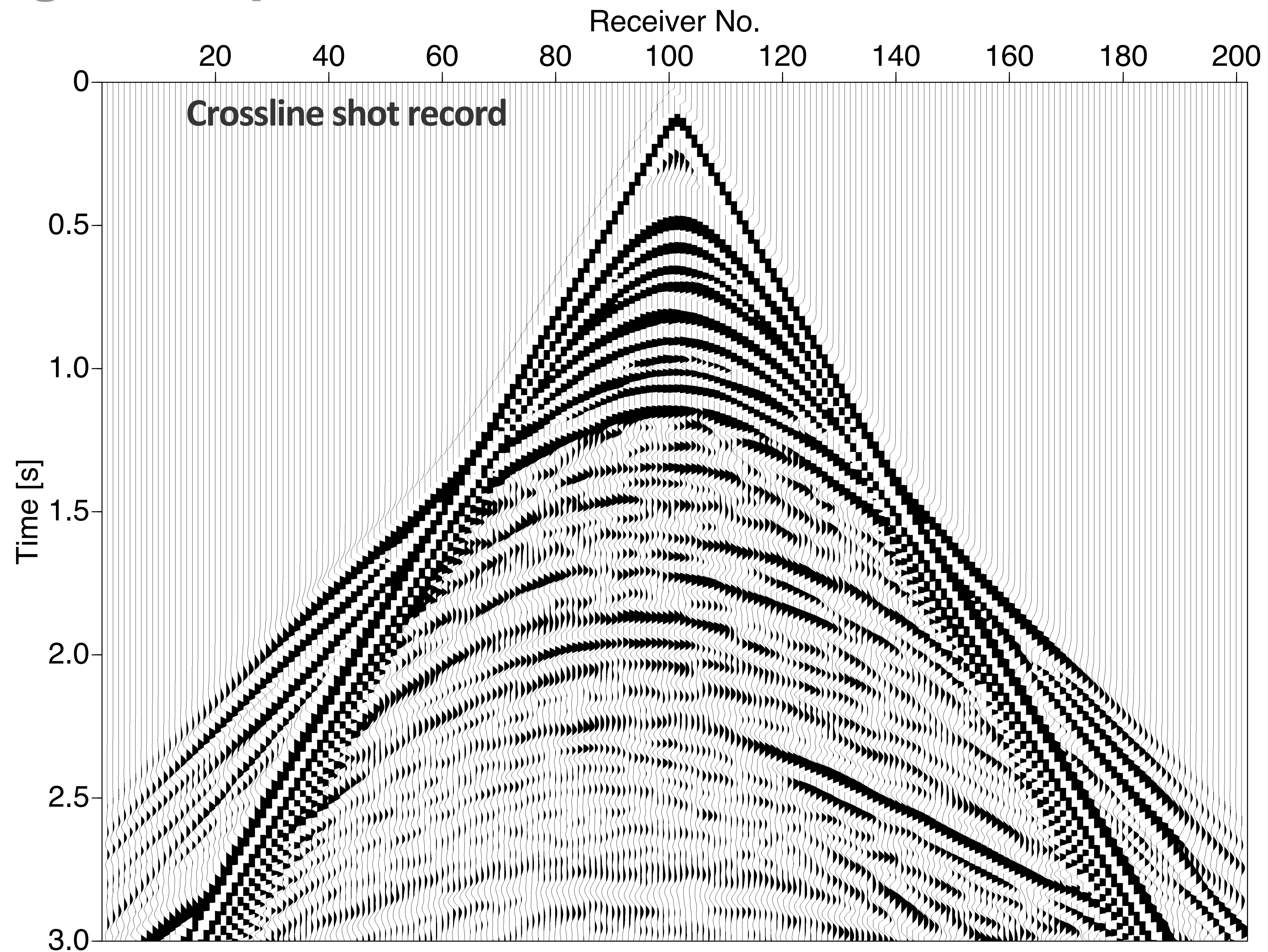
➔ Computational time:
50 minutes



Modeling example



Modeling example



Outlook

We're just getting started with Julia and there's still a lot to do:

- Reading/writing SEG-Y data
- Resolve memory issues (some memory leaks)
- Translate most important Matlab functions to Julia
- Devito: replace Python data/model objects with Julia objects (prevents data copies)

Acknowledgements

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