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Julia Devito: A scalable research framework for seismic inversion Philipp A. Witte, Mathias Louboutin and Felix J. Herrmann



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Motivation

Academic software frameworks:

- only for small 2D/3D problems (Madagascar, SeismicJulia) or
- unmaintainable low-level black-box spaghetti codes
- without detailed knowledge of code, hard to:
 - change a line search
 - keep history of gradients (e.g for SPG)
 - change parallelization
 - change the underlying physics, correct adjoints

But there is also iWave:

- well designed, abstractions
- high accuracy, testing framework, correct adjoints
- intuitive to use

but: written in C/C++, not primarily designed for performance, not very



Motivation

Potential applications of software: Inear least squares problems such as LS-RTM

 $\underset{\delta \mathbf{m}}{\text{minimize}} \quad \frac{1}{2} || \nabla \mathcal{F}(\mathbf{m}_0, \mathbf{q}) \ \delta \mathbf{m} - \delta \mathbf{d} ||_2^2$

non-linear optimization problems such as FWI

minimize $\phi \left(\mathcal{F}(\mathbf{m}, \mathbf{q}) - \mathbf{m} \right)$

Maintain flexibility:

- change $\mathcal{F}(\mathbf{m}, \mathbf{q})$, the underlying wave equation solver • change the formulation (different misfits $\phi(\mathbf{x})$, constraints, penalties) choose from large variety of optimization algorithms

$$-\, \mathbf{d} ig)$$
 , where $\,\, \phi(\mathbf{x}) = rac{1}{2} \|\mathbf{x}\|_2^2$



Julia Devito is a wave-equation based inversion framework:

- non proprietary Julia programming language (public license) uses Devito to express and solve underlying PDEs
- matrix-free linear operators and out-of-core SEG-Y data containers
- resilient parallelization
- unified 2D-3D environment
- can interact with variety of general-purpose optimization libraries
- designed to push inversion to the next scale
- scalable but also flexible











Linear algebra notation is intuitive for seismic operations: forward modeling/time reversal modeling

$$\mathbf{d} = \mathcal{P}_r \; \mathbf{F} \; \mathcal{P}_s^{ op} \mathbf{q}, \quad \widehat{\mathbf{q}}$$

- demigration/migration
 - $\delta \mathbf{d} = \mathbf{J} \ \delta \mathbf{m}, \quad \widehat{\delta \mathbf{m}} = \mathbf{J}^{\top} \delta \mathbf{d}$
- FWI gradients, Gauss-Newton step, etc.

$$\mathbf{g} = \mathbf{J}^{\top} (\mathcal{P}_r \ \mathbf{F} \ \mathcal{P}_s^{\top} \mathbf{q} \ \delta \mathbf{m} = (\mathbf{J}^{\top} \mathbf{J})^{-1} \mathbf{J}^{\top} \delta \mathbf{d}$$

- $\widehat{\mathbf{q}} = \mathcal{P}_s \ \mathbf{F}^\top \ \mathcal{P}_r^\top \mathbf{d}$
- $-\mathbf{d}_{obs}$)



- Challenges of this approach for time-domain modeling/inversion: seismic data is multidimensional volume with meta data simply vectorizing the input data not an option
- data typically too big to fit in memory

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$$\mathbf{d} = \mathcal{P}_r \mathbf{F} \mathcal{P}_s^{\mathsf{T}} \mathbf{q}$$

cannot be formed explicitly need physical information (model, source/receiver locations)



- Challenges of this approach for time-domain modeling/inversion: seismic data is multidimensional volume with meta data simply vectorizing the input data not an option data typically too big to fit in memory



cannot be kept in memory

►not a vector

- contains header information

cannot be formed explicitly need physical information (model, source/receiver locations)



Abstract in-core and out-of-core data vectors:

- inspired by iWave, RVL and others (Symes, Padula)
- can be formed directly from single/multiple SEG-Y files
- parallel read/write chunks of data

```
julia> container = segy_scan(pwd(), "overthrust_shots", ["GroupX","GroupY"]);
Scanning ... /home/slim/pwitte/overthrust_shots_41_60.segy
Scanning ... /home/slim/pwitte/overthrust_shots_21_40.segy
Scanning ... /home/slim/pwitte/overthrust_shots_61_80.segy
Scanning ... /home/slim/pwitte/overthrust_shots_1_20.segy
Scanning ... /home/slim/pwitte/overthrust_shots_81_97.segy
julia> d = joData(container)
(opesciSLIM.TimeModeling.joData{Float32}, "Julia seismic data container", 15029763, 1)
julia> size(d)
(15029763, 1)
julia> norm(d)
7371.35f0
julia> dot(d,d)
5.432854f7
julia> typeof(d.data[1])
SeisIO.SeisCon
```

(Instructional video at: <u>https://www.youtube.com/watch?v=tx530QOPeZo</u>)



(joint work with Keegan Lensink)



Matrix-free linear operators

- read necessary meta information from data objects
- use like explicit matrices

```
julia> F = joModeling(info,model0)
```

```
julia> Pr = joProjection(info,d.geometry)
```

```
julia> Ps = joProjection(info,q.geometry)
```

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

(opesciSLIM.TimeModeling.joModeling{Float32,Float32}, "forward wave equation", 27566740206, 27566740206)

(opesciSLIM.TimeModeling.joProjection{Float32,Float32}, "restriction operator", 15029763, 27566740206)

(opesciSLIM.TimeModeling.joProjection{Float32,Float32}, "restriction operator", 72847, 27566740206)







Parallelization

Modeling multiple shots happens in parallel:

```
julia> d = Pr*F*Ps'*q
       From worker 2: Nonlinear forward modeling (source no. 1)
       From worker 5: Nonlinear forward modeling (source no. 4)
       From worker 3: Nonlinear forward modeling (source no. 2)
       From worker 4: Nonlinear forward modeling (source no. 3)
(opesciSLIM.TimeModeling.joData{Float32}, "Seismic data vector", 240480, 1)
```

Same for adjoint modeling:

```
julia > \hat{q} = Ps*F'*Pr'*d
        From worker 2: Nonlinear adjoint modeling (source no. 2)
        From worker 3: Nonlinear adjoint modeling (source no. 3)
        From worker 4: Nonlinear adjoint modeling (source no. 1)
        From worker 5: Nonlinear adjoint modeling (source no. 4)
(opesciSLIM.TimeModeling.joData{Float32}, "Seismic data vector", 2004, 1)
```



Parallelization

Parallelization in our framework:

- 2 levels of parallelization
- distribution of sources/shots (shared/distributed memory)
- parallelization over modeling domain via OpenMP (shared memory)
- In future Devito release: domain decomposition for distributed memory

Julia's parallel framework has built-in resilience:

- processors
- program is not interrupted

in case of worker/node failure, workload is redistributed to remaining





Python



Interface to Devito

What is Devito?

- domain-specific language for Python
- symbolically set up variety of wave equations (acoustic, anisotropic)
- Devito compiler automatically generates optimized C code
- optimizes Flop count, loops, memory alignment, etc.
- details in the next talk by Mathias

Interfacing Devito from Julia:

- Julia allows direct Python and C function calls
- call Devito functions that generate optimized C code
- call generated C code directly from Julia (no data copies)



(joint work with Mathias Louboutin)

hon ve equations (acoustic, anisotropic) enerates optimized C code nory alignment, etc. s

function calls te optimized C code om Julia (no data copies)



Numerical case studies

Full-waveform inversion:

- vanilla FWI w/ gradient descent and line search
- FWI with different misfit functions
- Interfacing optimization libraries for more advanced algorithms

Least-squares migration:

- parallel algorithms: LS-RTM w/ elastic average SGD
- strategies for large-scale migration: compressive LS-RTM
- imaging in the presence of salt



Example 1: FWI with a line search

Full-waveform inversion w/ least squares misfit:

 $\underset{\mathbf{m}}{\text{minimize}} \quad \frac{1}{2} \| \mathcal{F}(\mathbf{m}, \mathbf{q}) - \mathbf{d} \|^2$

Optimization:

- gradient given by $\mathbf{g} = \mathbf{J}^{\top} (\mathcal{F}(\mathbf{m}, \mathbf{q}) \mathbf{d})$
- bound constraints for velocity

implement (stochastic) gradient descent w/ approximate line search



Example 1: FWI with a line search

Runnable Julia code:

```
# Main loop
   for j=1:maxiter
3
     # select current batch
4
     idx = randperm(dobs.nsrc)[1:batchsize]
5
     dsub = subsample(dobs,idx)
6
     qsub = subsample(q,idx)
7
8
     # get fwi objective function value and gradient
9
     f, g = fwi_objective(model0,qsub,dsub)
10
11
     # linesearch
12
     step = backtracking_linesearch(vec(model0.m), g; varargs...)
13
14
     # Update model and bound projection
15
     model0.m = proj(model0.m + step)
16
17
     # termination criteria
18
     if f <= fTerm || norm(g) <= gradTerm</pre>
19
        break
20
     end
21
22 end
```

alternatively:

- Ine search w/ (strong) Wolfe conditions
- Barzilai-Borwein step size
- constant step size
- ▶etc.



Example 1: FWI with a line search



23





Example 2: FWI with different misfit functions

Previous example:

9 f, g = fwi_objective(model0,qsub,dsub) 10

Change to different misfit:

if observed data has strong outliers: (pseudo-) Huber misfit

$$\phi(\mathbf{x}) = \epsilon^2 \sqrt{1 + \epsilon^2} \sqrt{1 +$$

gradient given by

$$\nabla \phi(\mathbf{x}) = \frac{\mathbf{x}}{\sqrt{1 + (\mathbf{x}/\epsilon)^2}}$$

- objective function that returns function value and gradient for ℓ_2 -misfit
 - # get fwi objective function value and gradient

 - $(\mathbf{x}/\epsilon)^2 1$ (Guitton and Symes, 2003; van Leeuwen et al., 2013)



Example 2: FWI with different misfit functions

```
Objective function w/ \ell_2-misfit
```

```
# FWI with least squares misfit function
  function fwi_objective_l2(model::Model,q::joData,d::joData)
     # Set up operators
     nt = get_computational_nt(q.geometry,d.geometry,model)
     info = Info(prod(model.n),d.nsrc,nt)
     F = joModeling(info,model,q.geometry,d.geometry)
     J = joJacobian(F,q)
     # Data residual, function value and gradient
10
     r = F * q - d
11
     f = .5*norm(r,2)^2
12
     g = J'*r
13
     return f,g
14
  end
15
```



change misfit independently from the rest of the code

Objective function w/ pseudo-Huber misfit:

```
# FWI with pseudo-huber misfit function
   function fwi_objective_huber(model::Model,q::joData,d::joData)
3
      # Set up operators
4
5
      • • •
6
     # Data residual, function value and gradient
\overline{7}
     r = F*q - d
8
     f = eps^2 + sqrt(1 + dot(r,r)/eps^2) - eps^2 # e.g. eps=1
9
     g = J'*r/sqrt(1 + dot(r,r)/eps^2)
10
     return f,g
11
  end
12
```



What if we want to use more complicated algorithms?

- previous misfit functions can be passed to third-party optimization libraries
- access to large variety of optimization methods
- no need to implement everything from scratch

Tested for various libraries:

- Julia implementation of minConf (included in software release) (Schmidt et al., 2009) Bas' framework for constrained optimization w/ projections onto intersections of convex sets (Peters and Herrmann, 2017)
- NLopt.jl (native Fortran library) (Johnson et al., 2017)
- Optim.jl (native Julia library) (White et al., 2017)



Does this scale to 3D?

- (100 billion data points, over 1.2 TB of data)
- case study w/ 3D Overthrust velocity model 801 x 801 x 207 grid points + PML (222 million unknowns) \sim 10k shot records, 8 km max. offset, 3 seconds recording time
- spectral-projected gradient algorithm from minConf library
- backtracking line search
- 15 iterations w/ 1080 shot records per iteration



```
Optimization parameters
  fevals = 15
  batchsize = 1080
    Objective function that is passed to library
  function objective_function(x)
7
     # update model
8
     model0.m = reshape(x,model0.n);
9
10
     # select batch
11
     idx = randperm(dobs.nsrc)[1:batchsize]
12
     dsub = subsample(dobs,idx)
13
     qsub = subsample(q,idx)
14
15
     # fwi function value and gradient
16
     fval, grad = fwi_misfit(model0,qsub,dsub;options=opt)
17
18
     # reset gradient in water column to 0.
19
     grad = reshape(grad,model0.n)
20
     grad[:,:,1:21] = 0.f0
21
22
     return fval, vec(grad)
23
  end
24
25
  # Bound projection
  Proj(x) = median([mmin x mmax],2)
28
    FWI with spectral projected gradient from minConf library
29
  x,fval = minConf_SPG(objective_function,vec(model0.m),Proj,opt)
30
```

Set up 3D FWI in < 50 lines of code:

- possible to work w/ subset of shots
- still access to gradient (mute, scale etc.)
- change from SPG to L-BFGS by modifying 2 lines of code
- works with out-of-core data containers (handle arbitrary sized data sets)
- 4 minutes per gradient (1 node, 20 threads)



x = 4 km



29





30

z = 400 m



Example 4: Serial and parallel SGD

What about parallel algorithms?

- parallel version of stochastic gradient descent: elastic average SGD (Zhang et al., 2015) change from serial to parallel version in few lines of code

Case study for LS-RTM (but could be used for FWI as well):

$$\underset{\widehat{\delta \mathbf{m}}}{\text{minimize}} \quad \frac{1}{2} || \mathbf{M}_l^{-1} \mathbf{J} \mathbf{M}_r^{-1} \mathbf{d}$$

- $\widehat{\delta \mathbf{m}} \mathbf{M}_l^{-1} \delta \mathbf{d} ||_2^2$ (e.g. Herrmann et al., 2008; Dai et al., 2012)
- \blacktriangleright $\mathbf{M}_{l}^{-1}, \mathbf{M}_{r}^{-1}$ are left- and right preconditioners (model-, data-topmute, scaling, etc.)



Example 4: LS-RTM w/ serial and parallel SGD



```
# Stochastic gradient descent
batchsize = 10
niter = 32
for j=1:niter
    # Select batch
    idx = randperm(dD.nsrc)[1:batchsize]
    Jsub = subsample(J,idx)
    dsub = subsample(dD,idx)
    # Compute residual and gradient
    r = Ml*Jsub*Mr*x - Ml*dsub
    g = Mr'*Jsub'*Ml'*r
```

```
# Step size and update variable
t = norm(r)^2/norm(g)^2
x -= t*g
d
```



Example 4: LS-RTM w/ serial and parallel SGD



```
# Gradient function
@everywhere function update_x(Ml,J,Mr,x,d,eta,alpha,xav)
  r = Ml*J*Mr*x - Ml*d
  g = Mr'*J'*Ml'*r
  return x - eta*g - alpha*(x - xav)
update_x_par = remote(update_x) # Parallel function wrapper
for j=1:niter
  @sync begin
     for k=1:p
        # Select batch
        idx = randperm(dD.nsrc)[1:batchsize]
        Jsub = subsample(J,idx)
        dsub = subsample(dD,idx)
        # Calculate x update in parallel
```

end

```
# Update average variable
xav = (1 - beta)*xav + beta*(1/p *sum(x,2))
x = copy(xnew)
```



Example 4: LS-RTM w/ serial and parallel SGD





34



Example 5: Compressive inversion

Challenges of large-scale 3D inversion:

- save forward wavefields for gradient
- domain decomposition, checkpointing, boundary reconstruction
- on-the-fly DFT for frequency domain gradients (Sirgue et al., 2010)

Devito allows to easily implement:

- boundary reconstruction
- on-the-fly DFT
- domain decomposition + checkpointing require more effort (w.i.p.)



Example 5: Compressive inversion

Implement inversion with on-the-fly DFT in Devito:

- sum wavefields in the forward time loop
- two extra lines of Python code

90	<pre># On-the-fly real-valued</pre>
91	$eqn_f_r = [Eq(ufr, ufr +$
92	eqn_f_i = [Eq(ufi, ufi +

similar change for gradients

Run FWI or LS-RTM <u>at any scale:</u>

- only save few frequency-domain wavefields
- integrates seamlessly into Julia framework

(e.g. Romero et al., 2000; Krebs et al., 2009; Herrmann et al., 2009; Dai et al., 2013)

DFT u*cos(2*np.pi*f*time*dt))] u*sin(2*np.pi*f*time*dt))]

applications: source encoded/simultaneous source FWI and LS-RTM



Example 5a: Compressive FWI



37



- overlapping frequency bands from 3-15 Hz



Imaging with frequency subsampling more challenging:

- subsampling creates noisy images
- want sharp image (broad frequency band) from few frequencies

- Sparsity-promoting "compressive" LS-RTM: (Herrmann and Li, 2012; Dai et al., 2013) frequency-domain imaging w/ time-domain modeling work with subsets of random shots and frequencies sparsity-promotion to address artifacts

$$\begin{array}{ccc} \text{minimize} & \lambda \| \mathbf{C} \, \delta \mathbf{m} \|_1 + \\ & \delta \mathbf{m} \end{array}$$

subject to: $\mathcal{F}\mathbf{J}\,\delta\mathbf{m} = \mathcal{F}\delta\mathbf{d}$

$$\frac{1}{2} \|\mathbf{C}\,\delta\mathbf{m}\|_2^2$$









Iteration 5





40





















Iteration 25





44









Example 6: Imaging in the presence of salt

Imaging with salt models:

- backscattered energy from salt interfaces causes low-frequency artifacts Laplacian filtering, wavefield filtering, alternative imaging conditions

SPLS-RTM with linearized inverse scattering imaging condition:

$$\widehat{\mathbf{J}}^{\top} \delta \mathbf{d} = \sum_{t} \left\{ \operatorname{diag} \left(\ddot{\mathbf{u}}[t] \odot \mathbf{m} \right) \left(\mathbf{F}^{\top} \mathcal{P}_{r}^{\top} \delta \mathbf{d} \right)[t] + \sum_{i=1}^{3} \operatorname{diag} \left(\frac{\partial \mathbf{u}[t]}{\partial \mathbf{x}_{i}} \right) \frac{\partial}{\partial \mathbf{x}_{i}} \left(\mathbf{F}^{\top} \mathcal{P}_{r}^{\top} \delta \mathbf{d} \right)[t] \right\}$$

$$\widehat{\mathbf{J}}\delta\mathbf{m} = \left\{ \mathcal{P}_r \mathbf{F} \operatorname{diag} \left(\ddot{\mathbf{u}}[t] \odot \mathbf{m} \right) \delta\mathbf{m} + \mathcal{P}_r \sum_{i=1}^3 \mathbf{F} \frac{\partial}{\partial \mathbf{x}_i} \operatorname{diag} \left(\frac{\partial \mathbf{u}[t]}{\partial \mathbf{x}_i} \right) \delta\mathbf{m} \right\}$$

- derive forward/adjoint pair of ISIC (Whitmore et al., 2012; Witte and Herrmann, 2017)



Example 6: Imaging in the presence of salt





(joint work with Mengmeng Yang)

- sparsity-promoting LS-RTM
- Inearized inverse scattering imaging condition
- 960 shots, 10 seconds recording
- 15 Hz peak frequency
- estimate source wavelet







Example 6: Imaging in the presence of salt

- sparsity-promoting LS-RTM
- Inearized Bregman w/ 18 iterations
- 960 shots, 10 seconds recording
- 100 shots per iteration, 2 data passes
- estimate source wavelet on the fly





(joint work with Mengmeng Yang)





Summary

Julia framework for seismic modeling and inversion

- modular software structure

- matrix-free linear operators and out-of-core SEG-Y data containers implement variety of inverse problems in few lines of code efficient and fast PDE solves through Devito parallelization w/ resilience to hardware failures
- interface optimization libraries
- all ingredients for LS-RTM: correct adjoints, artifact-free salt imaging scales to large-scale 3D problems



The road ahead

Map Julia Devito to the cloud:

- utilize full range of cloud services (auto-scaling, elastic cache, etc.)
- scale algorithms to ANY number of workers

Possible future workflows:

- data sets stored in cloud (already some SEG datasets available)
- bring algorithms to the cloud and to the data
- anyone can buy cloud time and run certain algorithms on a data set
- no need to buy and maintain expensive HPC clusters

provider independent (AWS, Google, Microsoft Azure or possibly others)



Reproducible examples

Examples from this talk can be found in the software release: FWI with a line search

https://github.com/SINBADconsortium/SLIM-release-jlapps/blob/master/WaveformInversion/TimeDomain/2DFWI/scripts/fwi overthrust 2D linesearch.jl

2D and 3D FWI with spectral-projected gradient descent

https://github.com/SINBADconsortium/SLIM-release-jlapps/blob/master/WaveformInversion/TimeDomain/3DFWI/scripts/fwi overthrust 3D.jl

Preconditioned LS-RTM w/ SGD

https://github.com/SINBADconsortium/SLIM-release-jlapps/blob/master/Imaging/TimeDomain/2DLSRTM/scripts/lsrtm marmousi.jl

more to come!



https://github.com/SINBADconsortium/SLIM-release-jlapps/blob/master/WaveformInversion/TimeDomain/2DFWI/scripts/fwi overthrust 2D.jl



Tutorial for data IO with SeisIO.jl

Demonstration and tutorial on Youtube:

- parallel scanning and reading of arbitrary size data sets



• SeisIO.jl on git: <u>https://github.com/slimgroup/SeisIO.jl</u>

• read and write SEG-Y in Julia (chunking, read/write blocks, create look-up tables)





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