Raising the abstraction to separate concerns: enabling different physics for geophysical exploration

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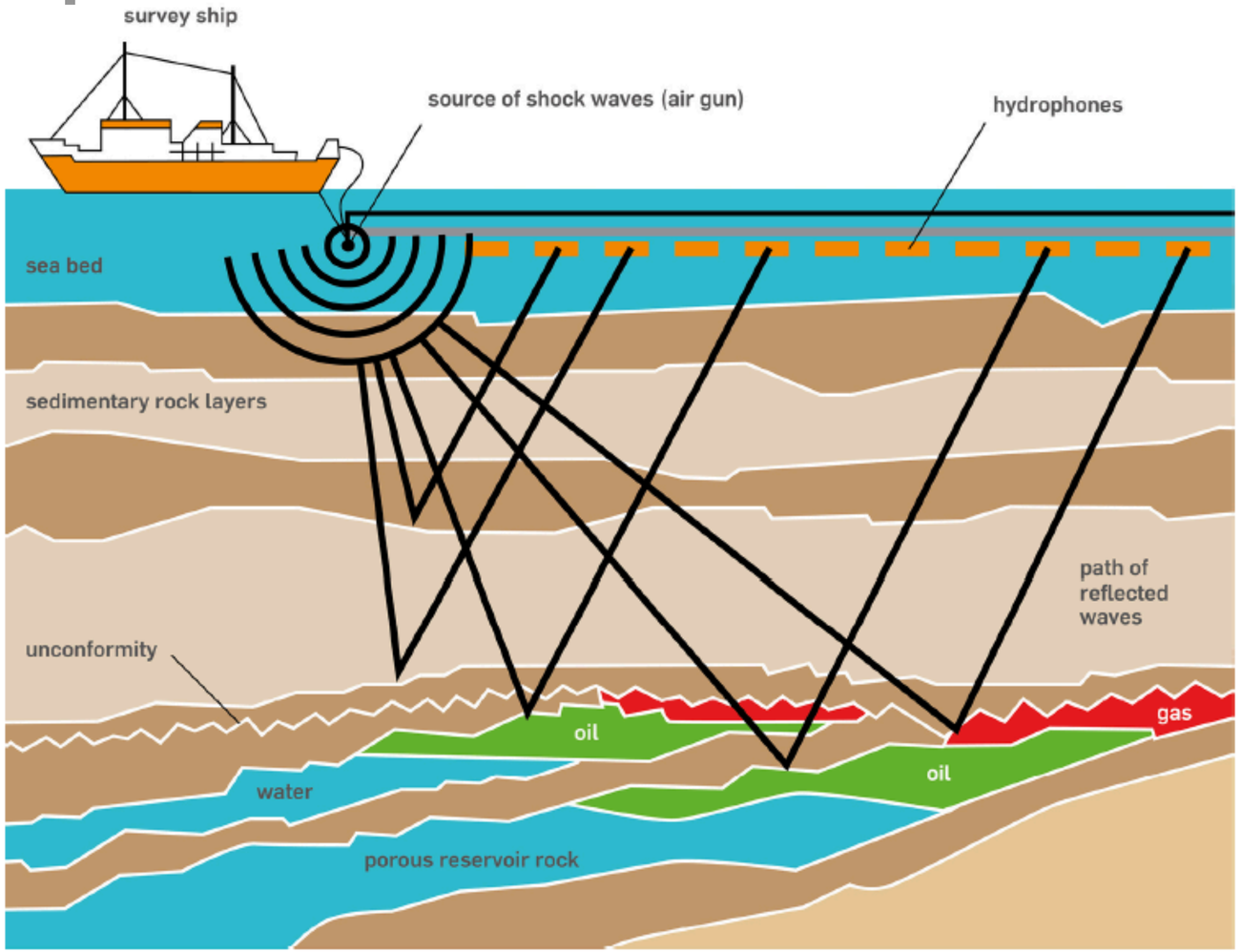
Wave-equation based geophysical exploration introduction

Physical problem



http://www.open.edu/openlearn/science-maths-technology/science/environmental-science/earths-physical-resources-petroleum/content-section-3.2.1

Mathematical problem

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

(Virieux and Operto, 2009)

$\mathbf{m}$: squared slowness

$\mathbf{d}$: field recorded data

$\mathbf{A}(\mathbf{m})$: discretized wave-equation

$\mathbf{q}$: source term

Challenges

- Multiple representations of the physics
- 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 ➡ $\mathbf{A}(\mathbf{m}) \in \mathbb{R}^{n \times n}, n = 1e16$
- Least square problem requires adjoints of the system matrix
- Discrete wave-equation can not be formed as an explicit matrix
  - stencil-based implementation
- Needs scalable, flexible, performant and portable discretization

Scientific motivations

Different physics

- Isotropic acoustic
- Isotropic acoustic with density
- Anisotropic acoustic
- Isotropic elastic
- Anisotropic elastic
- ...

Simulation for inversion

- Adjoint PDE
- Gradients
- ...

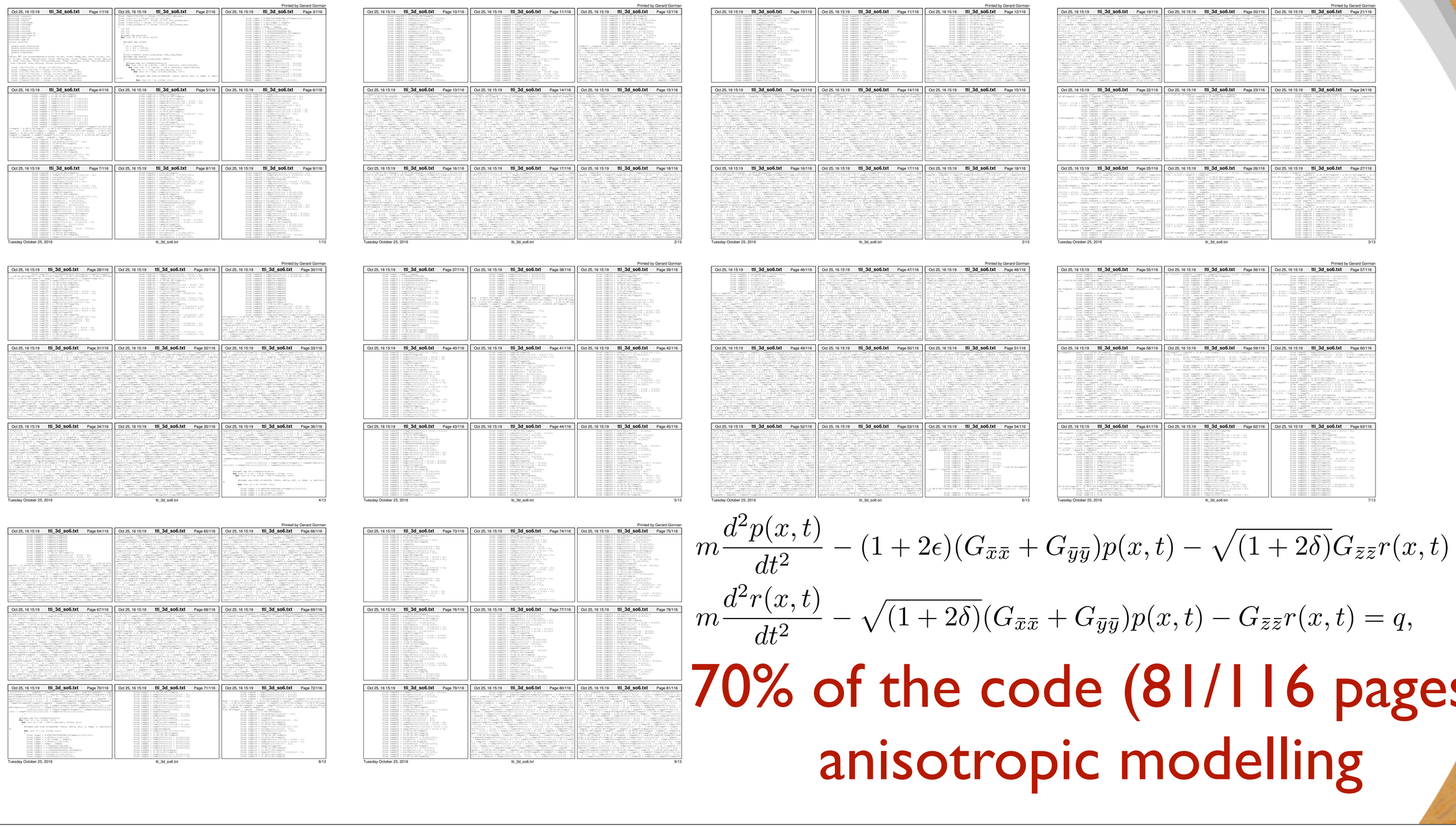
Design motivation

- Writing stencil codes is time consuming and hard for complicated equations. It is even harder because of the need for highly optimized implementations on a range of different computer architectures.

- **Separation of Concerns** with a finite-difference DSL

- Geophysicists need to be able to focus on the physics
- Computer scientists need to be able to focus on the software
- Mathematicians need to focus on numerical analysis

Design motivations



$$m\frac{d^2p(x,t)}{dt^2} - (1+2\epsilon)(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - \sqrt{(1+2\delta)}G_{\bar{z}\bar{z}}r(x,t) = q,$$

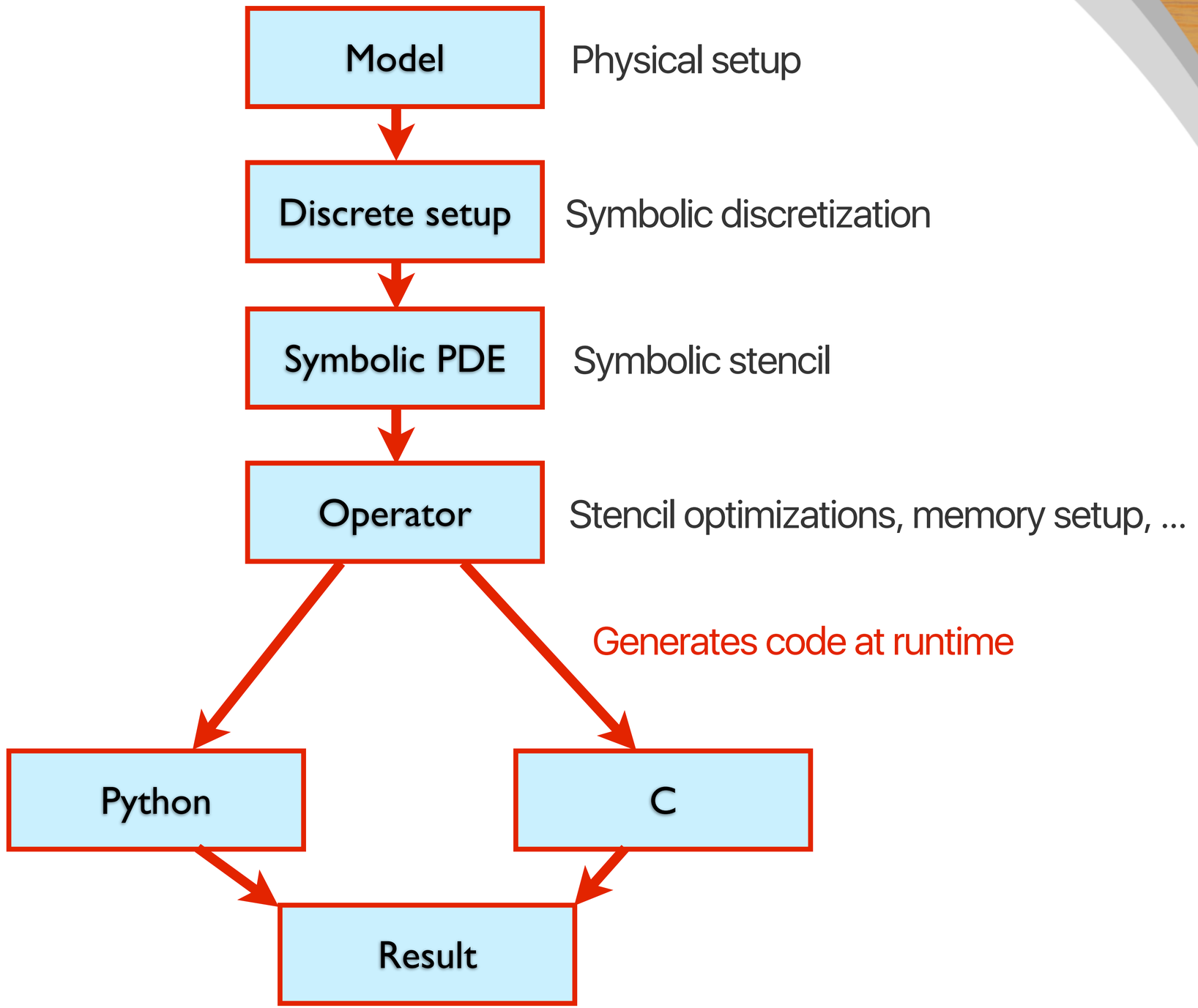
$$m\frac{d^2r(x,t)}{dt^2} - \sqrt{(1+2\delta)}(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - G_{\bar{z}\bar{z}}r(x,t) = q,$$

70% of the code (81/116 pages) anisotropic modelling

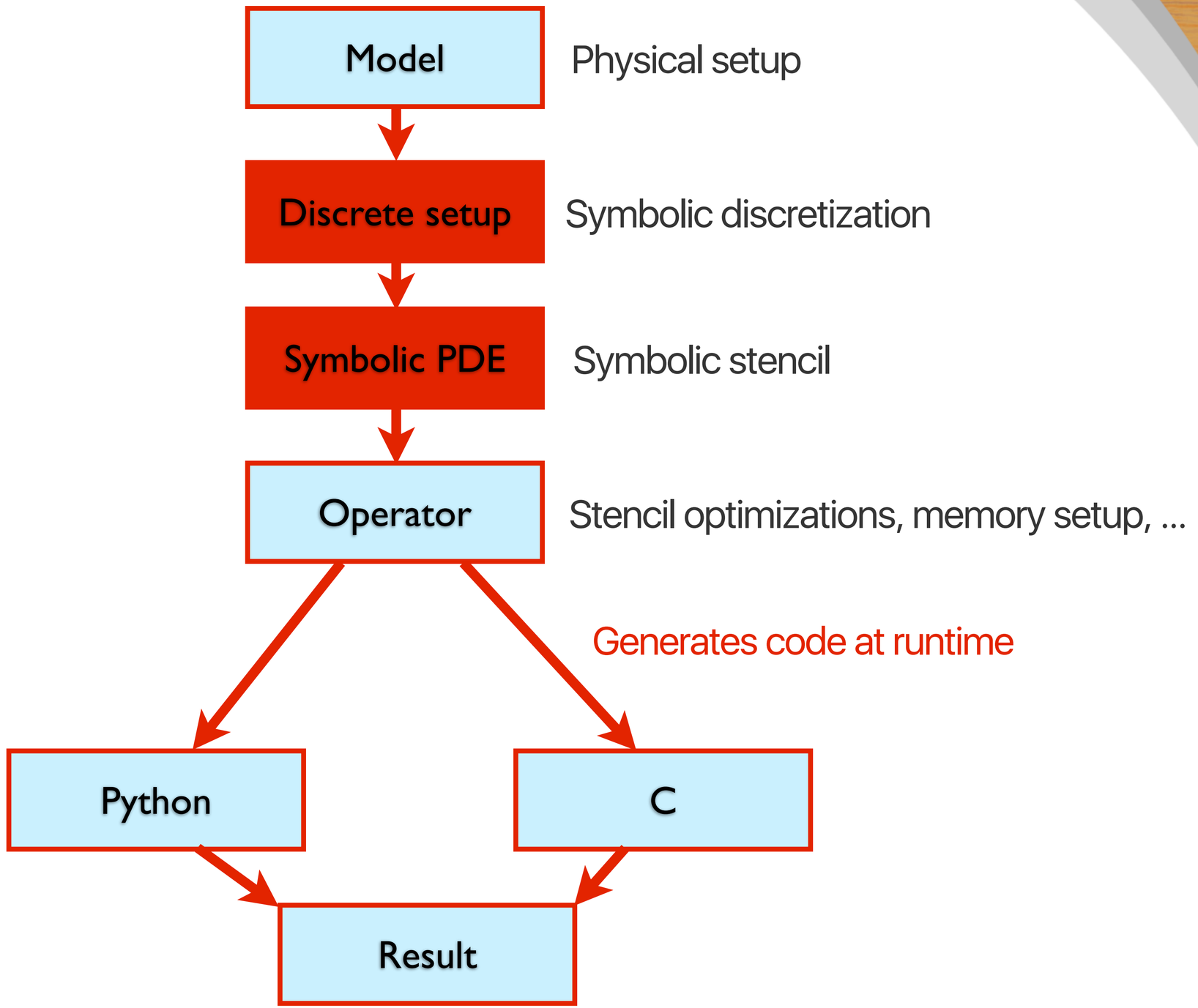
Objectives

- Flexible finite-differences discretization
- One framework for all equations
- Symbolic interface
  - easy to use
  - simple introduction of new PDEs

Summary


Model
Physical setup
Discrete setup
Symbolic discretization
Symbolic PDE
Symbolic stencil
Operator
Stencil optimizations, memory setup, ...
Generates code at runtime
Python
C
Result

Summary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Enabling different physics

Wave-equations

$$\frac{1}{c^2}\frac{d^2p(x,t)}{dt^2} - \Delta p(x,t) = 0$$

Acoustic isotropic

$$\frac{1}{\rho c^2}\frac{d^2p(x,t)}{dt^2} - \nabla.(\frac{1}{\rho}\nabla p(x,t)) = 0$$

Acoustic isotropic with density

$$m\frac{d^2p(x,t)}{dt^2} - (1+2\epsilon)(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - \sqrt{(1+2\delta)}G_{\bar{z}\bar{z}}r(x,t) = q,$$
$$m\frac{d^2r(x,t)}{dt^2} - \sqrt{(1+2\delta)}(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - G_{\bar{z}\bar{z}}r(x,t) = q,$$

Acoustic anisotropic

$$m\frac{d^2p(x,t)}{dt^2} - (1+2\epsilon)(D_{xx} + D_{yy})p(x,t) - \sqrt{(1+2\delta)}D_{zz}r(x,t) = q,$$
$$m\frac{d^2r(x,t)}{dt^2} - \sqrt{(1+2\delta)}(D_{xx} + D_{yy})p(x,t) - D_{zz}r(x,t) = q,$$

Acoustic tilted anisotropic

Zhang, Y., Zhang, H., and Zhang, G., 2011, A stable TTI reverse time migration and its implementation: Geophysics, 76

Symbolic discretization

Symbolic object with finite-difference discretization as a property

```
u =TimeData(name="u", shape=(nx, ny, nz),
            time_order=self.t_order,
            space_order=self.s_order)
```

is a symbolic object with derivatives properties

```
u.dx, u.dy, u.dz, u.dx2, ..., u.laplace,
```

In[69]: u.dx
Out[69]: -u(t - s, x - 3*h, y, z)/(60*h) + 3*u(t - s, x - 2*h, y, z)/(20*h) - 3*u(t - s, x - h, y, z)/(4*h) + 3*u(t - s, x + h, y, z)/(4*h) - 3*u(t - s, x + 2*h, y, z)/(20*h) + u(t - s, x + 3*h, y, z)/(60*h)

Symbolic wave-equations

Acoustic

$$0 = m\frac{d^2u(x,t)}{dt^2} - \Delta u(x,t) + \text{damp}\frac{du(x,t)}{dt}$$

```
eqn = m * u.dt2 - u.laplace + damp * u.dt
```

Acoustic 4th order in time

$$0 = m\frac{d^2u(x,t)}{dt^2} - \Delta u(x,t) - \frac{dt^2}{12}\Delta\left(\frac{1}{m}\Delta u(x,t)\right) + \text{damp}\frac{du(x,t)}{dt}$$

```
eqn = m * u.dt2 - u.laplace - (s**2)/12 * u.laplace2(1/m)+ damp * u.dt
```

Worked example

Acoustic modelling

Wave-equation setup

$$\mathbf{m}(\mathbf{x})\frac{\mathbf{u}(\mathbf{x},\mathbf{t}+dt)-2\mathbf{u}(\mathbf{x},t)+\mathbf{x},\mathbf{t}-dt)}{dt^2}-\Delta\mathbf{u}(\mathbf{x},\mathbf{t})=0$$

```
equation = m * u.dt2 - u.laplace + damp * u.dt
```

Absorbing boundary condition

$\mathbf{u}$: discretized wavefield

$\mathbf{m}$: discretized square slowness

Δ : discretized Laplacian

```
u = TimeData(name="u", shape=model.get_shape_comp(),
             time_dim=nt, time_order=time_order,
             space_order=spc_order,
             save=save, dtype=damp.dtype)

m = DenseData(name="m", shape=model.get_shape_comp(),
              dtype=damp.dtype)


Lap = u.laplace
```

Stencil

$$\mathbf{u}(\mathbf{x}, \mathbf{t} + dt) = 2\mathbf{u}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, \mathbf{t} - dt) + \frac{dt^2}{\mathbf{m}(\mathbf{x})}\Delta\mathbf{u}(\mathbf{x}, \mathbf{t})$$

u.forward = solve(equation, u.forward)

```
stencil = Eq(u.forward, solve(equation, u.forward))
```

Forward operator

```
# Create a forward operator
super(ForwardOperator, self).__init__(nt, m.shape,
                                      stencils=stencil,
                                      subs=subs,
                                      spc_border=spc_order/2,
                                      time_order=time_order,
                                      forward=True,
                                      dtype=m.dtype,
                                      **kwargs)

# Insert source and receiver terms post-hoc
self.propagator.time_loop_stencils_a = source.add(m, u) + rec.read(u)
```

Generate code at runtime

Application developer

```
(rec, u) = Acoustic.Forward()
```

Generated code

```
#include <cassert>
#include <cstdlib>
#include <cmath>
#include <iostream>
#include <fstream>
#include <vector>
#include <cstdio>
#include <string>
#include <inttypes.h>
#include <sys/time.h>
#include <math.h>
struct profiler
{
  double loop_stencils_a;
  double loop_body;
  double kernel;
} ;
struct flops
{
  long long loop_stencils_a;
  long long loop_body;
  long long kernel;
} ;
extern "C" int ForwardOperator(double *m_vec, double *u_vec, double *damp_vec, double *src_vec, float
*src_coords_vec, double *rec_vec, float *rec_coords_vec, long i1block, struct profiler *timings, struct flops *flops)
{
  double (*m)[280] = (double (*)[280]) m_vec;
  double (*u)[280][280] = (double (*)[280][280]) u_vec;
  double (*damp)[280] = (double (*)[280]) damp_vec;
  double (*src)[2] = (double (*)[2]) src_vec;
  float (*src_coords)[2] = (float (*)[2]) src_coords_vec;
  double (*rec)[101] = (double (*)[101]) rec_vec;
  float (*rec_coords)[2] = (float (*)[2]) rec_coords_vec;
  {
    struct timeval start_kernel, end_kernel;
    gettimeofday(&start_kernel, NULL);
    int t0;
    int t1;
    int t2;
    ;
    for (int i3 = 0; i3<500; i3+=1)
    {
      flops->kernel += 2.000000;
      {
        {
          t0 = (i3)%(3);
          t1 = (t0 + 1)%(3);
          t2 = (t1 + 1)%(3);
        }
        struct timeval start_loop_body, end_loop_body;
        gettimeofday(&start_loop_body, NULL);
        {
          for (int i1b = 1; i1b<279 - (278 % i1block); i1b+=i1block)
            for (int i1 = i1b; i1<i1b+i1block; i1++)
              {
```

Scientific motivations

Multi-physics

- Isotropic acoustic
- Isotropic acoustic with density
- Anisotropic acoustic
- Isotropic elastic
- Anisotropic elastic
- ...

Simulation for inversion

- Adjoint PDE
- Gradients
- ...

Adjoint-state

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

(Virieux and Operto, 2009)

Gradient with respect to $\mathbf{m}$ requires adjoint

$$\mathbf{g} = -\left(\frac{\partial \mathbf{u}}{\partial m}\right)^\top \mathbf{A}^{-\top}(\mathbf{m})(\mathbf{A}^{-1}(\mathbf{m}).\mathbf{q} - \mathbf{d})$$

Discretization for inversion

Extend symbolic discretization to adjoints

```
first_derivative(u,  dim=x, side=centered, order=spc_order, matvec=transpose)
```

CRITICAL for odd order derivatives (anti-symmetric stencil)

Not required for acoustic (self-adjoint equation)

Acoustic adjoint operator

Self-adjoint => Same stencil

Backward in time

Data as source

```
# Create a forward operator
super(AdjointOperator, self).__init__(nt, m.shape,
                                      stencils=stencil,
                                      subs=subs,
                                      spc_border=spc_order/2,
                                      time_order=time_order,
                                      forward=False,
                                      dtype=m.dtype,
                                      **kwargs)

# Insert source and receiver terms post-hoc
self.propagator.time_loop_stencils_a = source.read(m, u) + rec.add(u)
```

Generate code at runtime

Application developer

```
srca = Acoustic.Adjoint(dSyn - dObs)
```

Generated code

```
#include <cassert>
#include <cstdlib>
#include <cmath>
#include <iostream>
#include <fstream>
#include <vector>
#include <cstdio>
#include <string>
#include <inttypes.h>
#include <sys/time.h>
#include <math.h>
struct profiler
{
  double loop_stencils_a;
  double loop_body;
  double kernel;
} ;
struct flops
{
  long long loop_stencils_a;
  long long loop_body;
  long long kernel;
} ;
extern "C" int AdjointOperator(double *m_vec, double *u_vec, double *damp_vec, double *src_vec, float
*src_coords_vec, double *rec_vec, float *rec_coords_vec, long i1block, struct profiler *timings, struct flops *flops)
{
  double (*m)[280] = (double (*)[280]) m_vec;
  double (*u)[280][280] = (double (*)[280][280]) u_vec;
  double (*damp)[280] = (double (*)[280]) damp_vec;
  double (*src)[2] = (double (*)[2]) src_vec;
  float (*src_coords)[2] = (float (*)[2]) src_coords_vec;
  double (*rec)[101] = (double (*)[101]) rec_vec;
  float (*rec_coords)[2] = (float (*)[2]) rec_coords_vec;
  {
    struct timeval start_kernel, end_kernel;
    gettimeofday(&start_kernel, NULL);
    int t0;
    int t1;
    int t2;
    ;
    for (int i3 = 500; i3>0; i3-=1)
    {
      flops->kernel += 2.000000;
      {
        {
          t0 = (i3)%(3);
          t1 = (t0 + 1)%(3);
          t2 = (t1 + 1)%(3);
        }
        struct timeval start_loop_body, end_loop_body;
        gettimeofday(&start_loop_body, NULL);
        {
          for (int i1b = 1; i1b<279 - (278 % i1block); i1b+=i1block)
            for (int i1 = i1b; i1<i1b+i1block; i1++)
              {
```

Standardized verification for optimization

Rigorousness tests used as unit tests

Verify implementation

Allows stable continuous software integration with automated testing (TRAVIS)

Testing framework

Forward-adjoint test:

for any random $\mathbf{x} \in \text{span}(\mathbf{P}_s\mathbf{A}^T\mathbf{P}_r^T), \mathbf{y} \in \text{span}(\mathbf{P}_r\mathbf{A}\mathbf{P}_s^T)$

$$< \mathbf{P}_r\mathbf{A}\mathbf{P}_s^T\mathbf{x}, \mathbf{y} > - < \mathbf{x}, \mathbf{P}_s\mathbf{A}^T\mathbf{P}_r^T\mathbf{y} >= 0$$

$$\frac{< \mathbf{P}_r\mathbf{A}\mathbf{P}_s^T\mathbf{x}, \mathbf{y} >}{< \mathbf{x}, \mathbf{P}_s\mathbf{A}^T\mathbf{P}_r^T\mathbf{y} >} = 1$$

Gradient test:

for any small model perturbation $\mathbf{dm}$

$$\Phi_s(\mathbf{m} + h\mathbf{dm}) = \Phi_s(\mathbf{m}) + \mathcal{O}(h)$$

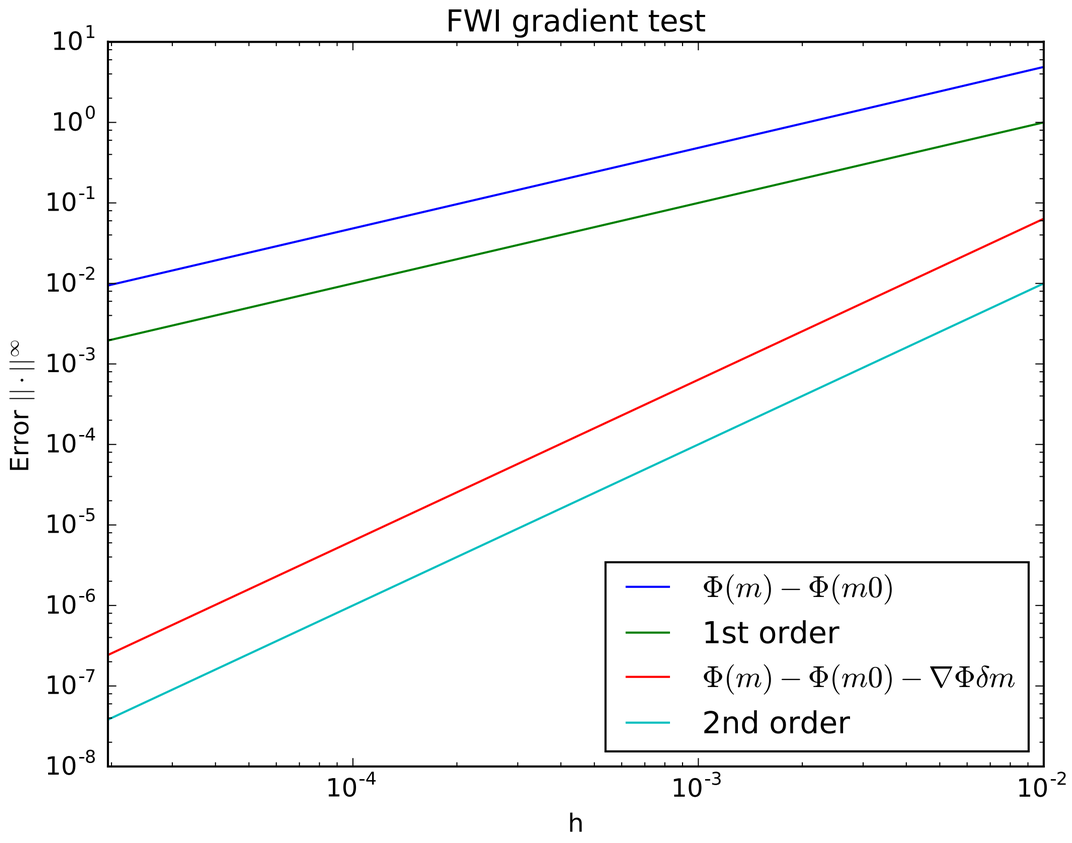
$$\Phi_s(\mathbf{m} + h\mathbf{dm}) = \Phi_s(\mathbf{m}) + h(\mathbf{J}[\mathbf{m}]^T\delta\mathbf{d})\mathbf{dm} + \mathcal{O}(h^2)$$

Adjoint test

Order	Dimension	$< \mathbf{F}\vec{x}, \vec{y} >$	$< \vec{x}, \mathbf{F}^t\vec{y} >$	Difference	ratio
2nd order	2D:	373323.7976042	373323.7975435	6.07169350e-05	1.0
4th order	2D:	340158.1486528	340158.1485253	0.00012756	1.0
6th order	2D:	341557.3948828	341557.3947399	0.00014287	1.0
8th order	2D:	358240.8513606	358240.8511932	0.00016741	1.0
10th order	2D:	393488.5561654	393488.5559270	0.00023841	1.0
12th order	2D:	439561.4005613	439561.4002034	0.00035794	1.0
2nd order	3D:	2.17496552	2.17496553	-1.23030883e-08	0.99999999
4th order	3D:	3.64447937	3.64447939	-2.13132316e-08	0.99999999
6th order	3D:	3.78730372	3.78730375	-2.22477072e-08	0.99999999
8th order	3D:	3.80286229	3.80286231	-2.23545817e-08	0.99999999
10th order	3D:	3.80557957	3.80557959	-2.23736993e-08	0.99999999
12th order	3D:	3.80318675	3.80318677	-2.23587757e-08	0.99999999

Gradient test

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



$\Leftarrow \quad \Phi(\mathbf{m} + h\mathbf{dm}) - \Phi(\mathbf{m})$

$\Leftarrow \quad \Phi(\mathbf{m} + h\mathbf{dm}) - \Phi(\mathbf{m}) - h(\mathbf{J}[\mathbf{m}]^T \delta\mathbf{d})\mathbf{dm}$

Future tests

Discretization tests

- test the finite-difference scheme generated against polynomials

Accuracy test

- test against analytical solution
- method of manufactured solutions (MMS)

...

Computational performance and optimization

MS84
Domain-Specific Abstractions for Full-Waveform Inversion
Symbolic Math for Automated Fast Finite Difference Computations

Navjot Kukreja, Imperial College London, United Kingdom

MS44
Efficiency of High-Order Methods on the 2nd Generation Intel Xeon Phi Processor

Vectorization and Locality Optimizations for Seismic Imagining Methods Through Automated Code Generation

Fabio Luporini, Imperial College, United Kingdom; Gerard J Gorman, Paul Kelly, and Michael Lange, Imperial College London, United Kingdom

Slides available upon request

Conclusions

Flexible physics with a simple finite-difference interface

- weeks, months, ... of development time saved
- write your own problem

Minimal coding required for geophysicists/mathematicians

- domain specialists only focus on their own problem
- improves collaborations with a high-level common ground

Simulation for inversion with adjoint-aware discretization

- not only restricted to modelling
- adjoints are inherently hard, specially for complicated physics

And all advantages of code generation with Devito (performance, architecture portability, ...)

References and link

OPESCI : http://www.opesci.org/

- documentation
- list of publications
- examples
- link to DEVITO source code

SLIM : https://www.slim.eos.ubc.ca/

- examples
- documentation
- list of publications

Acknowledgements

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