Devito

Automated fast finite difference computation

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Finite Difference Methods

$$f'(a) \approx \frac{f(a+h) - f(a)}{h} \qquad (1)$$

- Taylor series expansion
- Calculate derivatives of any order with relative simplicity
- Mathematically simple method for solving PDEs

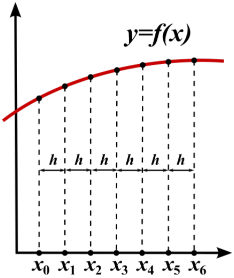


Figure: Discretizing a function on a grid (Wikipedia)

Why FD?

The acoustic wave equation

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0 \qquad (2)$$

Discretized:

$$u_i^{n+1} = -u_i^{n-1} + 2u_i^n + C^2(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \qquad (3)$$

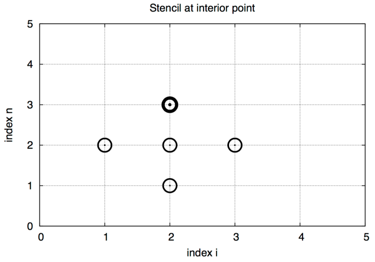


Figure: Mesh in space and time for a 1D wave equation

Why the wave equation?

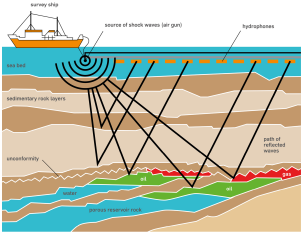


Figure: Offshore seismic survey

Seismic imaging

- RTM
  - Inputs: Velocity Model, Seismic Data
  - Output: Seismic image
- FWI
  - Inputs: Initial Velocity Model, Seismic Data
  - Output: Improved Velocity Model

Pure Python Implementation

```
for ti in range(0, nt):
    for a in range(1, nx-1):
        for b in range(1, ny-1):
            if ti == 0:
                u[ti, a, b] = self.ts(0, 0, 0, 0, 0, 0,
                                      m[a, b], dt, h, damp[a, b])
            elif ti == 1:
                u[ti, a, b] = self.ts(0, u[ti - 1, a - 1, b],
                                      u[ti - 1, a, b],
                                      u[ti - 1, a + 1, b],
                                      u[ti - 1, a, b - 1],
                                      u[ti - 1, a, b + 1],
                                      m[a, b], dt, h, damp[a, b])
            else:
                u[ti, a, b] = self.ts(u[ti - 2, a, b],
                                      u[ti - 1, a - 1, b],
                                      u[ti - 1, a, b],
                                      u[ti - 1, a + 1, b],
                                      u[ti - 1, a, b - 1],
                                      u[ti - 1, a, b + 1],
                                      m[a, b], dt, h, damp[a, b])
```

Why does it need to be fast?

- Large number of operations: $\approx$ 5000 FLOPs per loop iteration of a 16th order TTI Kernel
- Realistic problems have large grids: 1580 x 1580 x 1130 $\approx$ 2.82 Billion points (SEAM Benchmark)
- $2.82 \times 10^9 \times 5000 \times 3000(t) \times 2$ (forward-reverse) $\approx 8.5 \times 10^{16}$ per iteration of FWI
- Typically $\approx$ 30000 FWI iterations ($\approx 2.5 \times 10^{21} = 2.5 \times 10^9$ TFLOPs)

$\approx$ 135 wall-clock hours on the TACC Stampede (ideally)

Why automated

Computer Science

- Fast code is complex
  - Loop blocking
  - OpenMP clauses
  - Vectorisation - intrinsics
  - Memory - alignment, NUMA
  - Factorization
  - FMA
- Fast code is platform dependent
  - Intrinsics
  - CUDA
  - OpenCL
- Fast code is error prone

Geophysics

- Change of discretizations
- Change of physics
  - Anisotropy - VTI/TTI
  - Elastic equation
- Boundary conditions
- Continuous acquisition

SymPy - Symbolic computation in Python

- Symbolic computer algebra system written in pure Python
- Features
  - Complex symbolic expressions as Python object trees
  - Symbolic manipulation routines and interfaces
  - Convert symbolic expressions to numeric functions
    - Python or NumPy functions
    - C or Fortran kernels

For specialised domains generating C code is not enough!

Devito - a prototype Finite Difference DSL

Devito - A Finite Difference DSL for seismic imaging

- Aimed at creating fast high-order inversion kernels
- Development is driven by "real world" problems

Based on SymPy expressions

- The acoustic wave equation:

$$m\frac{\partial^2 u}{\partial t^2} + \eta\frac{\partial u}{\partial t} - \nabla u = 0 \tag{4}$$

  can be written as

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

Devito auto-generates optimised C kernel code

- OpenMP threading and vectorisation pragmas
- Cache blocking and auto-tuning
- Symbolic stencil optimisation (eg. CSE, hoisting)

Devito

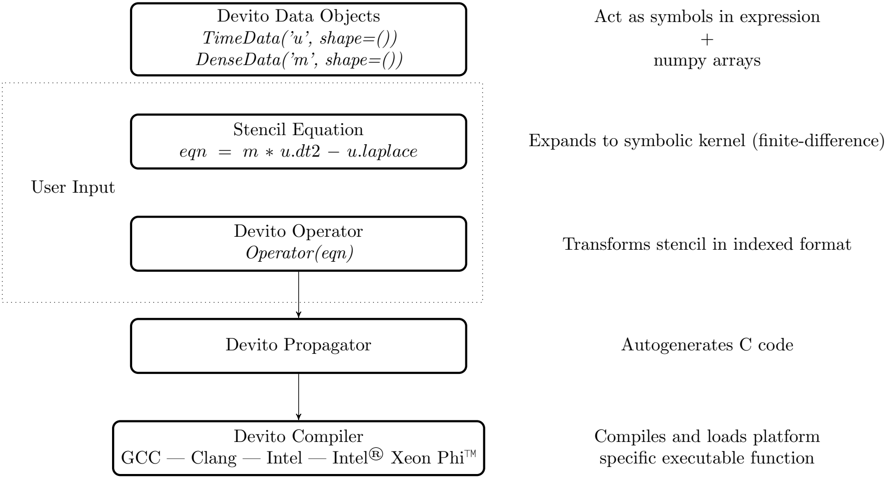


Figure: An overview of Devito's architecture

Devito

Real-world applications need more than PDE solvers

- File I/O and support for large datasets
- Non PDE kernel code e.g. sparse point interpolation
- Ability to easily interface with complex outer code

Devito follows the principle of graceful degradation

- Circumvent restrictions to the high-level API by customisation
- Devito translates high-level PDE-based stencils into "matrix index" format in steps

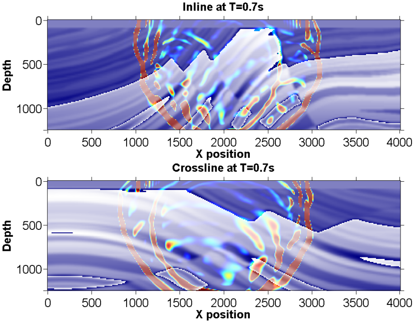
```
# High-level expression equivalent to f.dx2
(-2*f(x, y) + f(x - h, y) + f(x + h, y)) / h**2
# Low-level expression with explicit indexing
(-2*f[x, y] + f[x - 1, y] + f[x + 1, y]) / h**2
```

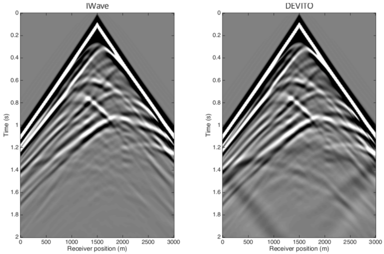
- Allows custom functionality in auto-generated kernels

Seismic Imaging

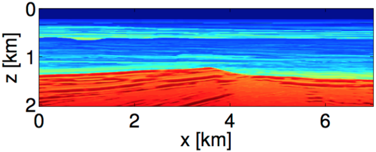
Full waveform inversion

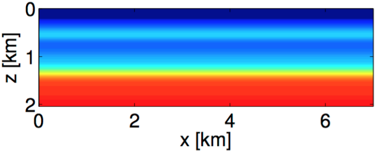
- Acoustic and TTI wave equations of varying spatial order
- Numerically verified against Industrial standard software on standard datasets
- Achieved performance is also comparable to industrial standard software





FWI





Example code for forward propagation

```
def forward(model, nt, dt, h, order=2):
        shape = model.shape
        m = DenseData(name="m", shape=shape,
                space_order=order)
        m.data[:] = model
        u = TimeData(name="u", shape=shape,
                time_dim=nt, time_order=2,
                space_order=order, save=True)
        eta = DenseData(name="eta", shape=shape,
                space_order=order)
        # Derive stencil from symbolic equation
        eqn = m * u.dt2 - u.laplace + eta * u.dt
        stencil = solve(eqn, u.forward)[0]
        op = Operator(stencils=Eq(u.forward , stencil),
                nt=nt, subs={s: dt, h: h}, shape=shape ,
                forward=True)
        # Source injection code omitted for brevity
        op.apply()
```

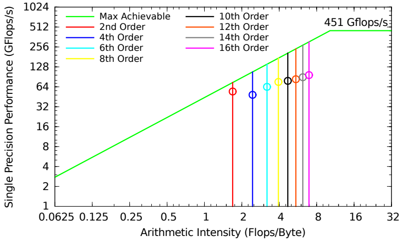
```
// #include directives omitted for brevity
extern "C" int ForwardOperator(double *u_vec, double *damp_vec, double *m_vec, double *src
{
  double (*u)[130][130][130] = (double (*)[130][130][130]) u_vec;
  double (*damp)[130][130] = (double (*)[130][130]) damp_vec;
  double (*m)[130][130] = (double (*)[130][130]) m_vec;
  double (*src)[1] = (double (*)[1]) src_vec;
  float (*src_coords)[3] = (float (*)[3]) src_coords_vec;
  double (*rec)[101] = (double (*)[101]) rec_vec;
  float (*rec_coords)[3] = (float (*)[3]) rec_coords_vec;
  {
    #pragma omp parallel
    for (int i4 = 0; i4<149; i4+=1)
    {
      {
        #pragma omp for schedule(static)
        for (int i1b = 1; i1b<129 - (128 % i1block); i1b+=i1block)
          for (int i2b = 1; i2b<129 - (128 % i2block); i2b+=i2block)
            for (int i1 = i1b; i1<i1b+i1block; i1++)
              for (int i2 = i2b; i2<i2b+i2block; i2++)
              {
                #pragma omp simd aligned(damp, m, u:64)
                for (int i3 = 1; i3<129; i3++)
                {
                  double temp1 = damp[i1][i2][i3];
                  double temp2 = m[i1][i2][i3];
                  double temp4 = u[i4 - 1][i1][i2][i3];
                  double temp5 = u[i4 - 2][i1][i2][i3];
                  u[i4][i1][i2][i3] = ...
                }
              }
        for (int i1 = 129 - (128 % i1block); i1<129; i1++)
          for (int i2 = 1; i2<129 - (128 % i2block); i2++)
```

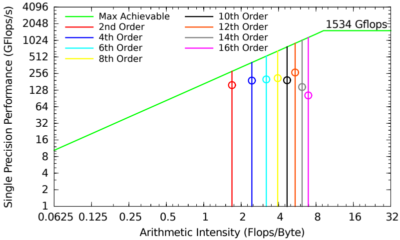
```python
def adjoint(model, nt, dt, h, spc_order=2):
    m = DenseData("m", model.shape)
    m.data[:] = model
    v = TimeData(name='v', shape=model.shape, time_dim=nt,
                 time_order=2, space_order=spc_order,
                 save=False)
    damp = DenseData("damp", model.shape)

    # Derive stencil from symbolic equation
    eqn = m * v.dt2 - v.laplace - damp * v.dt
    stencil = solve(eqn, v.backward)[0]

    # Add spacing substitutions
    subs = {s: dt, h: h}
    op = Operator(stencils=Eq(u.backward, stencil), nt=nt,
                 shape=model.shape, subs=subs, forward=False)
    op.apply()
```

Performance

Performance of acoustic forward operator

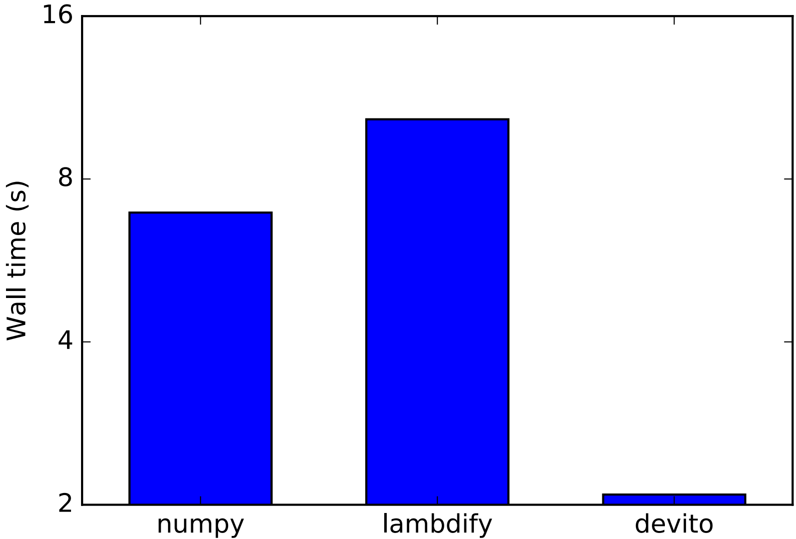
- Intel Xeon E5-2690v2 10C 3GHz and a Intel® Xeon Phi™Knightscorner
- Model size 201 x 201 x 70 + 40 ABC
- Grid size 15m 10Hz Ricker wavelet source





Performance

2D Diffusion equation on a single core



Performance Optimizations

Automated code optimizations:

- OpenMP and vectorization pragmas
- Loop blocking and auto-tuning for block size
- Automated roofline plotting for performance analysis

Symbolic Optimizations

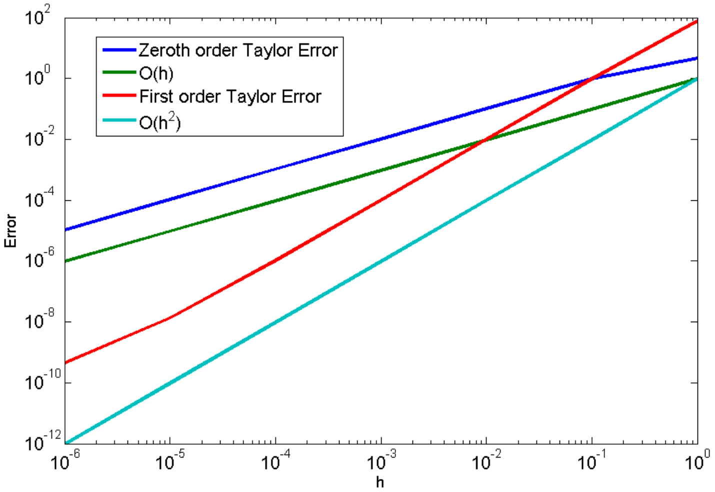
- Common Subexpression elimination
  - Reduces compilation time from hours to seconds for large stencils
  - Enables further factorization techniques to reduce flops

Potential future optimizations

- Polyhedral compilation (time blocking)
- Automated data layout optimizations

Verification

Adjoint Test and Gradient Test



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Conclusions

- Devito: A finite difference DSL for seismic imaging
  - Symbolic problem description (PDEs) via SymPy
  - Low-level API for kernel customisation
  - Automated performance optimisation
- Devito is driven by real-world scientific problems
  - Not yet another stencil compiler
  - Bridge the gap between stencil compilers and real world applications
- Future work:
  - Extend feature range to facilitate more science
  - MPI parallelism for larger models
  - Integrate stencil or polyhedral compiler backends
  - Additional symbolic optimisation (factorisation, hoisting, etc.)
  - Integrate automated verification tools to catch compiler bugs

Thank you

Publications

- N. Kukreja, M. Louboutin, F. Vieira, F. Luporini, M. Lange, and G. Gorman. Devito: automated fast finite difference computation. Accepted for WOLFHPC16, to appear in ACM SIGHPC, 2016
- M. Lange, N. Kukreja, M. Louboutin, F. Luporini, F. Vieira, V. Pandolfo, P. Velesko, P. Kazakas, and G. Gorman. Devito: Towards a generic Finite Difference DSL using Symbolic Python. Accepted for PyHPC2016, to appear in ACM SIGHPC, 2016
- M. Louboutin, M. Lange, N. Kukreja, F. Herrmann, and G. Gorman. Performance prediction of finite-difference solvers for different computer architectures. Submitted to Computers and Geosciences, 2016

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