Optimised finite difference computation from symbolic equations

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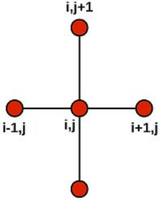
Symbolic computation is a powerful tool

Solving simple PDEs is (kind of) easy...

First-order diffusion equation:

```
for ti in range(timesteps):
    t0 = ti % 2
    t1 = (ti + 1) % 2
    for i in range(1, nx-1):
        for j in range(1, ny-1):
            uxx = (u[t0, i+1, j] -2 * u[t0, i, j] + u[t0, i-1, j]) / dx2
            uyy = (u[t0, i, j+1] -2 * u[t0, i, j] + u[t0, i, j-1]) / dy2
            u[t1, i, j] = u[t0, i, j] + dt * a * (uxx + uyy)
```



Symbolic computation is a powerful tool

Solving complicated PDEs is not easy!

12th-order acoustic wave equation:

```
for (int i4 = 0; i4<149; i4+=1) {
  for (int i1 = 6; i1<64; i1++) {
    for (int i2 = 6; i2<64; i2++) {
      for (int i3 = 6; i3<64; i3++) {
        u[i4][i1][i2][i3] = 6.01250601250601e-9F*(2.80896e+8F*damp[i1][i2][i3]*u[i4-2][i1
              ][i2][i3]-3.3264e+8F*m[i1][i2][i3]*u[i4-2][i1][i2][i3]+6.6528e+8F*m[i1][i2][
              i3]*u[i4-1][i1][i2][i3]-2.12255421155556e+7F*u[i4-1][i1][i2][i3
              ]-1.42617283950617e+2F*u[i4-1][i1][i2][i3-6]+2.46442666666667e+3F*u[i4-1][i1
              ][i2][i3-5]-2.11786666666667e+4F*u[i4-1][i1][i2][i3-4]+1.25503209876543e+5F*
              u[i4-1][i1][i2][i3-3]-6.3536e+5F*u[i4-1][i1][i2][i3-2]+4.066304e+6F*u[i4-1][
              i1][i2][i3-1]+4.066304e+6F*u[i4-1][i1][i2][i3+1]-6.3536e+5F*u[i4-1][i1][i2][
              i3+2]+1.25503209876543e+5F*u[i4-1][i1][i2][i3+3]-2.11786666666667e+4F*u[i4
              -1][i1][i2][i3+4]+2.46442666666667e+3F*u[i4-1][i1][i2][i3
              +5]-1.42617283950617e+2F*u[i4-1][i1][i2][i3+6]-1.42617283950617e+2F*u[i4-1][
              i1][i2-6][i3]+2.46442666666667e+3F*u[i4-1][i1][i2-5][i3]-2.11786666666667e+4
              F*u[i4-1][i1][i2-4][i3]+1.25503209876543e+5F*u[i4-1][i1][i2-3][i3]-6.3536e+5
              F*u[i4-1][i1][i2-2][i3]+4.066304e+6F*u[i4-1][i1][i2-1][i3]+4.066304e+6F*u[i4
              -1][i1][i2+1][i3]-6.3536e+5F*u[i4-1][i1][i2+2][i3]+1.25503209876543e+5F*u[i4
              -1][i1][i2+3][i3]-2.11786666666667e+4F*u[i4-1][i1][i2+4][i3
              ]+2.46442666666667e+3F*u[i4-1][i1][i2+5][i3]-1.42617283950617e+2F*u[i4-1][i1
              ][i2+6][i3]-1.42617283950617e+2F*u[i4-1][i1-6][i2][i3]+2.46442666666667e+3F*
              u[i4-1][i1-5][i2][i3]-2.11786666666667e+4F*u[i4-1][i1-4][i2][i3
              ]+1.25503209876543e+5F*u[i4-1][i1-3][i2][i3]-6.3536e+5F*u[i4-1][i1-2][i2][i3
              ]+4.066304e+6F*u[i4-1][i1-1][i2][i3]+4.066304e+6F*u[i4-1][i1+1][i2][i3
              ]-6.3536e+5F*u[i4-1][i1+2][i2][i3]+1.25503209876543e+5F*u[i4-1][i1+3][i2][i3
              ]-2.11786666666667e+4F*u[i4-1][i1+4][i2][i3]+2.46442666666667e+3F*u[i4-1][i1
              +5][i2][i3]-1.42617283950617e+2F*u[i4-1][i1+6][i2][i3])/(1.68888888888889F*
              damp[i1][i2][i3]+2*m[i1][i2][i3]);
    }
  }
```

Symbolic computation is a powerful tool

We can solve PDEs symbolically

- Domain-specific languages provide high levels of abstraction
- Separation of concerns between scientists and computational experts

SymPy: Symbolic computer algebra system in pure Python[1]

Enables automation of stencil generation

- Complex symbolic expressions as Python object trees
- Programmatic manipulation of symbolic expressions
- Built-in code generation for variety of languages

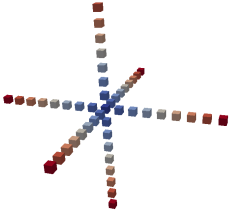
- For a great overview see A. Meurer's talk at SciPy 2016

[1] A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M. J. Curry, A. R. Terrel, Š. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3:e103, January 2017

Devito: Finite difference DSL based on SymPy

Devito generates highly optimized stencil code...

- OpenMP threading and vectorisation pragmas
- Cache blocking and auto-tuning
- Symbolic stencil optimization



... from concise mathematical syntax!

Example: acoustic wave equation with dampening

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

can be written as

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

CFD Python: Step 5 - Linear convection

Governing equation:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} + c\frac{\partial u}{\partial y} = 0$$

Discretized:

$$u_{i,j}^{n+1} = u_{i,j}^{n} - c\frac{\Delta t}{\Delta x}(u_{i,j}^{n} - u_{i-1,j}^{n}) - c\frac{\Delta t}{\Delta y}(u_{i,j}^{n} - u_{i,j-1}^{n})$$

SymPy stencil (assume $\Delta t = s$, $\Delta x = \Delta y = h$):

```
from devito import *
from sympy import solve

c = 1.
grid = Grid(shape=(nx, ny))
u = TimeFunction(name='u', grid=grid)
eq = Eq(u.dt + c * u.dxl + c * u.dyl)
stencil = solve(eq, u.forward)[0]

[In] print(stencil)
[Out] (h*u(t, x, y) - 2.0*s*u(t, x, y)
     + s*u(t, x, y - h) + s*u(t, x - h, y))/h
```

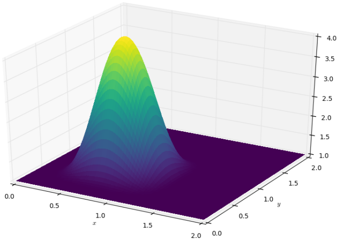
CFD Python: Step 5 - Linear convection

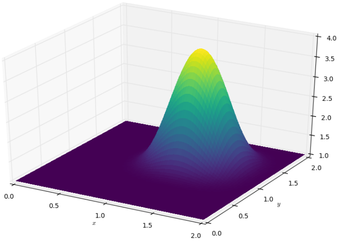
Simple advection example:

```
op = Operator(Eq(u.forward, stencil))

# Set initial condition as a smooth bump
init_smooth(u.data, dx, dy)

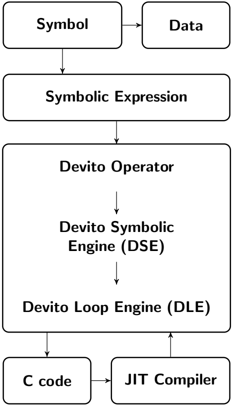
op(u=u, time=100, dt=dt)  # Apply for 100 timesteps
```





http://nbviewer.jupyter.org/github/barbagroup/CFDPython/blob/master/lessons/07_Step_5.ipynb

Devito - Automated code optimizations




```
u = TimeFunction(name='u', grid=grid)
m = Function(name='m', grid=grid)
```

High-level function symbols associated with user data

```
eqn = m * u.dt2 - u.laplace
```

Symbolic equations that expand finite difference stencils

```
op = Operator(expressions)
op.apply(time=ntime)
```

Automatic code generation and execution from high-level expressions

Symbolic optimization to reduce computation per stencil point

Loop-level optimization for efficient parallel execution

Just-in-time compilation of optimized C code

Motivation: Inversion problems for seismic imaging

Seismic imaging is a challenging problem for HPC

Big data meets big compute

- Very large amounts of data, huge amount of compute
- HPC architectures, often with accelerators (eg. Intel® Xeon Phi)
- Require highly optimized solvers code

Often use complex finite difference operators

- Different high-order formulations of wave equations
- Unknown topology and high wave frequencies
- Large, complicated stencils, often **written by hand!**

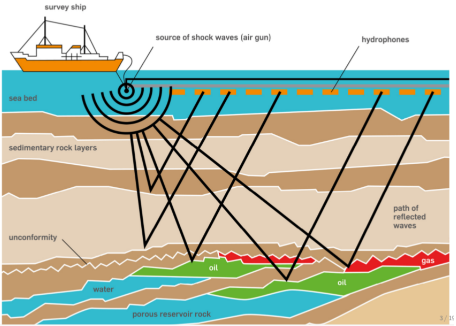
Pure stencil DSLs are not enough

- Generating stencils still has to be done by hand
- Many special-cases that do not fit the "stencil" abstraction

The aim is to derive an image of the earth's subsurface

Solve a PDE-constrained optimization problem

- Using wave propagation operators and their adjoints
- Wave is inserted and read at unaligned points
  Inject sparse point interpolation into kernels!



High-performance wave propagators for seismic imaging

```
def forward(model, m, eta, src, rec, order=2):
    # Create the wavefeld function
    u = TimeFunction(name='u', grid=model.grid,
                     time_order=2, space_order=order)

    # Derive stencil from symbolic equation
    eqn = m * u.dt2 - u.laplace + eta * u.dt
    stencil = solve(eqn, u.forward)[0]
    update_u = [Eq(u.forward, stencil)]

    # Inject wave as source term
    src_term = src.inject(field=u, expr=src * dt**2 / m)

    # Interpolate wavefield onto receivers
    rec_term = rec.interpolate(expr=u)

    # Create operator with source and receiver terms
    return Operator(update_u + src_term + rec_term)
```

Acoustic wave equation:

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

High-performance wave propagators for seismic imaging

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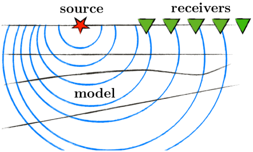
    update_u = [Eq(u.forward, stencil)]

    # Inject wave as source term
    src_term = src.inject(field=u, expr=src * dt**2 / m)

    # Interpolate wavefield onto receivers
    rec_term = rec.interpolate(expr=u)

    # Create operator with source and receiver terms
    return Operator(update_u + src_term + rec_term)
```



High-performance wave propagators for seismic imaging

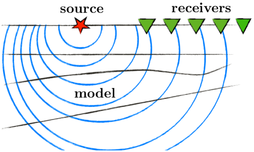
```
def gradient(model, m, eta, srca, rec, order=2):
    # Create the adjoint wavefeld function
    v = TimeFunction(name='v', grid=model.grid,
                     time_order=2, space_order=order)

    # Derive stencil from symbolic equation
    eqn = m * v.dt2 - v.laplace — eta * v.dt
    stencil = solve(eqn, u.forward)[0]
    update_v = [Eq(v.backward, stencil)]

    # Inject the previous receiver readings
    rec_term = rec.inject(field=v, expr=rec * dt**2 / m)

    # Gradient update terms
    grad = Function(name='grad', grid=model.grid)
    grad_update = Eq(grad, grad — u.dt2 * v)

    # Create operator with source and receiver terms
    return Operator(update_v + [grad_update] + rec_term,
                    time_axis=Backward)
```



Devito - Automated finite difference propagators

Reverse time migration in $<$ 100 lines of Python

```
# Define acquisition geometry and timestepping
model = Model(...)
dt, nt = <timestepping parameters>
src = RickerSource(...)
rec = Receiver(...)

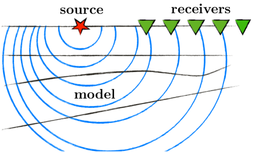
# Create forward and gradient operators
op_fwd = forward(model, src, rec, order)
op_grad = gradient(model, rec, order)

grad = Function(name='grad', grid=model.grid)

for shot in shots:
    # Create wavefield for forward propagation
    u = TimeFunction(name='u', grid=model.grid,
                     space_order=order)

    # Update source location and compute forward
    src.coordinates.data[0. :] = source_loc[i]
    op_forward(u=u, src=src, rec=rec, m=model.m)

    # Compute gradient update from the residual
    residual = measurement_data - rec.data[:]
    op_gradient(u=u, v=v, grad=grad,
                rec=residual, m=model.m)
```

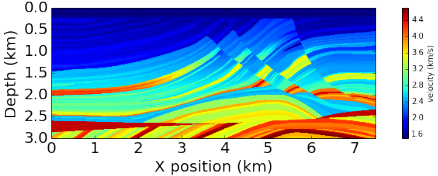


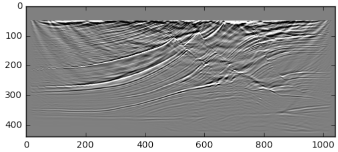
High-performance wave propagators for seismic imaging

Efficient development

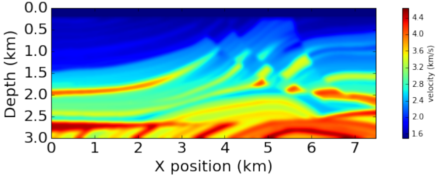
- Test and verify in Python
- Operators in $<$ 20 lines
- RTM loop in $<$ 100 lines
- Variable stencil order

Subsurface model (Marmousi 2D)





Inverted subsurface image



Initial pertubation (Gaussian filter)

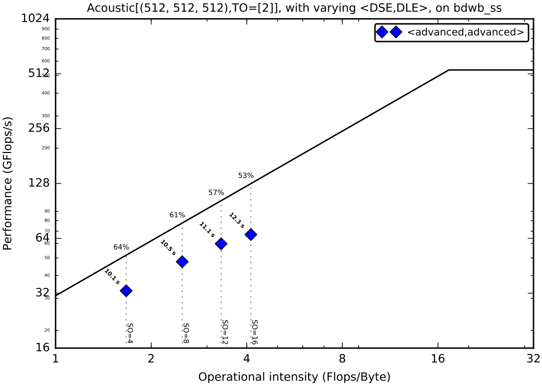
http://www.opesci.org/devito/tutorials.html

Devito - Performance of acoustic operators

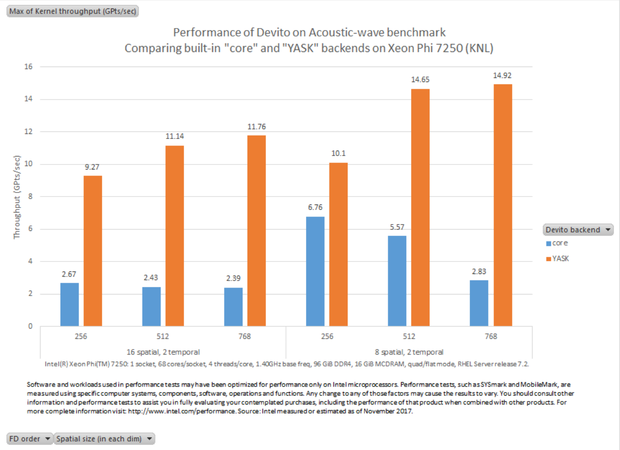
Performance benchmark:

- Second order in time with boundary dampening
- 3D domain (512 × 512 × 512), grid spacing = 20.
- Varying space order (SO)

- Xeon E5-2620 v4 2.1Ghz (Broadwell) 8 cores @ 2.1GHz, single socket



Devito - YASK integration



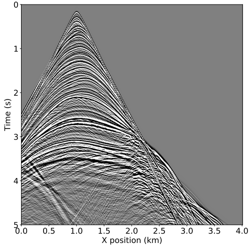
Y*A*S*K
Yet Another Stencil Kernel

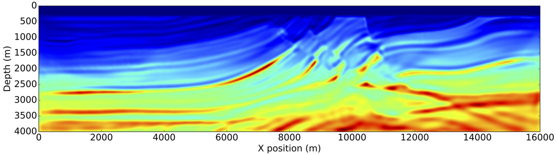
Imperial College London

Summary

- **Devito: High-performance finite difference DSL**
  - Symbolic finite difference stencils via SymPy
  - Fully executable via JIT compilation
  - **Increased productivity through high-level API**
  - **Fully composable with scientific Python ecosystem**

- **Fast wave propagators for inversion problems**
  - Seismic inversion operators in < 20 lines
  - Complete problem setups in 200 lines
  - **Automated performance optimisation!**





Thank You

Useful links:

- http://www.opesci.org
- https://github.com/opesci/devito
- http://www.sympy.org

Tutorials:

- Recorded version of this talk given at SciPy17
- Devito tutorials: http://www.opesci.org/devito/tutorials.html
- CFD Python tutorial: http://lorenabarba.com/blog/cfd-python-12-steps-to-navier-stokes/

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