Automatic code generation - developing high performance propagators better, faster and cheaper.

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[3]Intel Corporation

Devito - Automated finite difference propagators

Something is rotten in the state of Denmark...

Seismic inversion is extremely computationally demanding!

Yet new models are built around bespoke operators...

- Discretization and numerical methods are chosen a priori [1]
- Performance optimization repeated for each architecture
- Requires many person-months (years) to develop new algorithms

Complex algorithms need end-to-end optmization

- Optimization at various levels of expertise
- Domain-specialists, numericists and compiler experts ...
- But we can't all be polymaths. We need separation of concerns!

[1] M. Louboutin, M. Lange, F. J. Herrmann, N. Kukreja, and G. Gorman. Performance prediction of finite-difference solvers for different computer architectures. *Computers and Geosciences*, 105:148 – 157, 2017

Devito - Automated finite difference propagators

Symbolic computation is a powerful tool!

- **FEniCS / Firedrake** - Finite element DSL packages

  Velocity-stress formulation of elastic wave equation, with isotropic stress:

$$\rho \frac{\partial \mathbf{u}}{\partial t} = \nabla \cdot \mathbb{T}$$

$$\frac{\partial \mathbb{T}}{\partial t} = \lambda \left(\nabla \cdot \mathbf{u}\right) \mathbb{I} + \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}\right)$$

  Weak form of equations written in UFL [1]:

```
F_u = density*inner(w, (u - u0)/dt)*dx - inner(w, div(s0))*dx
solve(lhs(F_u) == rhs(F_u), u)
```

[1] Anders Logg, Kent-Andre Mardal, and Garth Wells. *Automated Solution of Differential Equations by the Finite Element Method: The FEniCS Book*. Springer Publishing Company, Incorporated, 2012

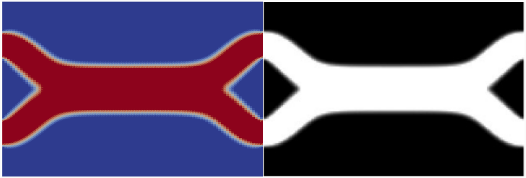
Devito - Automated finite difference propagators

Symbolic computation is a powerful tool!

Dolfin-Adjoint: Symbolic adjoints from symbolic PDEs[1]

- Solves complex optimisation problems
- 2015 Wilkinson prize winner

Below is the optimal design of a double pipe that minimises the dissipated power in the fluid.



[1] P. E. Farrell, D. A. Ham, S. W. Funke, and M. E. Rognes. Automated derivation of the adjoint of high-level transient finite element programs. *SIAM Journal on Scientific Computing*, 35(4):C369–C393, 2013

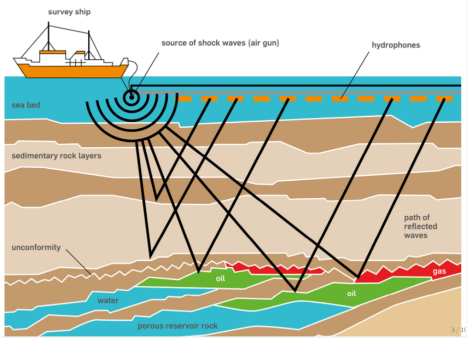
Devito - Automated finite difference propagators

For Seismic imaging we need to solve inversion problems

- Finite difference solvers for forward and adjoint runs
- Different types of wave equations with large complicated stencils

Many stencil languages exist, but few are practical

- Stencil still written by hand!



Devito - Automated finite difference propagators

- **SymPy** - Symbolic computer algebra system in pure Python[1]
- Features:
  - Complex symbolic expressions as Python object trees
  - Symbolic manipulation routines and interfaces
  - Convert symbolic expressions to numeric functions
    - Python (NumPy) functions; C or Fortran kernels
  - For a great overview see A. Meuer's talk at SciPy 2016

For specialised domains generating C code is not enough!

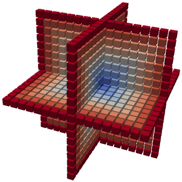
- Compiler-level optimimizaton to leverage performance
- Stencil optimization is a research field of its own

[1] Aaron Meurer, Christopher P Smith, Mateusz Paprocki, Ondřej Čertík, Matthew Rocklin, AMiT Kumar, Sergiu Ivanov, Jason K Moore, Sartaj Singh, Thilina Rathnayake, et al. Sympy: Symbolic computing in python. Technical report, PeerJ Preprints, 2016

Devito - Automated finite difference propagators

Devito: a finite difference DSL for seismic imaging

- Generates highly optimized stencil code
  - OpenMP threading and vectorisation pragmas
  - Cache blocking and auto-tuning
  - Symbolic stencil optimisation



- From concise mathematical syntax

Acoustic wave equation:

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

can be written as

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

Devito - Automated finite difference propagators

Development is driven by real-world problems!

- Productivity through code generation
  - Variable numerical discretisation stencil size
  - Individual operators in 10s of lines of code
  - Complete problem setups in a few 100 lines

- Fast high-order operators for inversion problems
  - Automated performance optimisation
  - Customization through hierarchical API

Devito - Automated finite difference propagators

Development is driven by real-world problems!

Devito Data Objects

`u = TimeData('u', shape=(nx, ny))`

`m = DenseData('m', shape=(nx, ny))`

High-level function symbols associated with user data

↓

Stencil Equation

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

Symbolic equations that expand Finite Difference stencils

↓

Devito Operator

`op = Operator(eqn)`

Transform stencil expressions into explicit array accesses

↓

Devito Compiler

GCC — Clang — Intel®— Intel®Xeon Phi™

`op.compiler = IntelMIC`

Compiles and loads Platform specific executable function

Devito - Automated finite difference propagators

Wave propagators in less than 100 lines

```
def forward(model, m, eta, src, rec, order=2, save=True):
    # Create the wavefeld function
    u = TimeData(name='u', shape=model.shape, save=save,
                 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,
                    subs={s: dt, h: model.spacing})
```

Devito - Automated finite difference propagators

Wave propagators in less than 100 lines

```
def adjoint(model, m, eta, srca, rec, order=2):
    # Create the adjoint wavefeld function
    v = TimeData(name='v', shape=model.shape,
                 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)

    # Interpolate the adjoint-source
    srca_term = srca.interpolate(expr=v)

    # Create operator with source and receiver terms
    return Operator(update_v + rec_term + srca_term,
                    subs={s: dt, h: model.spacing},
                    time_axis=Backward)
```

Devito - Automated finite difference propagators

Wave propagators in less than 100 lines

```
def gradient(model, m, eta, srca, rec, order=2):
    # Create the adjoint wavefeld function
    v = TimeData(name='v', shape=model.shape,
                 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 = DenseData(name='grad', shape=model.shape)
    grad_update = Eq(grad, grad - u.dt2 * v)

    # Create operator with source and receiver terms
    return Operator(update_v + [grad_update] + rec_term
                    subs={s: dt, h: model.spacing},
                    time_axis=Backward)
```

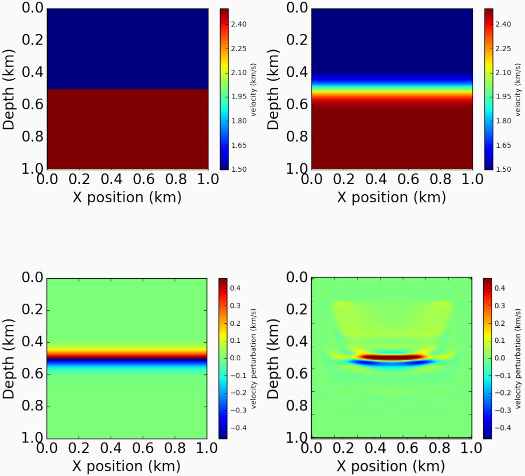
Devito - Automated finite difference propagators

Reverse time migration in less than 100 lines

```
# Create the true and a smoothed model
m_true = Model(...)
m_smooth = Model(...)

# Create operators for forward and gradient
op_forward = forward(...)
op_gradient = forward(...)

# Create gradient field and loop over shots
grad = DenseData(name='grad', shape=model.shape)

for shot in shots:
    # Create receiver data from true model
    src = PointData(shot.source, ...)
    rec_true = PointData(shot.receiver.coordinates, ...)
    op_forward(src=src, rec=rec_true, m=m_true)

    # Run forward modelling operator with smooth model
    u = TimeData(name='u', shape=model.shape,
                 time_order=2, space_order=order)
    rec_smooth = PointData(shot.receiver.coordinates, ...)
    op_forward(u=u, src=src, rec=rec_smooth, m=m_smooth)

    # Compute gradient update from the residual
    v = TimeData(name='v', shape=model.shape,
                 time_order=2, space_order=order)
    residual = rec_true.data[:] - rec_smooth.data[:]
    op_gradient(u=u, v=v, grad=grad, rec=residual, m=m_smooth)
```

Rapid propagator development and integration

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



Devito - Automated finite difference propagators

From math to tuned HPC code in a few lines:

$$\frac{m}{\rho}\frac{d^2p(x,t)}{dt^2} - (1+2\epsilon)(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - \sqrt{(1+2\delta)}G_{\bar{z}\bar{z}}r(x,t) = q,$$
$$\frac{m}{\rho}\frac{d^2r(x,t)}{dt^2} - \sqrt{(1+2\delta)}(G_{\bar{x}\bar{x}} + G_{\bar{y}\bar{y}})p(x,t) - G_{\bar{z}\bar{z}}r(x,t) = q,$$
$$p(.,0) = 0,$$
$$\frac{dp(x,t)}{dt}|_{t=0} = 0,$$
$$r(.,0) = 0,$$
$$\frac{dr(x,t)}{dt}|_{t=0} = 0,$$

(incomplete) specification of a TTI (Tilted Transverse Isotropy) forward operator

$$D_{x1} = cos(\theta)cos(\phi)\frac{d}{dx}\bigg|_l + cos(\theta)sin(\phi)\frac{d}{dy} - sin(\theta)\frac{d}{dz}$$
$$D_{x2} = cos(\theta)cos(\phi)\frac{d}{dx} + cos(\theta)sin(\phi)\frac{d}{dy}\bigg|_l - sin(\theta)\frac{d}{dz}|_l$$
$$G_{\bar{x}\bar{x}} = \frac{1}{2}\left(D^T_{x1}(\frac{1}{\rho})D_{x1} + D^T_{x2}(\frac{1}{\rho})D_{x2}\right)$$

rotated second order differential operators [1]

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[1] Y. Zhang and F. Mueller. Auto-generation and auto-tuning of 3d stencil codes on gpu clusters. In *Proceedings of the Tenth International Symposium on Code Generation and Optimization*, CGO '12, pages 155–164, New York, NY, USA, 2012. ACM

Devito - Automated finite difference propagators

From math to tuned HPC code in a few lines:

```
ang0, ang1 = cos(theta), sin(theta)
ang2, ang3 = cos(phi), sin(phi)
Gyp = (ang3 * u.dx - ang2 * u.dyr)
Gyy = (first_derivative(Gyp * ang3, dim=x, side=centered, order=space_order, matvec=transpose) -
       first_derivative(Gyp * ang2, dim=y, side=right, order=space_order, matvec=transpose))
Gyp2 = (ang3 * u.dxr - ang2 * u.dy)
Gyy2 = (first_derivative(Gyp2 * ang3, dim=x, side=right, order=space_order, matvec=transpose) -
        first_derivative(Gyp2 * ang2, dim=y, side=centered, order=space_order, matvec=transpose))
Gxp = (ang0 * ang2 * u.dx + ang0 * ang3 * u.dyr - ang1 * u.dzr)
Gzr = (ang1 * ang2 * v.dx + ang1 * ang3 * v.dyr + ang0 * v.dzr)
Gxx = (first_derivative(Gxp * ang0 * ang2, dim=x, side=centered, order=space_order, matvec=transpose) +
       first_derivative(Gxp * ang0 * ang3, dim=y, side=right, order=space_order, matvec=transpose) -
       first_derivative(Gxp * ang1, dim=z, side=right, order=space_order, matvec=transpose))
Gzz = (first_derivative(Gzr * ang1 * ang2, dim=x, side=centered, order=space_order, matvec=transpose) +
       first_derivative(Gzr * ang1 * ang3, dim=y, side=right, order=space_order, matvec=transpose) +
       first_derivative(Gzr * ang0, dim=z, side=right, order=space_order, matvec=transpose))
Gxp2 = (ang0 * ang2 * u.dxr + ang0 * ang3 * u.dy - ang1 * u.dz)
Gzr2 = (ang1*ang2*v.dxr+ang1*ang3*v.dy+ang0*v.dz) dim=x, side=right, order=space_order, matvec=transpose) +
        first_derivative(Gxp2 * ang0 * ang3, dim=y, side=centered, order=space_order, matvec=transpose) -
        first_derivative(Gxp2 * ang1,dim=z, side=centered, order=space_order, matvec=transpose))
Gzz2 = (first_derivative(Gzr2 * ang1 * ang2, dim=x, side=right, order=space_order, matvec=transpose) +
        first_derivative(Gzr2 * ang1 * ang3, dim=y, side=centered, order=space_order, matvec=transpose) +
        first_derivative(Gzr2 * ang0, dim=z, side=centered, order=space_order, matvec=transpose))

Hp = -(.5*Gxx + .5*Gxx2 + .5 * Gyy + .5*Gyy2)
Hzr = -(.5*Gzz + .5 * Gzz2)
stencilp = 1.0 / (2.0 * m + s * damp) * (4.0 * m * u + (s * damp - 2.0 * m) * u.backward
         + 2.0 * s**2 * (epsilon * Hp + delta * Hzr))
stencilr = 1.0 / (2.0 * m + s * damp) * (4.0 * m * v + (s * damp - 2.0 * m) * v.backward
         + 2.0 * s**2 * (delta * Hp + Hzr))
```

Devito - Automated finite difference propagators

From math to tuned HPC code in a few lines:

```python
def forward(model, m, eta, epsilon, delta, theta, phi, src, rec, order=2):

    # Create two wavefelds
    u = TimeData(name='u', shape=model.shape, time_order=2, space_order=order)
    v = TimeData(name='v', shape=model.shape, time_order=2, space_order=order)

    # Create update expressions from stencil
    stencilp, stencilr = ...
    update_u = Eq(u.forward, stencilp)
    update_v = Eq(v.forward, stencilr)

    # Inject wave as source term
    src_term = src.inject(field=u, expr=src * dt**2 / m)
    src_term += src.inject(field=v, 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, update_v] + src_term + rec_term,
                    subs={s: dt, h: model.spacing})
```

Devito - Automated finite difference propagators

Summary:

- **Productivity through code generation**
  - Acoustic operators in < 20 lines
  - TTI operators in < 100 lines
  - Variable discretization and stencil order
  - Fully executable Python code, easy to experiment
  - Complete problem setups in < 1000 lines

- Fast wave propagators for inversion problems
  - Highly efficient development through automation
  - Interoperability: Generated code is low-level C
  - **Automated performance optimisation**

OPESCI

intel

SINBAD

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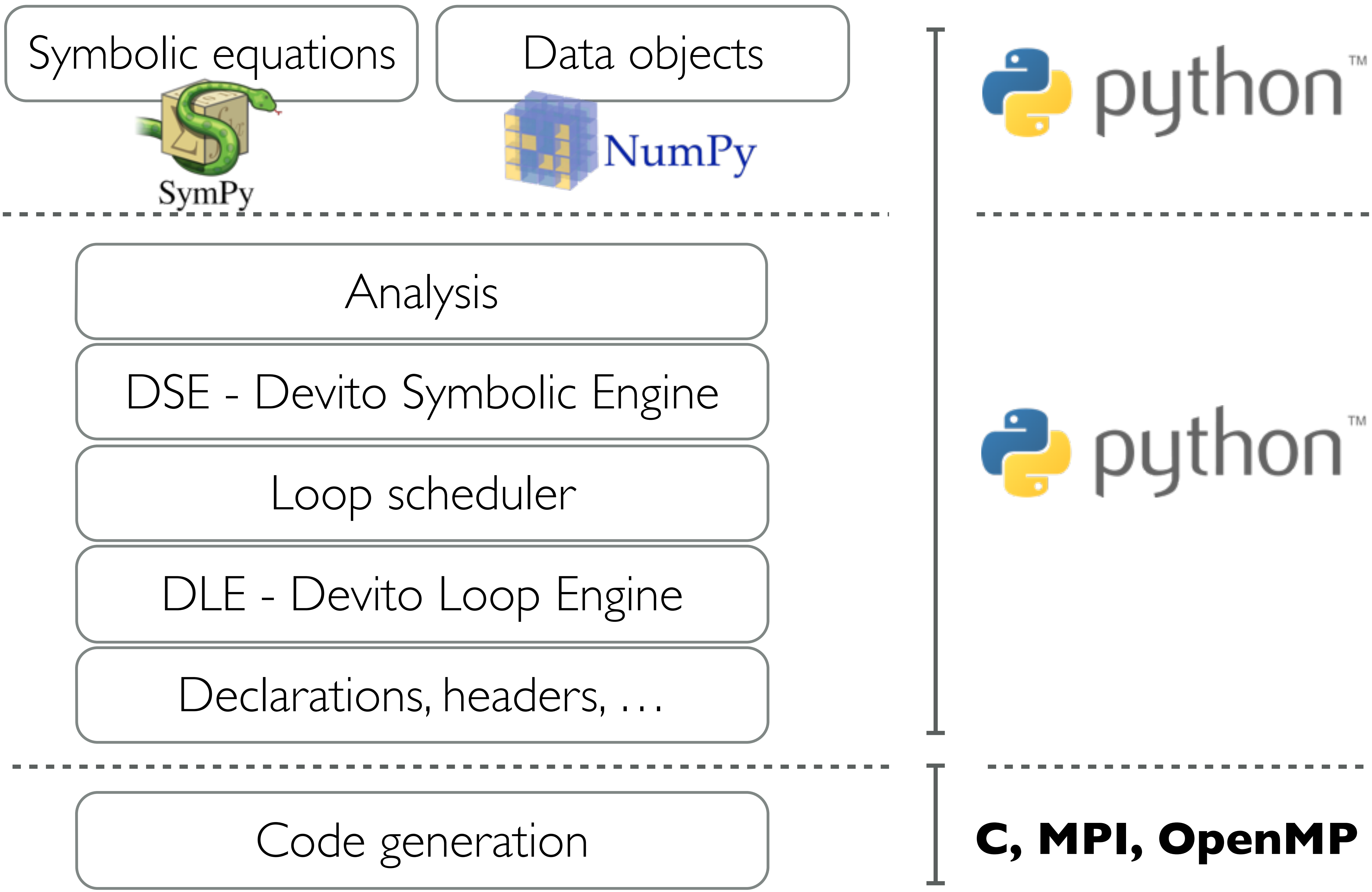
Engineering and Physical Sciences
Research Council

The compilation flow: from symbolics to HPC code



The compilation flow: from symbolics to HPC code

Symbolic equations | Data objects

SymPy | NumPy

python

Analysis

DSE - Devito Symbolic Engine

Loop scheduler

DLE - Devito Loop Engine

Declarations, headers, . . .

"FLOPS" OPTIMIZATIONS

python

Code generation

C, MPI, OpenMP

The compilation flow: from symbolics to HPC code

Symbolic equations

Data objects

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python™

Analysis

DSE - Devito Symbolic Engine

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Declarations, headers, …

Code generation

“FLOPS” OPTIMIZATIONS

“MEMORY” OPTIMIZATIONS

C, MPI, OpenMP

Devito Symbolic Engine

A sequence of compiler passes to reduce FLOPS (no loops at this stage!)

Devito Symbolic Engine

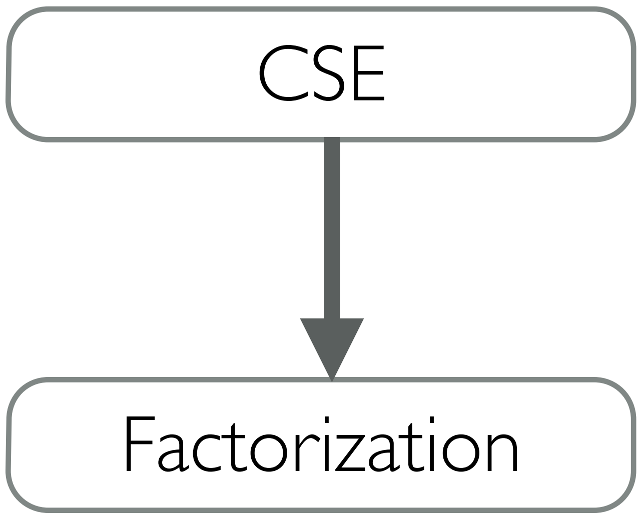
A sequence of compiler passes to reduce FLOPS (no loops at this stage!)

CSE

- Common sub-expressions elimination
  - C compilers do it already… but necessary for symbolic processing and compilation speed

Devito Symbolic Engine

A sequence of compiler passes to reduce FLOPS (no loops at this stage!)

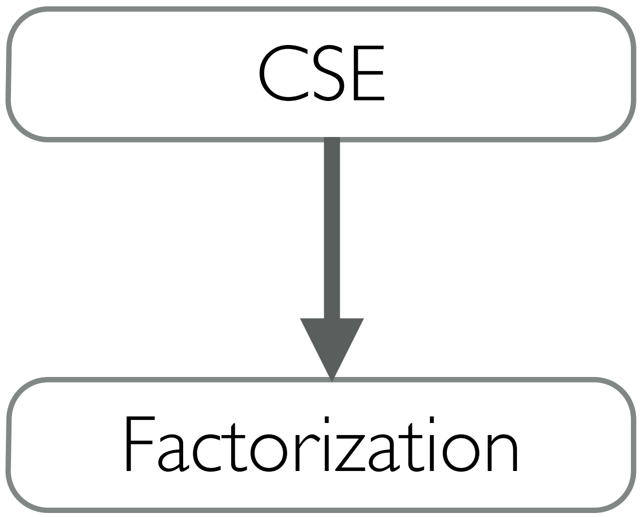


- Common sub-expressions elimination
  - C compilers do it already… but necessary for symbolic processing and compilation speed

- Heuristic factorization of recurrent terms
  - E.g., finite difference weights: `0.3*a + … + 0.3*b => 0.3*(a+b)`
  - Many possibilities (doesn’t leverage domain properties yet!)

Devito Symbolic Engine

A sequence of compiler passes to reduce FLOPS (no loops at this stage!)



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Factorization impact:

TTI, space order 4: 1100 → 950

TTI, space order 8: 2380 → 2120

TTI, space order 12: 4240 → 3760

TTI, space order 16: 6680 → 5760

Devito Symbolic Engine

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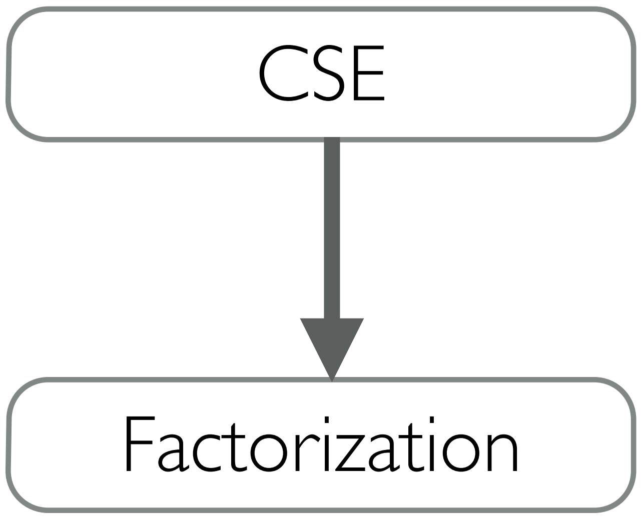

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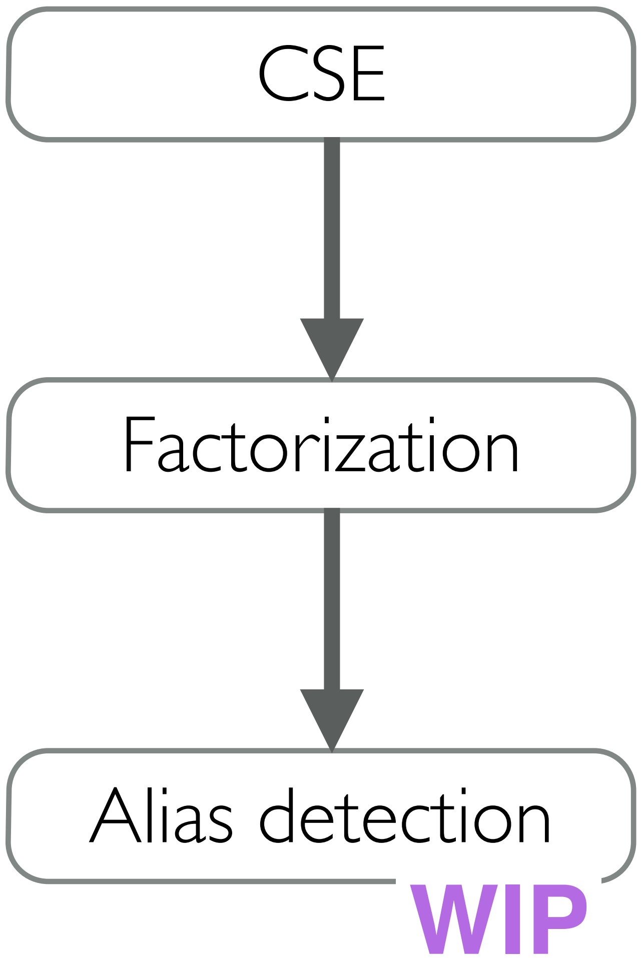

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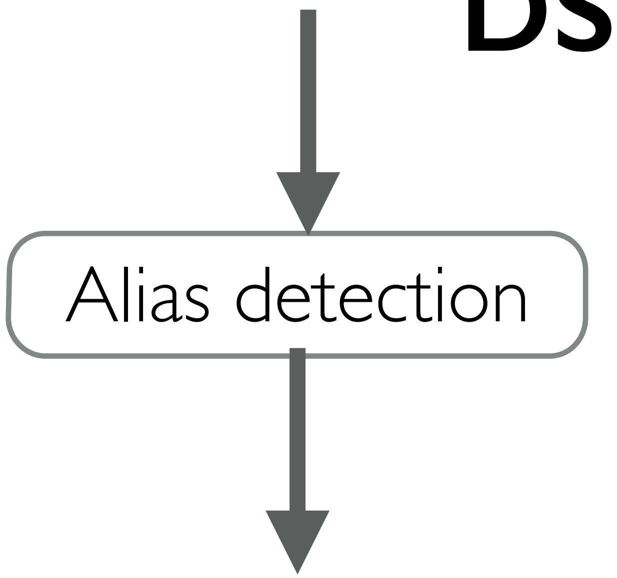
- Fundamental in compute-bound stencil codes (e.g., TTI)
  - E.g., `sin(phi[i,j,k]), sin(phi[i-1,j-1,k-1])`

DSE's aliases detection algorithms



Fundamental in compute-bound stencil codes (e.g., TTI)

```
tmp1 = …*sin(phi[i,j,k]) + … + 0.4*sin(phi[i-1,j-1,k-1]) + … +
        …0.1*sin(phi[i+2,j+2,k+2]) + …
```

Observations (focus on <u>underlined</u> sub-expressions)

- Same operators `(sin)`
- Same operands `(phi)`
- Same indices `(i, j, k)`
- Linearly dependent index vectors `([i, j, k], [i-1, j-1, k-1], [i+2, j+2, k+2])`

DSE's aliases detection algorithms

Alias detection

Fundamental in compute-bound stencil codes (e.g., TTI)

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Observations (focus on underlined sub-expressions)

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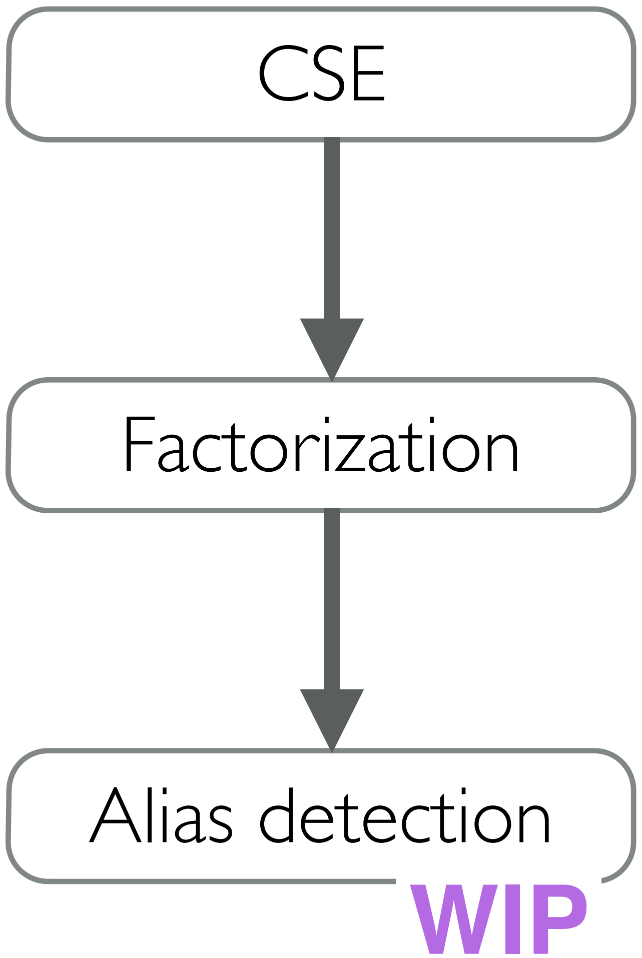
```
B[i,j,k] = sin(phi[i,j,k])
tmp1 = …*B[i,j,k] + … + 0.4*B[i-1,j-1,k-1] + … + … + 0.1*B[i+2,j+2,k+2] + …
```

Devito Symbolic Engine

A sequence of compiler passes to reduce FLOPS (no loops at this stage!)



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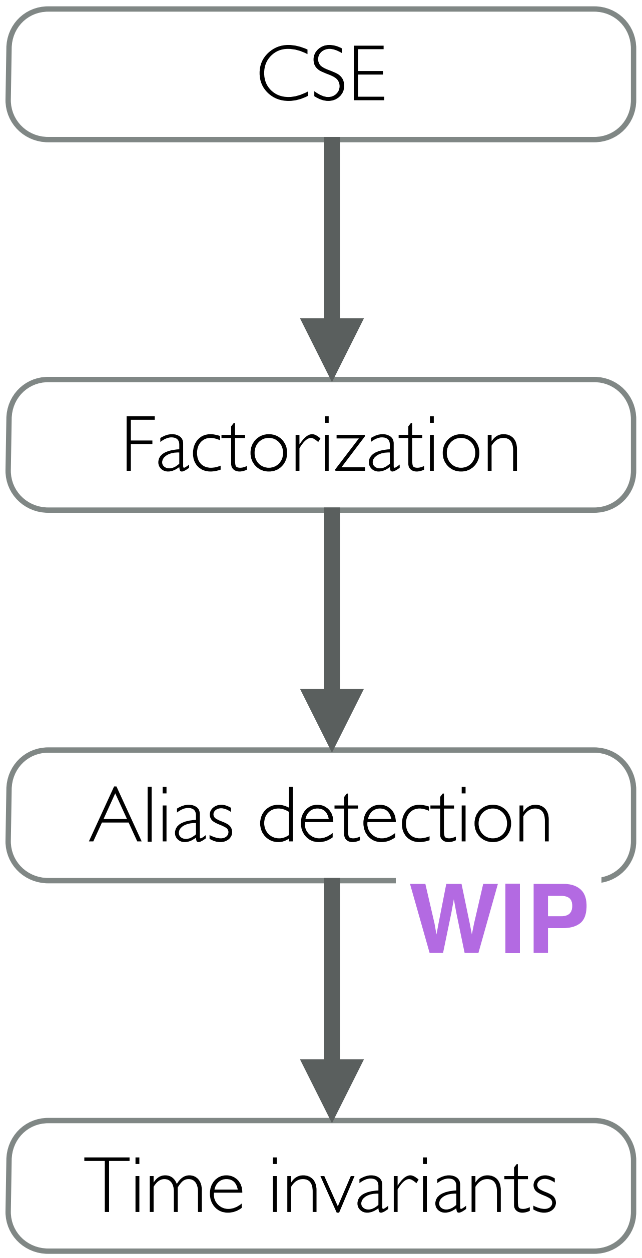

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  - E.g., `sin(phi[i,j,k])`, `sin(phi[i-1,j-1,k-1])`

- Heuristic hoisting of time-invariant quantities
  - Currently, only (expensive) trigonometric functions applied to space-varying quantities

Devito Loop Engine

A sequence of compiler passes to introduce parallelism, SIMD vectorization and to improve data locality

Devito Loop Engine

A sequence of compiler passes to introduce parallelism, SIMD vectorization and to improve data locality

Cache opts

- Cache optimizations (mostly L1 cache)
  - Loop fission + elemental functions (register locality)
  - Padding + data alignment (split loads)

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Intel VTune, Broadwell E5-2620 v4, TTI space orders 4-8-12

eneral Exploration General Exploration viewpoint

Collection Log | Analysis Target | Analysis Type | Summary

Elapsed Time: 487.651s

Clockticks:	5,099,766,000,000
Instructions Retired:	4,963,350,000,000
CPI Rate:	1.027
MUX Reliability:	0.754
Front-End Bound:	1.7%
Bad Speculation:	0.3%
Back-End Bound:	77.5%
Memory Bound:	54.7%
L1 Bound:	31.0%
DTLB Overhead:	3.0%
Loads Blocked by Store Forwarding:	0.0%
Lock Latency:	0.0%
Split Loads:	13.5%
4K Aliasing:	22.8%
FB Full:	22.1%
L2 Bound:	0.0%
L3 Bound:	3.3%
DRAM Bound:	24.7%
Memory Bandwidth:	24.1%
Memory Latency:	34.7%
Local DRAM:	95.0%
Remote DRAM:	0.0%
Remote Cache:	0.0%
Store Bound:	1.8%
Core Bound:	22.7%
Retiring:	20.5%
Total Thread Count:	205

Front-End Bound:	2.0%
Bad Speculation:	0.2%
Back-End Bound:	79.0%
Memory Bound:	55.2%
L1 Bound:	31.4%
DTLB Overhead:	3.9%
Loads Blocked by Store Forwarding:	0.0%
Lock Latency:	0.0%
Split Loads:	68.3%
4K Aliasing:	31.4%
FB Full:	89.2%
L2 Bound:	0.0%
L3 Bound:	4.0%
DRAM Bound:	24.5%
Memory Bandwidth:	15.3%
Memory Latency:	37.5%
Local DRAM:	19.3%
Remote DRAM:	0.0%
Remote Cache:	0.0%
Store Bound:	3.5%

Front-End Bound:	2.2%
Bad Speculation:	0.3%
Back-End Bound:	76.0%
Memory Bound:	53.1%
L1 Bound:	28.5%
DTLB Overhead:	5.0%
Loads Blocked by Store Forwarding:	0.0%
Lock Latency:	0.0%
Split Loads:	38.7%
4K Aliasing:	36.6%
FB Full:	100.0%
L2 Bound:	0.0%
L3 Bound:	11.2%
Contested Accesses:	0.0%
Data Sharing:	0.0%
L3 Latency:	5.2%
SQ Full:	0.3%
DRAM Bound:	12.1%
Memory Bandwidth:	12.1%
Memory Latency:	40.1%

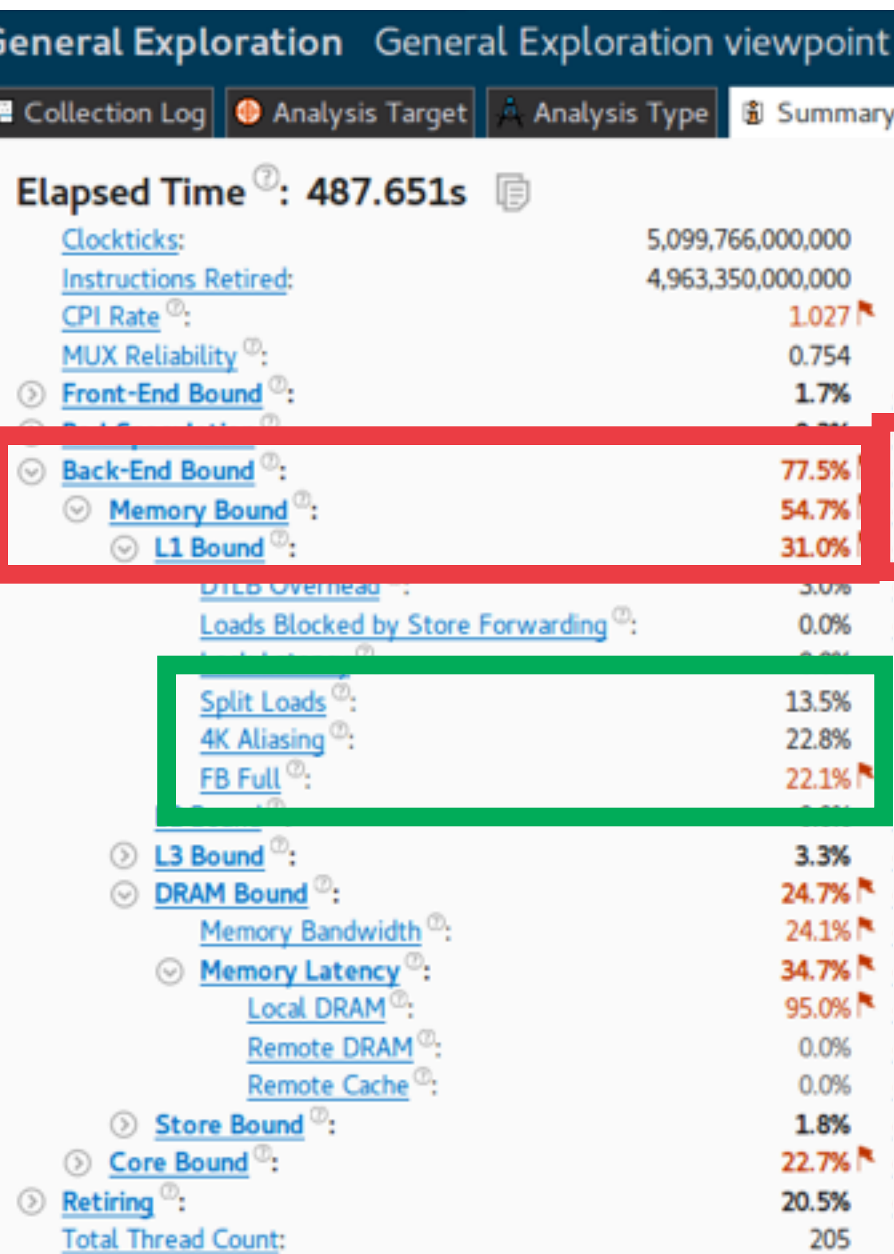
Devito Loop Engine

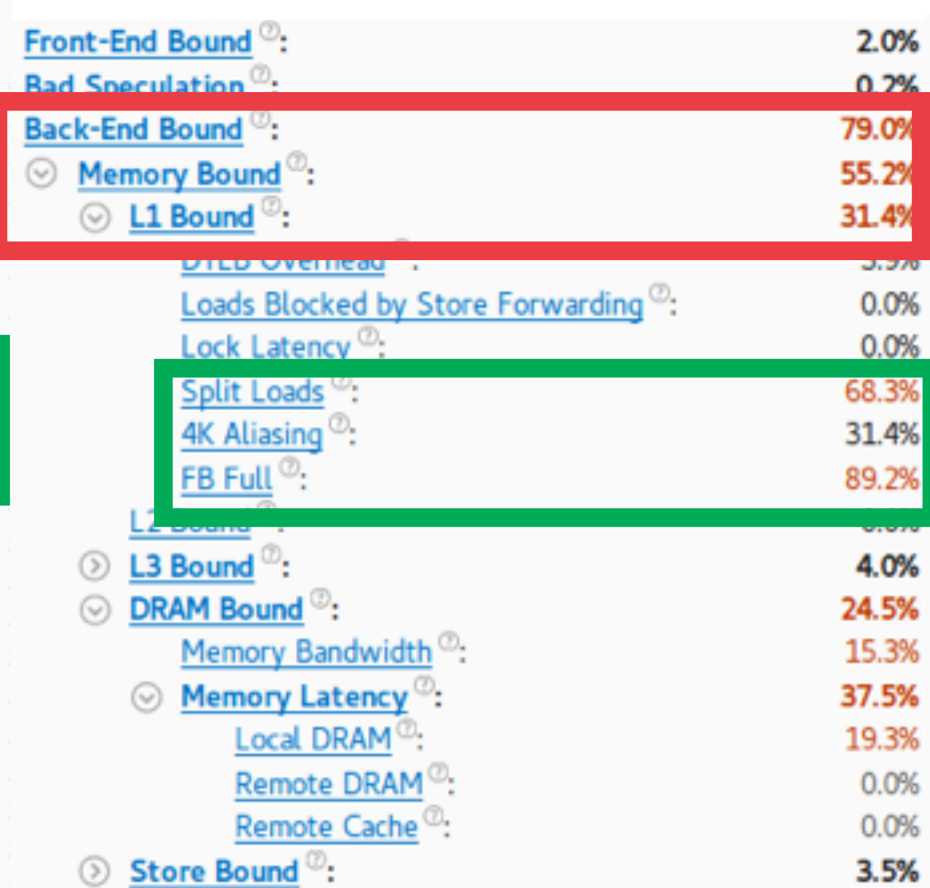
A sequence of compiler passes to introduce parallelism, SIMD vectorization and to improve data locality

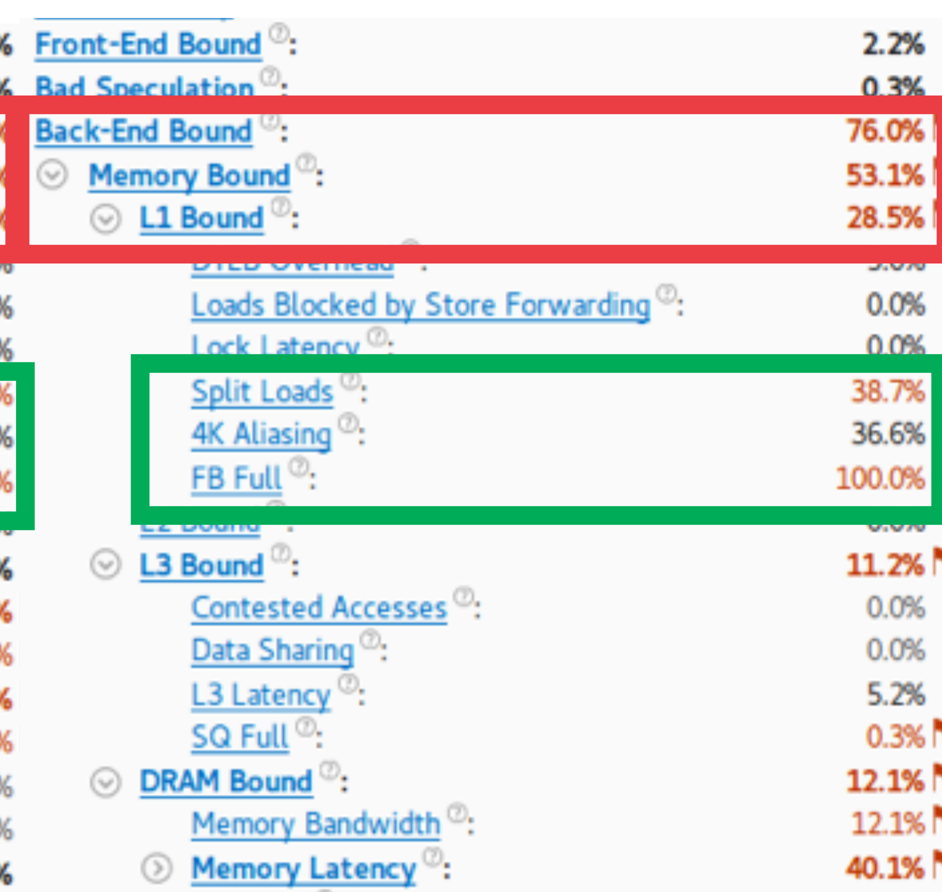
Cache opts

- Cache optimizations (mostly L1 cache)
  - Loop fission + elemental functions (register locality)
  - Padding + data alignment (split loads)

Intel VTune, Broadwell E5-2620 v4, TTI space orders 4-8-12







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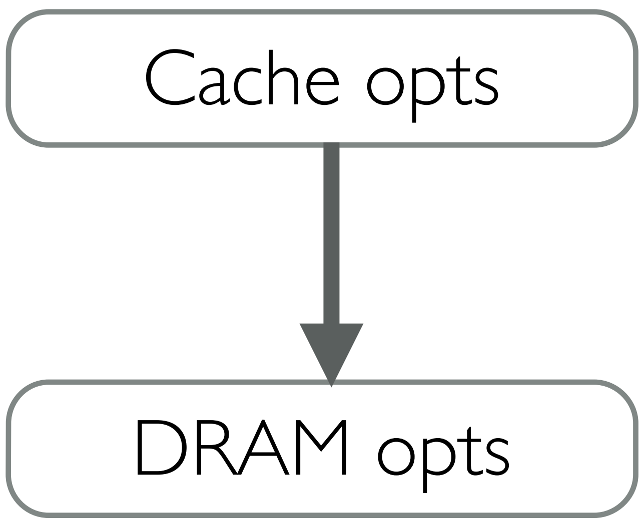

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Devito Loop Engine

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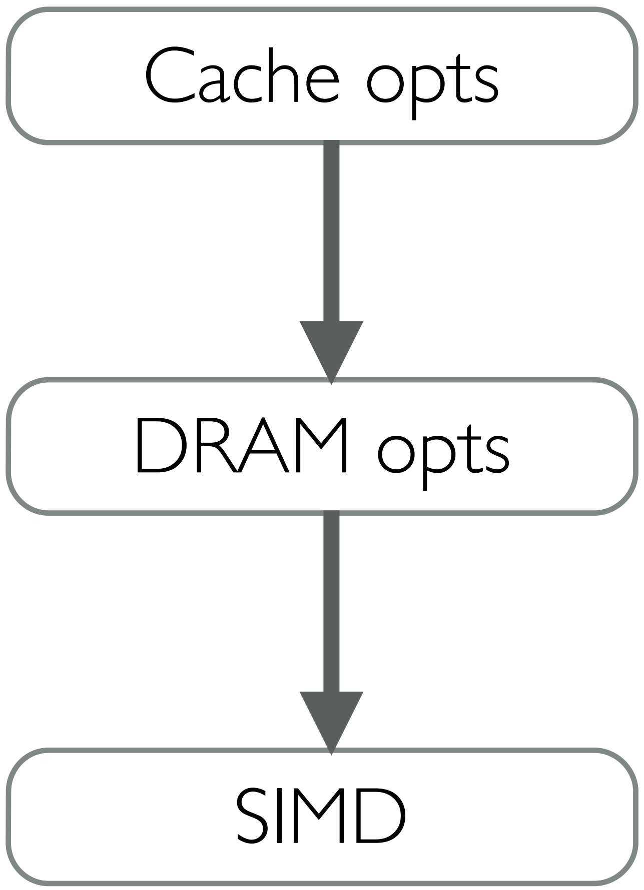

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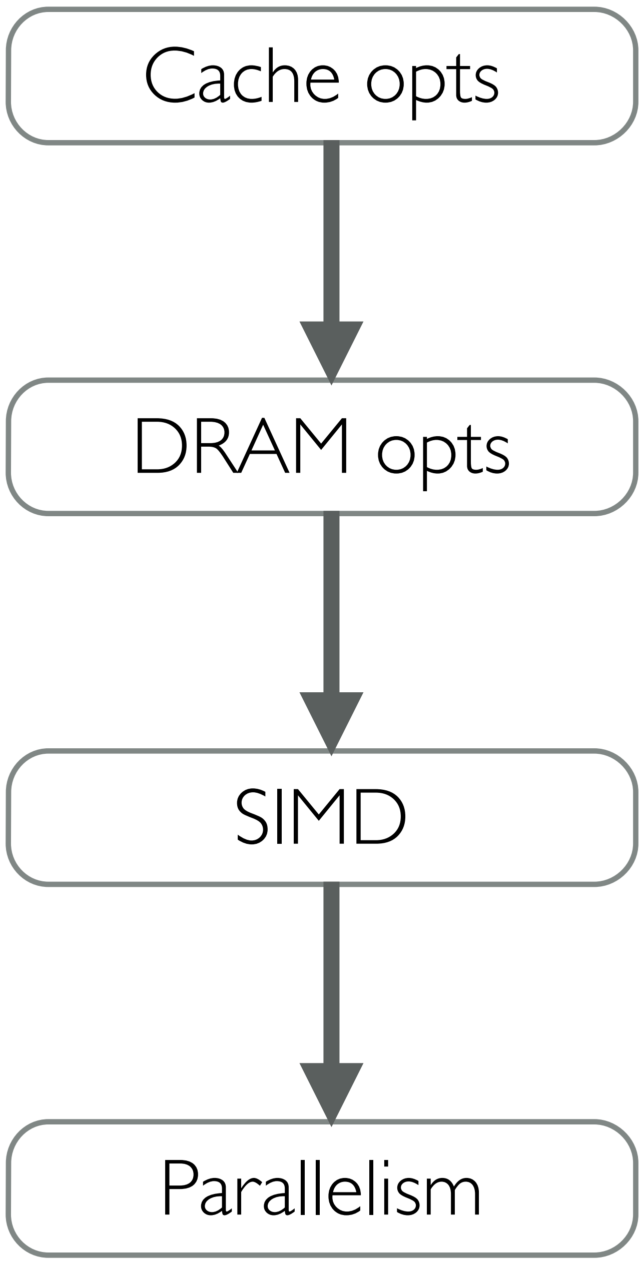
A sequence of compiler passes to introduce parallelism, SIMD vectorization and to improve data locality



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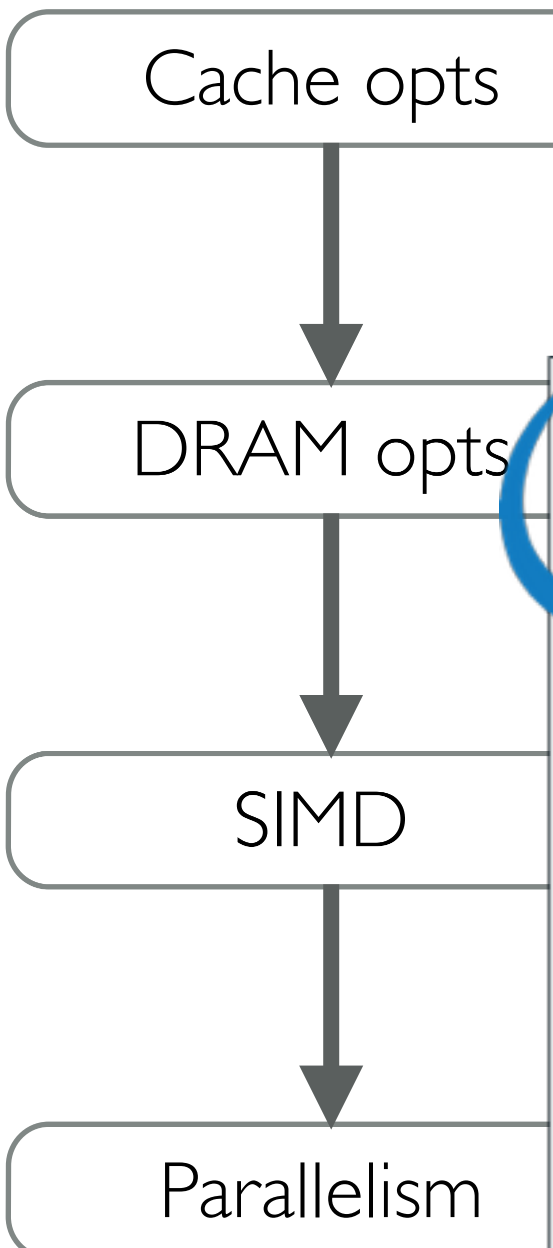
- OpenMP
  - *#pragma collapse* clause on the Xeon Phi

Devito Loop Engine

A sequence of compiler passes to introduce parallelism, SIMD vectorization and to improve data locality



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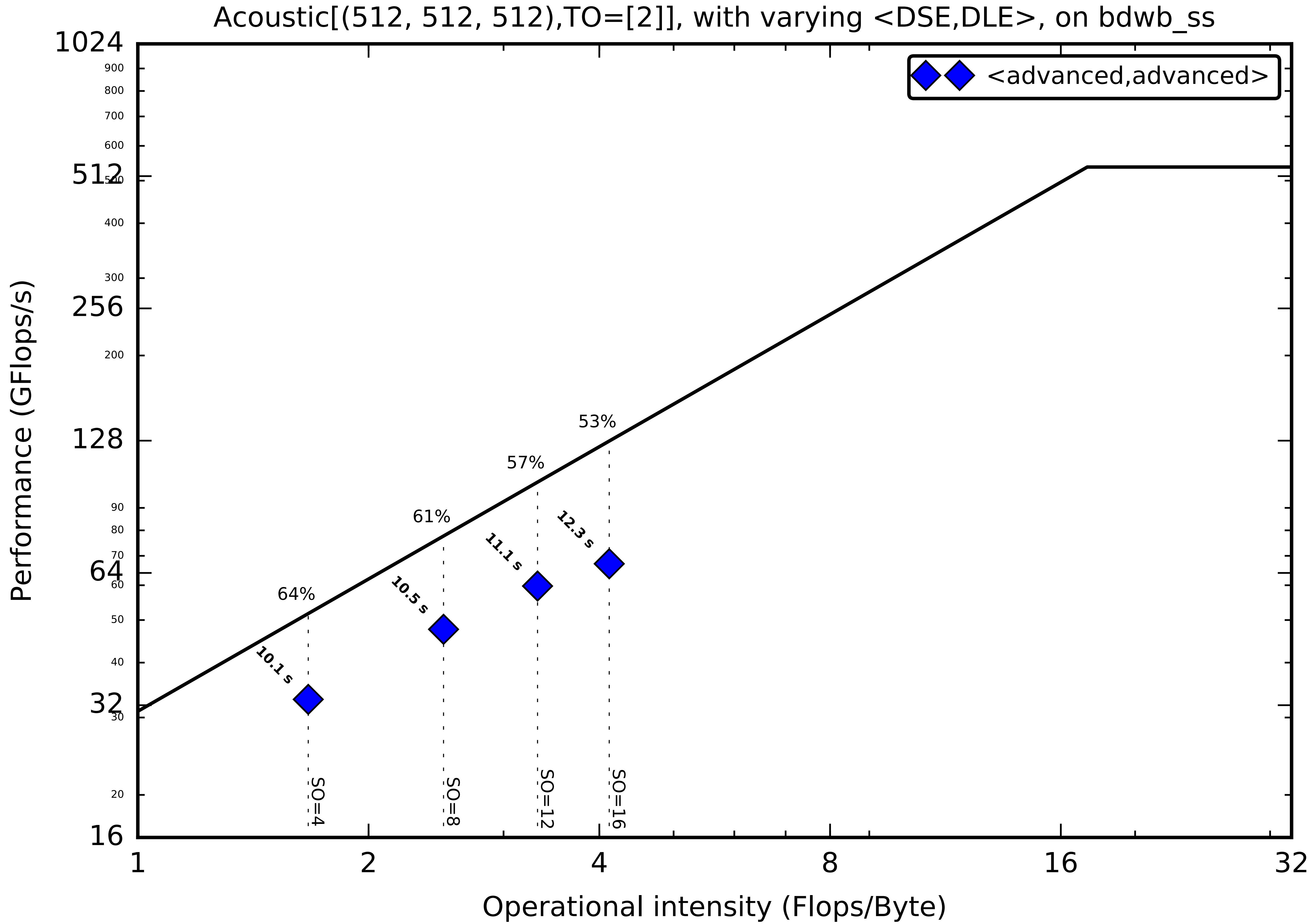
  - Padding + data alignment (split loads)

WIP

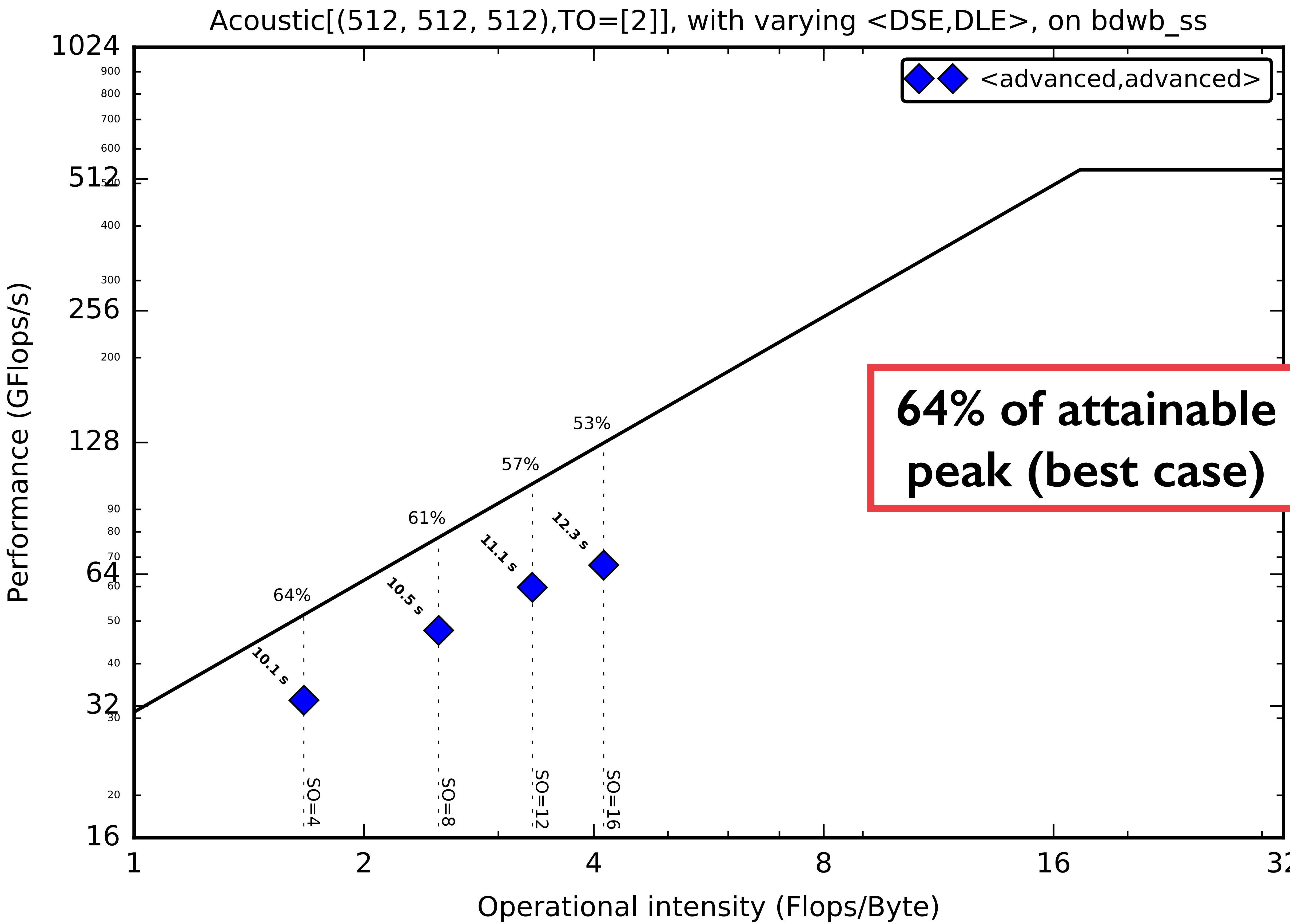
Y*A*S*K

Yet Another Stencil Kernel

Acoustic on Broadwell

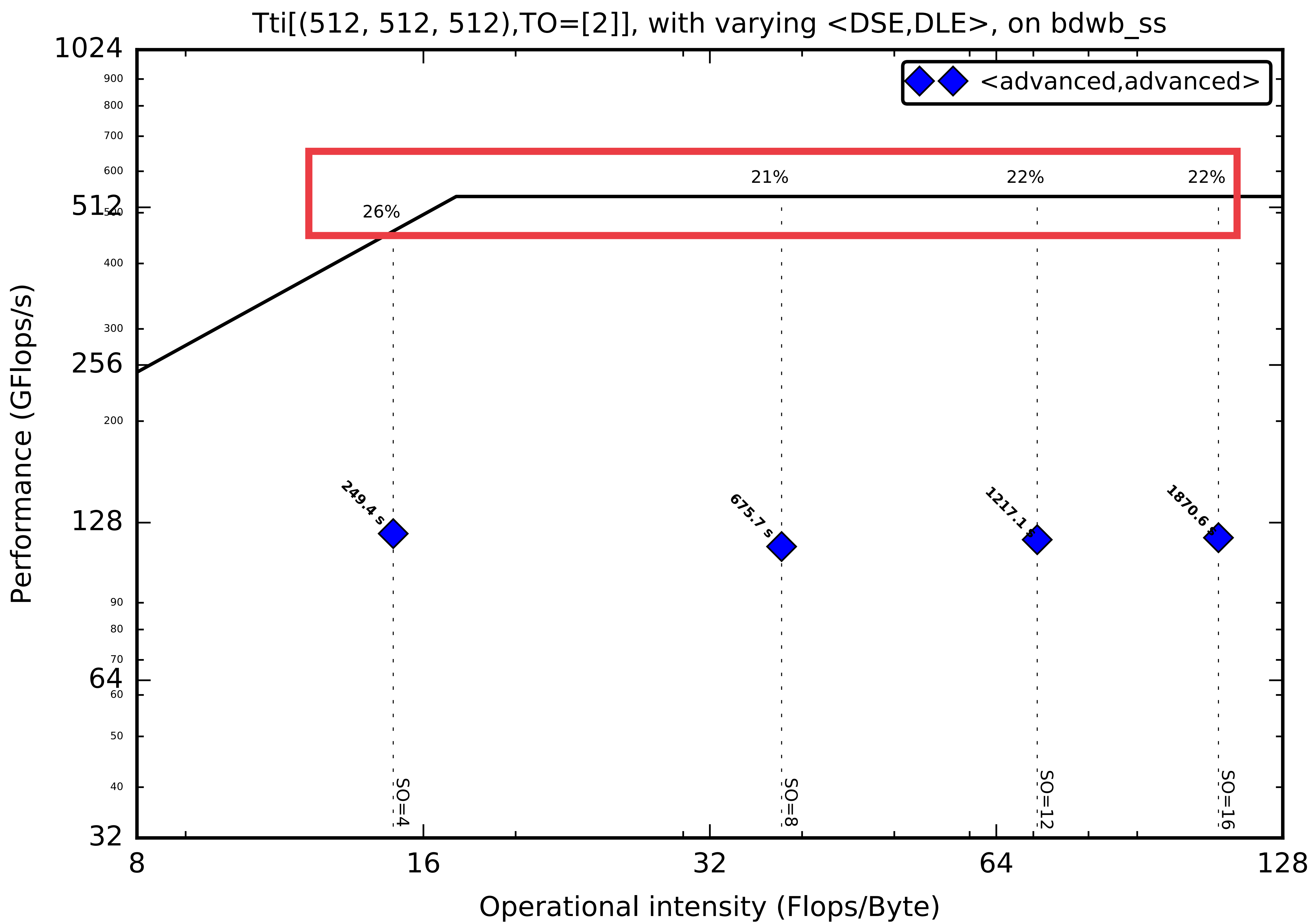


Acoustic on Broadwell

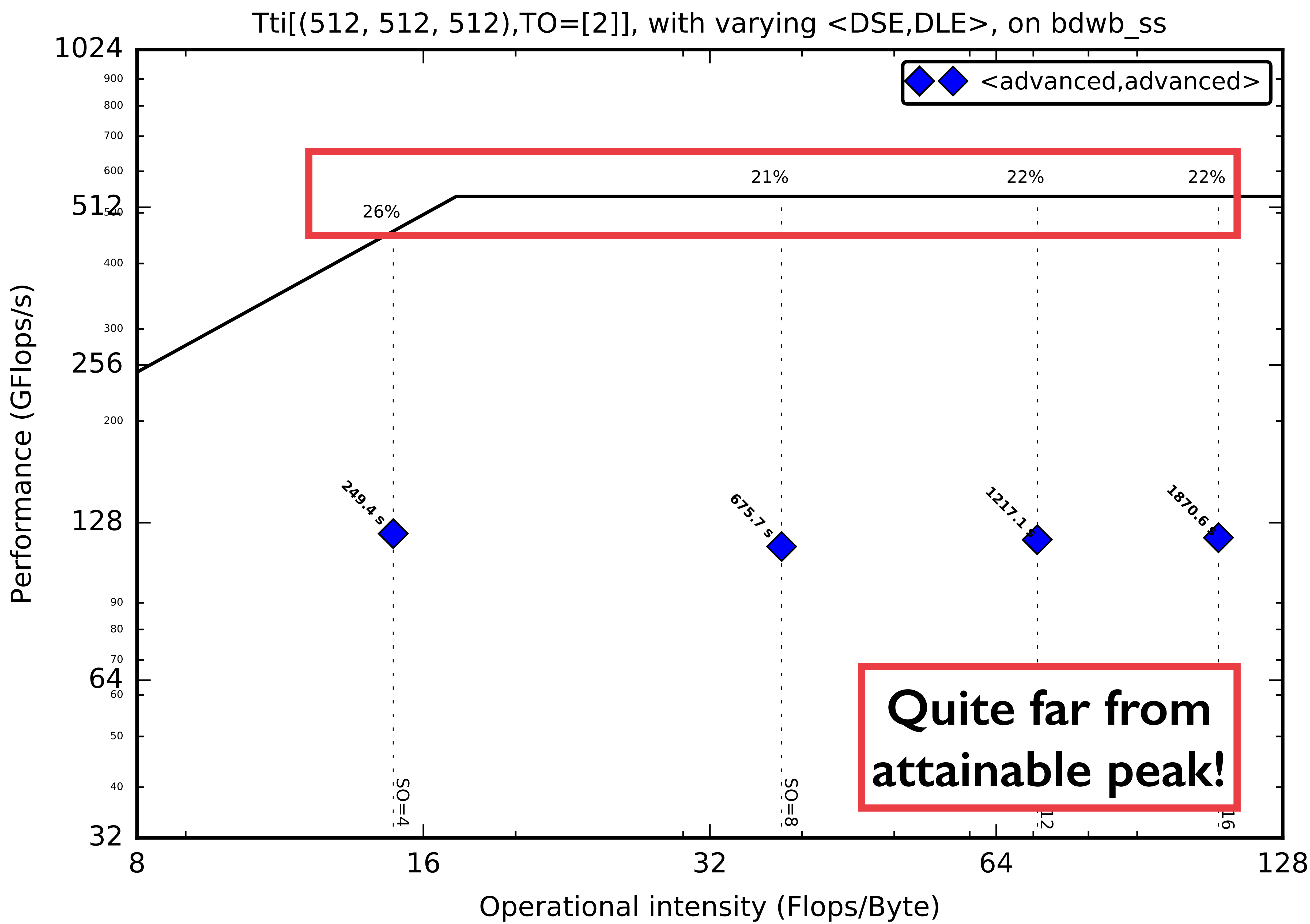


64% of attainable peak (best case)

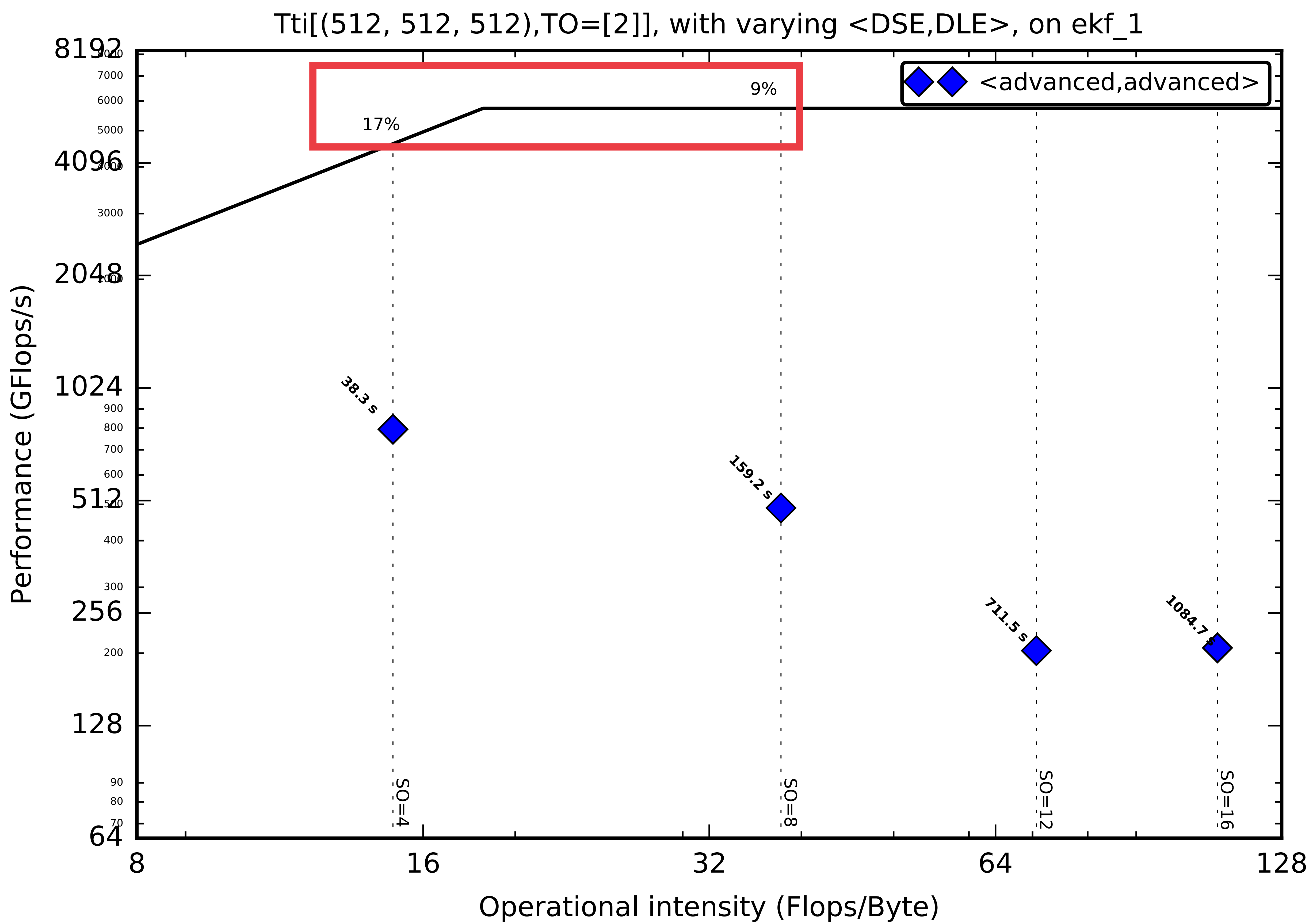
TTI on Broadwell (8 threads, single socket)



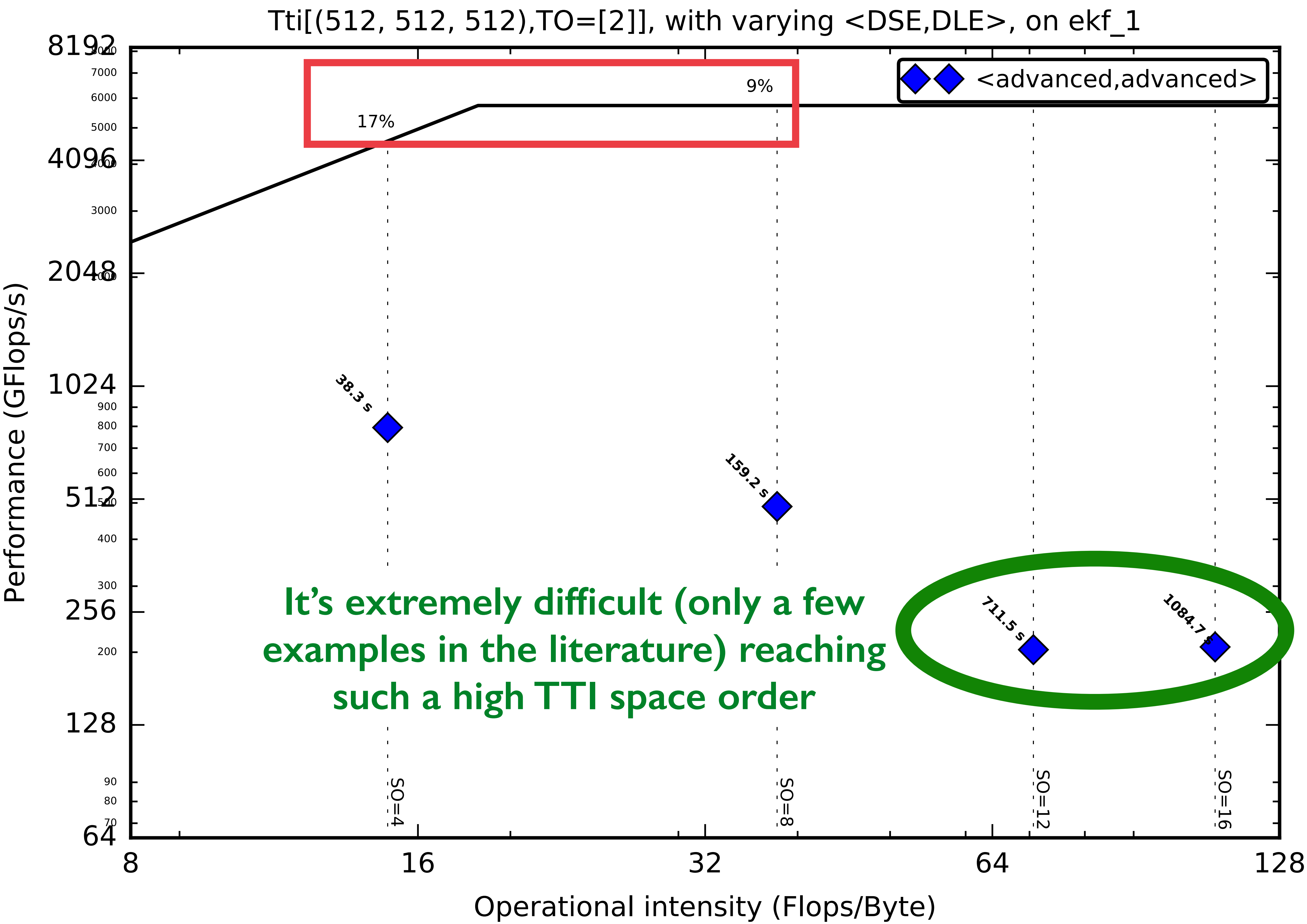
TTI on Broadwell (8 threads, single socket)



TTI on Xeon Phi (64 threads, cache mode, quadrant)



TTI on Xeon Phi (64 threads, cache mode, quadrant)



It's extremely difficult (only a few examples in the literature) reaching such a high TTI space order

Conclusions and resources

- Devito: an efficient and sustainable finite difference DSL
- Driven/inspired by **real-world seismic imaging**
- **Interdisciplinary research effort**
- Based on **actual compiler technology**

Useful links

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