AUTOMATED LOOP GENERATION FOR HIGH-PERFORMANCE FINITE DIFFERENCES (AND BEYOND)

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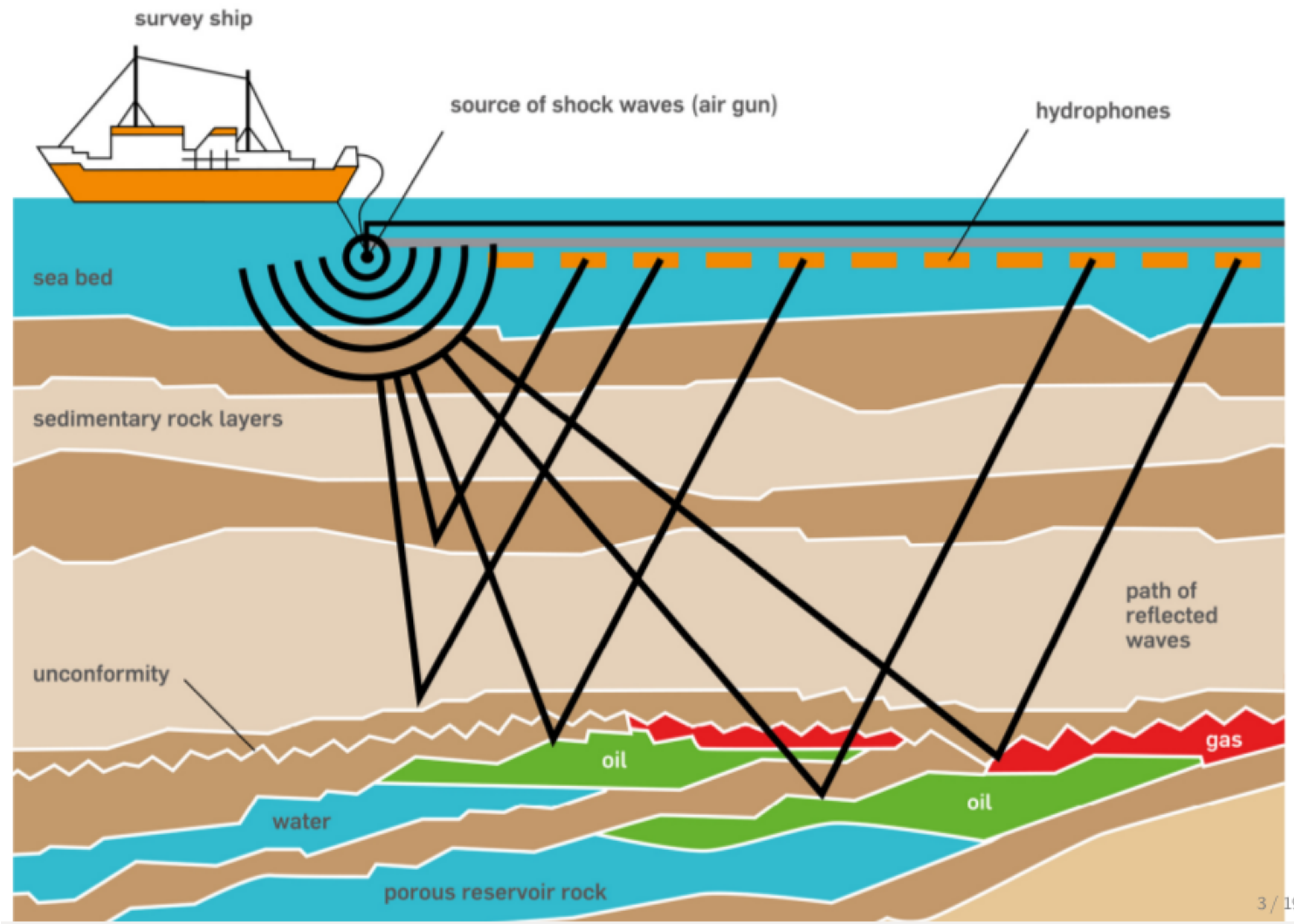
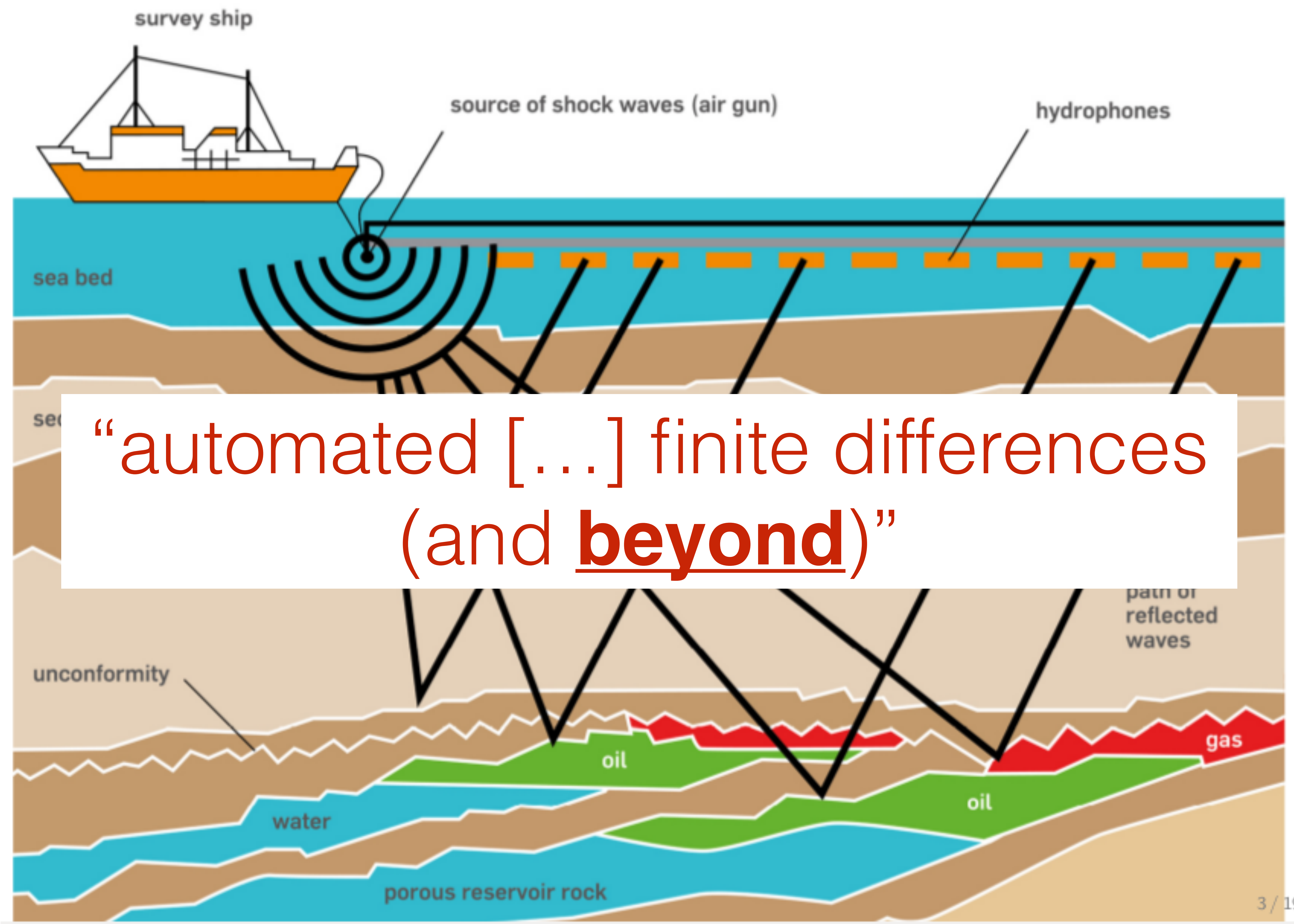
Dagstuhl Seminar, March 2018

Driving application: inversion algorithms for seismic imaging



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

Driving application: inversion algorithms for seismic imaging



“automated [...] finite differences (and **<u>beyond</u>**)”

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Issue 1: Computational cost

Realistic full-waveform inversion (FWI) scenario:

- **O(10^3) FLOPs per loop iteration** or **high memory pressure**
- Realistic 3D grids with **>10^9 grid points**
- Often more than **3000 time steps**
- **Two** operators: forward + adjoint, to be executed **~15 times**
- Usually **30000 shots**
- ≈ **O(billions) TFLOPs**
- **>>> Days, weeks, months on supercomputers**

Issue 2: Variations in physics and mathematics

- Overarching strategy for inversion
- Formulations of wave equations
- Space and time discretizations
- Boundary conditions, data acquisition, sources/receivers …

Issue 3: Time flies…

- Proliferation of computer architectures
- Unmaintainable, impenetrable, non-portable legacy code
- Skepticism: C/C++/Fortran **IS** the way

Raising the level of abstraction

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

```
void kernel(…) {
  …
  <impenetrable code with crazy
   performance optimizations>
  …
}
```

Raising the level of abstraction

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eqn = m * u.dt2 + eta * u.dt - u.laplace
solve(eqn, u.forward)
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Raising the level of abstraction

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

Devito

```
eqn = m * u.dt2 + eta * u.dt - u.laplace
solve(eqn, u.forward)
```

```
void kernel(…) { … }
```

1) Flexibility in space/time discretization

```
u = TimeFunction(…, space_order=so)
eqn = m * u.dt2 + eta * u.dt - u.laplace
solve(eqn, u.forward)
```

so=4

```
  for (int time = time_m, t0 = (time)%(3), t1 = (time + 1)%(3), t2 = (time +
2)%(3); time <= time_M; time += 1, t0 = (time)%(3), t1 = (time + 1)%(3), t2 =
(time + 2)%(3)) {
    for (int x = x_m; x <= x_M; x += 1) {
      for (int y = y_m; y <= y_M; y += 1) {
        for (int z = z_m; z <= z_M; z += 1) {
          u[t1][x + 4][y + 4][z + 4] = 2*pow(dt,
3)*(-2.08333333333333e-4F*u[t0][x + 2][y + 4][z + 4] +
3.33333333333333e-3F*u[t0][x + 3][y + 4][z + 4] - 2.08333333333333e-4F*u[t0]
[x + 4][y + 2][z + 4] + 3.33333333333333e-3F*u[t0][x + 4][y + 3][z + 4] -
2.08333333333333e-4F*u[t0][x + 4][y + 4][z + 2] + 3.33333333333333e-3F*u[t0]
[x + 4][y + 4][z + 3] - 1.875e-2F*u[t0][x + 4][y + 4][z + 4] +
3.33333333333333e-3F*u[t0][x + 4][y + 4][z + 5] - 2.08333333333333e-4F*u[t0]
[x + 4][y + 4][z + 6] + 3.33333333333333e-3F*u[t0][x + 4][y + 5][z + 4] -
2.08333333333333e-4F*u[t0][x + 4][y + 6][z + 4] + 3.33333333333333e-3F*u[t0]
[x + 5][y + 4][z + 4] - 2.08333333333333e-4F*u[t0][x + 6][y + 4][z + 4])/
(pow(dt, 2)*damp[x + 1][y + 1][z + 1] + 2*dt*m[x + 4][y + 4][z + 4]) +
pow(dt, 2)*damp[x + 1][y + 1][z + 1]*u[t2][x + 4][y + 4][z + 4]/(pow(dt,
2)*damp[x + 1][y + 1][z + 1] + 2*dt*m[x + 4][y + 4][z + 4]) + 4*dt*m[x + 4][y
+ 4][z + 4]*u[t0][x + 4][y + 4][z + 4]/(pow(dt, 2)*damp[x + 1][y + 1][z + 1]
+ 2*dt*m[x + 4][y + 4][z + 4]) - 2*dt*m[x + 4][y + 4][z + 4]*u[t2][x + 4][y +
4][z + 4]/(pow(dt, 2)*damp[x + 1][y + 1][z + 1] + 2*dt*m[x + 4][y + 4][z +
4]);
        }
      }
    }
  }
```

so=12

```
  for (int time = time_m, t0 = (time)%(3), t1 = (time + 1)%(3), t2 = (time +
2)%(3); time <= time_M; time += 1, t0 = (time)%(3), t1 = (time + 1)%(3), t2 =
(time + 2)%(3)) {
    for (int x = x_m; x <= x_M; x += 1) {
      for (int y = y_m; y <= y_M; y += 1) {
        for (int z = z_m; z <= z_M; z += 1) {
          u[t1][x + 12][y + 12][z + 12] = 2*pow(dt,
3)*(-1.5031265031265e-7F*u[t0][x + 6][y + 12][z + 12] +
2.5974025974026e-6F*u[t0][x + 7][y + 12][z + 12] - 2.23214285714286e-5F*u[t0][x
+ 8][y + 12][z + 12] + 1.32275132275132e-4F*u[t0][x + 9][y + 12][z + 12] -
6.69642857142857e-4F*u[t0][x + 10][y + 12][z + 12] + 4.28571428571429e-3F*u[t0]
[x + 11][y + 12][z + 12] - 1.5031265031265e-7F*u[t0][x + 12][y + 6][z + 12] +
2.5974025974026e-6F*u[t0][x + 12][y + 7][z + 12] - 2.23214285714286e-5F*u[t0][x
+ 12][y + 8][z + 12] + 1.32275132275132e-4F*u[t0][x + 12][y + 9][z + 12] -
6.69642857142857e-4F*u[t0][x + 12][y + 10][z + 12] + 4.28571428571429e-3F*u[t0]
[x + 12][y + 11][z + 12] - 1.5031265031265e-7F*u[t0][x + 12][y + 12][z + 6] +
2.5974025974026e-6F*u[t0][x + 12][y + 12][z + 7] - 2.23214285714286e-5F*u[t0][x
+ 12][y + 12][z + 8] + 1.32275132275132e-4F*u[t0][x + 12][y + 12][z + 9] -
6.69642857142857e-4F*u[t0][x + 12][y + 12][z + 10] + 4.28571428571429e-3F*u[t0]
[x + 12][y + 12][z + 11] - 2.23708333333333e-2F*u[t0][x + 12][y + 12][z + 12] +
4.28571428571429e-3F*u[t0][x + 12][y + 12][z + 13] - 6.69642857142857e-4F*u[t0]
[x + 12][y + 12][z + 14] + 1.32275132275132e-4F*u[t0][x + 12][y + 12][z + 15] -
2.23214285714286e-5F*u[t0][x + 12][y + 12][z + 16] + 2.5974025974026e-6F*u[t0]
[x + 12][y + 12][z + 17] - 1.5031265031265e-7F*u[t0][x + 12][y + 12][z + 18] +
4.28571428571429e-3F*u[t0][x + 12][y + 13][z + 12] - 6.69642857142857e-4F*u[t0]
[x + 12][y + 14][z + 12] + 1.32275132275132e-4F*u[t0][x + 12][y + 15][z + 12] -
2.23214285714286e-5F*u[t0][x + 12][y + 16][z + 12] + 2.5974025974026e-6F*u[t0]
[x + 12][y + 17][z + 12] - 1.5031265031265e-7F*u[t0][x + 12][y + 18][z + 12] +
4.28571428571429e-3F*u[t0][x + 13][y + 12][z + 12] - 6.69642857142857e-4F*u[t0]
[x + 14][y + 12][z + 12] + 1.32275132275132e-4F*u[t0][x + 15][y + 12][z + 12] -
2.23214285714286e-5F*u[t0][x + 16][y + 12][z + 12] + 2.5974025974026e-6F*u[t0]
[x + 17][y + 12][z + 12] - 1.5031265031265e-7F*u[t0][x + 18][y + 12][z + 12])/
(pow(dt, 2)*damp[x + 1][y + 1][z + 1] + 2*dt*m[x + 12][y + 12][z + 12]) +
```

2) Backward propagation

```
u = TimeFunction(…, space_order=so)
eqn = m * u.dt2 - eta * u.dt - u.laplace
solve(eqn, u.backward)
```

produces

```
u[t-1, …] = f(u[t, …], u[t+1, …], …)
```

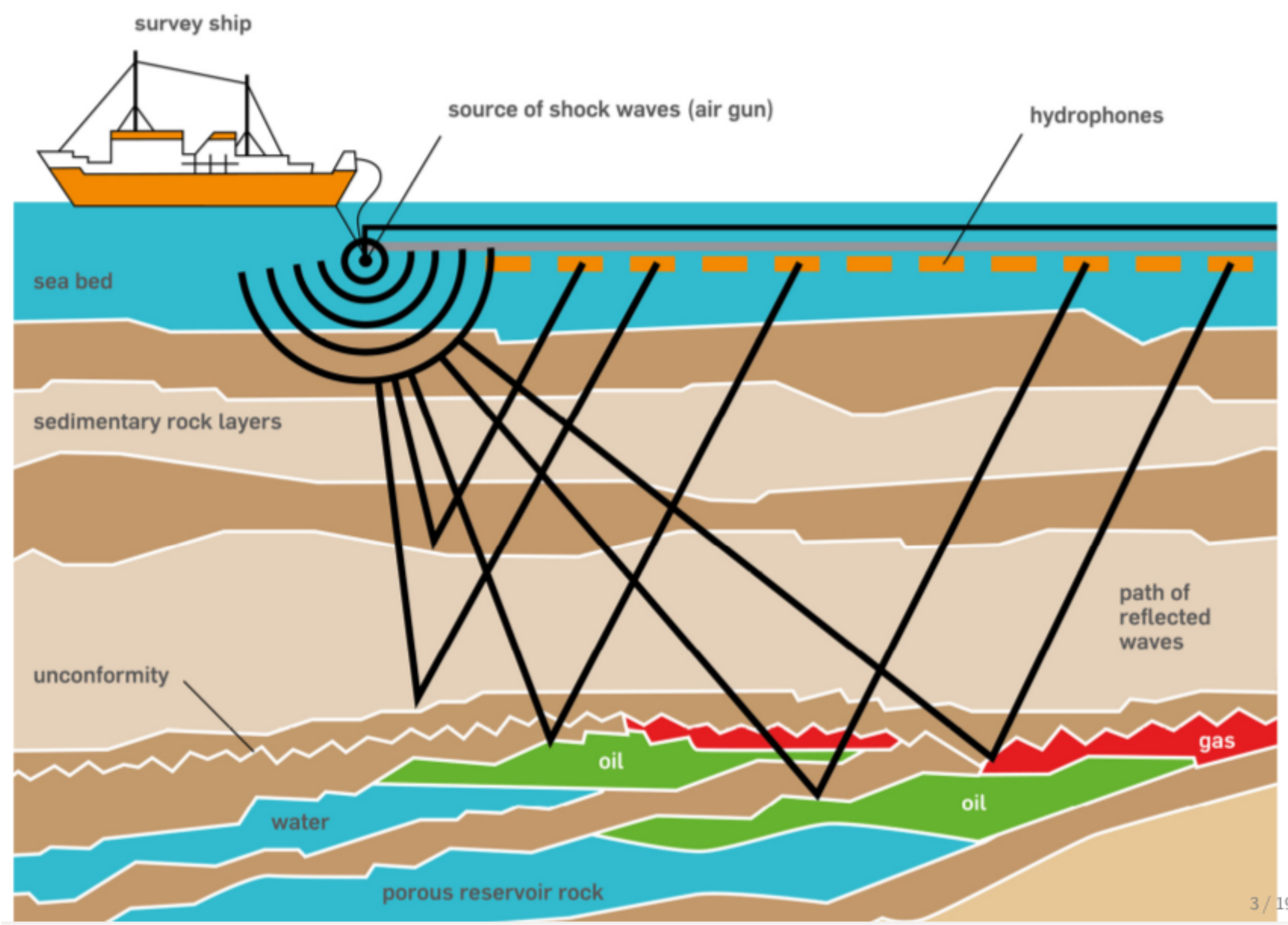
instead of

```
u[t+1, …] = f(u[t, …], u[t-1, …], …)
```

So we must march backwards in time to let the information flow from an iteration to another ("true" flow dependences)

3) beyond finite differences (sparse functions)

```
u = TimeFunction(…, space_order=so)
src = SparseFunction(…)
rec = SparseFunction(…)
eqns = […, src.inject(…), rec.interpolate(…)]
```



Example
Hydrophones only at the top of a 3D grid, but in general unaligned with the computational grid

Eventually, the generated loop nest can be quite complex

```
for (int time = time_m, t0 = …, t1 = …, …) {
  for (int x = x_m; x <= x_M; x += 1) {
    for (int y = y_m; y <= y_M; y += 1) {
      for (int z = z_m; z <= z_M; z += 1) {
        u[t1][x + 12][y + 12][z + 12] = …
      }
    }
  }
  for (int p_src = p_src_m; p_src <= p_src_M; p_src += 1) {
    u[t1][map[…]][map[…]][map[…]] = …
  }
  for (int p_rec = p_rec_m; p_rec <= p_rec_M; p_rec += 1) {
    rec[time][p_rec] = …
  }
}
```

Indirection array

4) beyond finite differences (chained BLAS/contractions)

```
A = Function(…)
B = Function(…)
…
eqns = [Eq(D, A*B + A*C), Eq(F, D*E)]
```

4) beyond finite differences (chained BLAS/contractions)

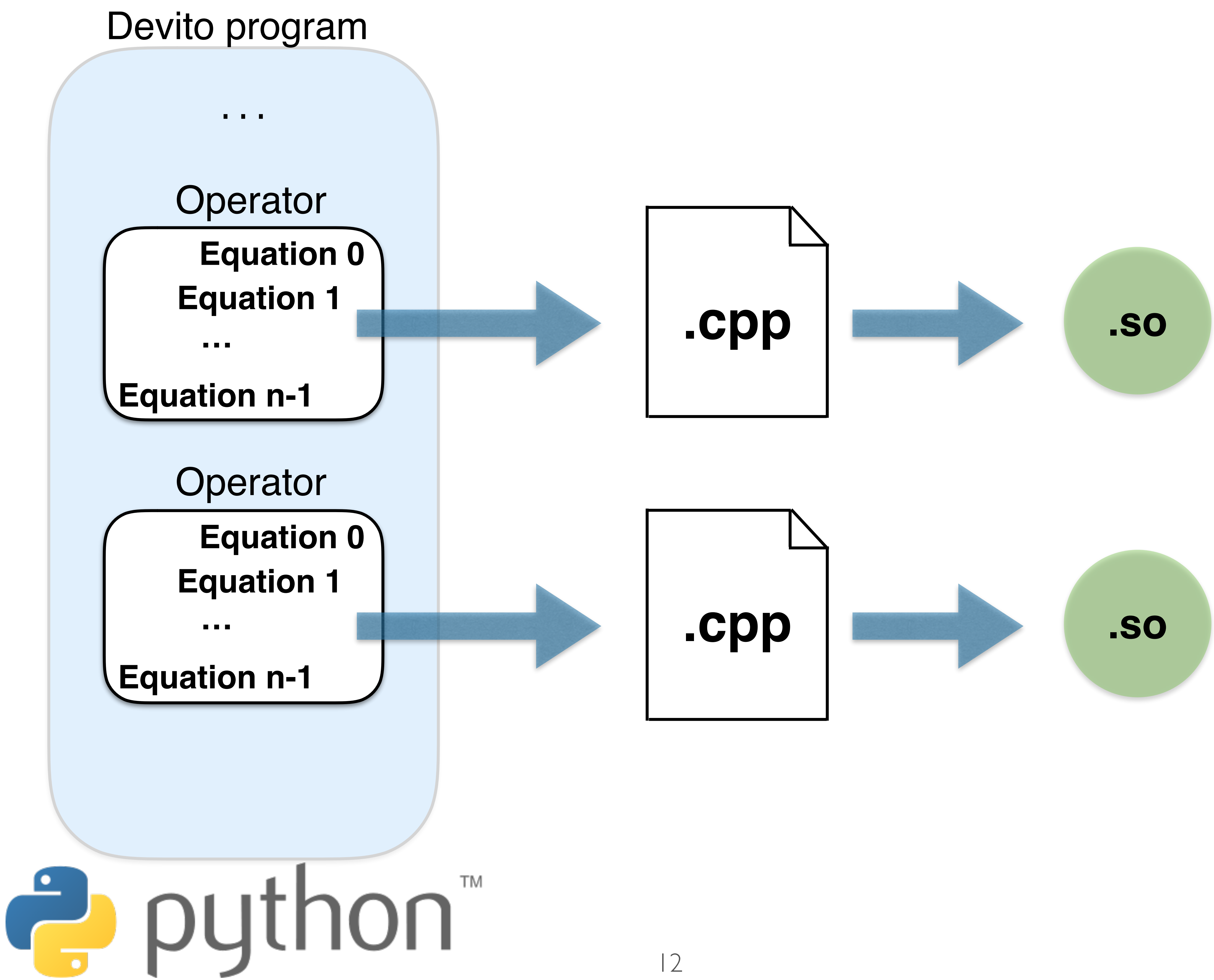
```
A = Function(…)
B = Function(…)
…
eqns = [Eq(D, A*B + A*C), Eq(F, D*E)]
```

Reuse D along i

```
for (int i = i_s; i < i_e; i += 1) {
  for (int k = k_s; k < k_e; k += 1) {
    for (int j = j_s; j < j_e; j += 1) {
      D[i][k] = A[i][j]*B[j][k] + A[i][j]*C[j][k];
    }
  }
  for (int l = l_s; l < l_e; l += 1) {
    for (int k = k_s; k < k_e; k += 1) {
      F[i][l] = D[i][k]*E[k][l];
    }
  }
}
```

Inlined sum

Devito: program model

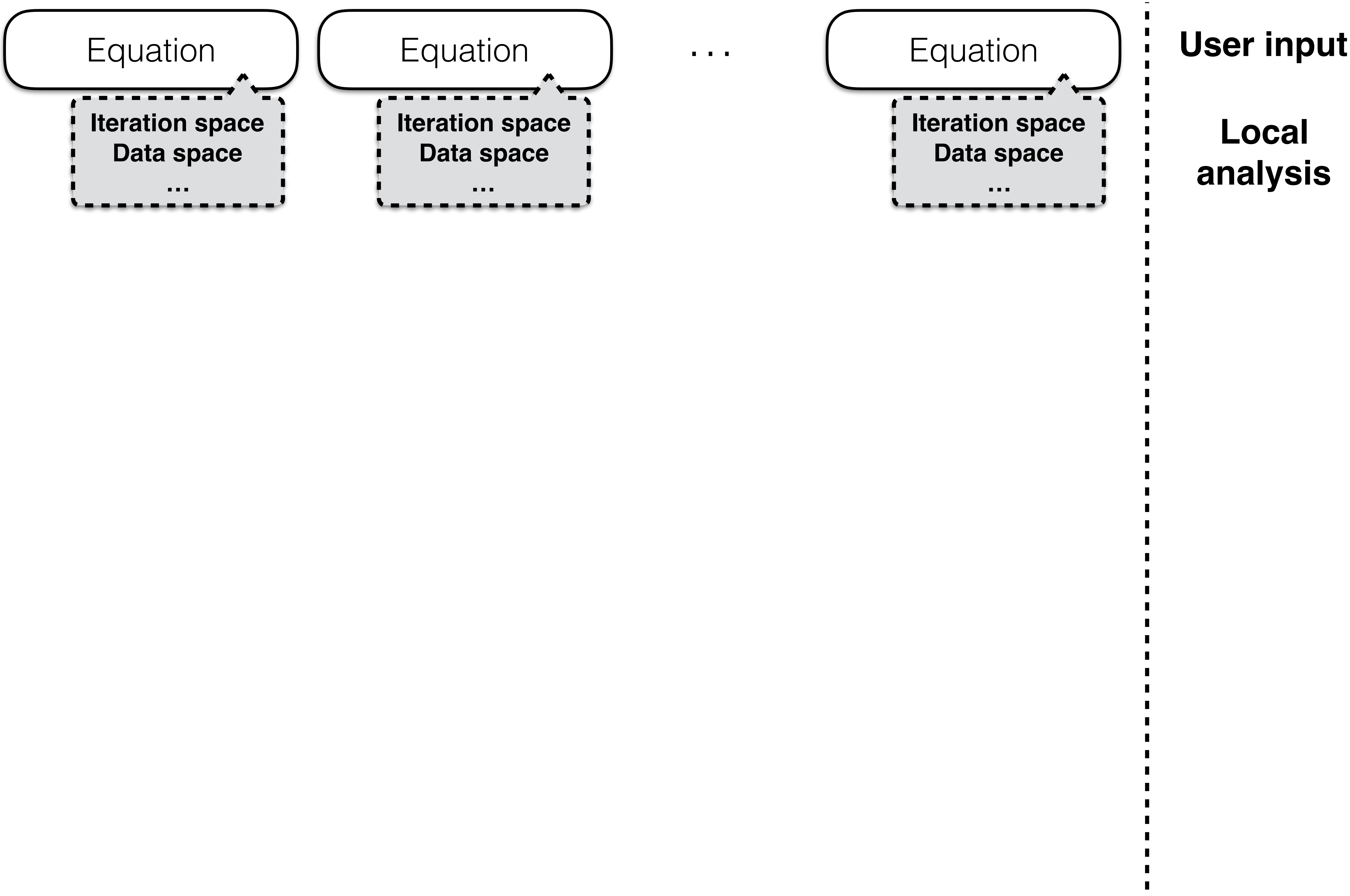


Devito: compilation passes and IRs overview

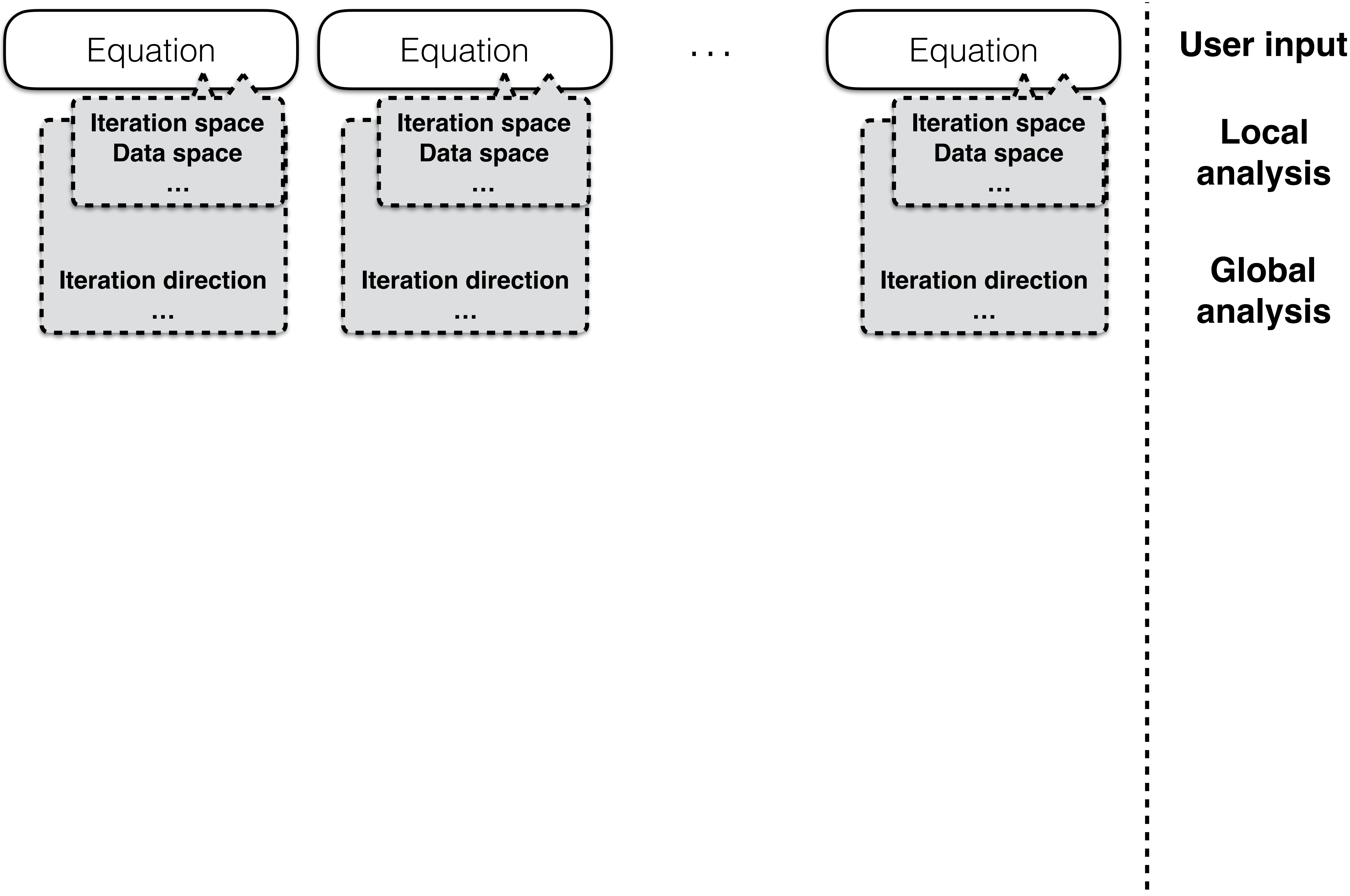
Equation | Equation | . . . | Equation

User input

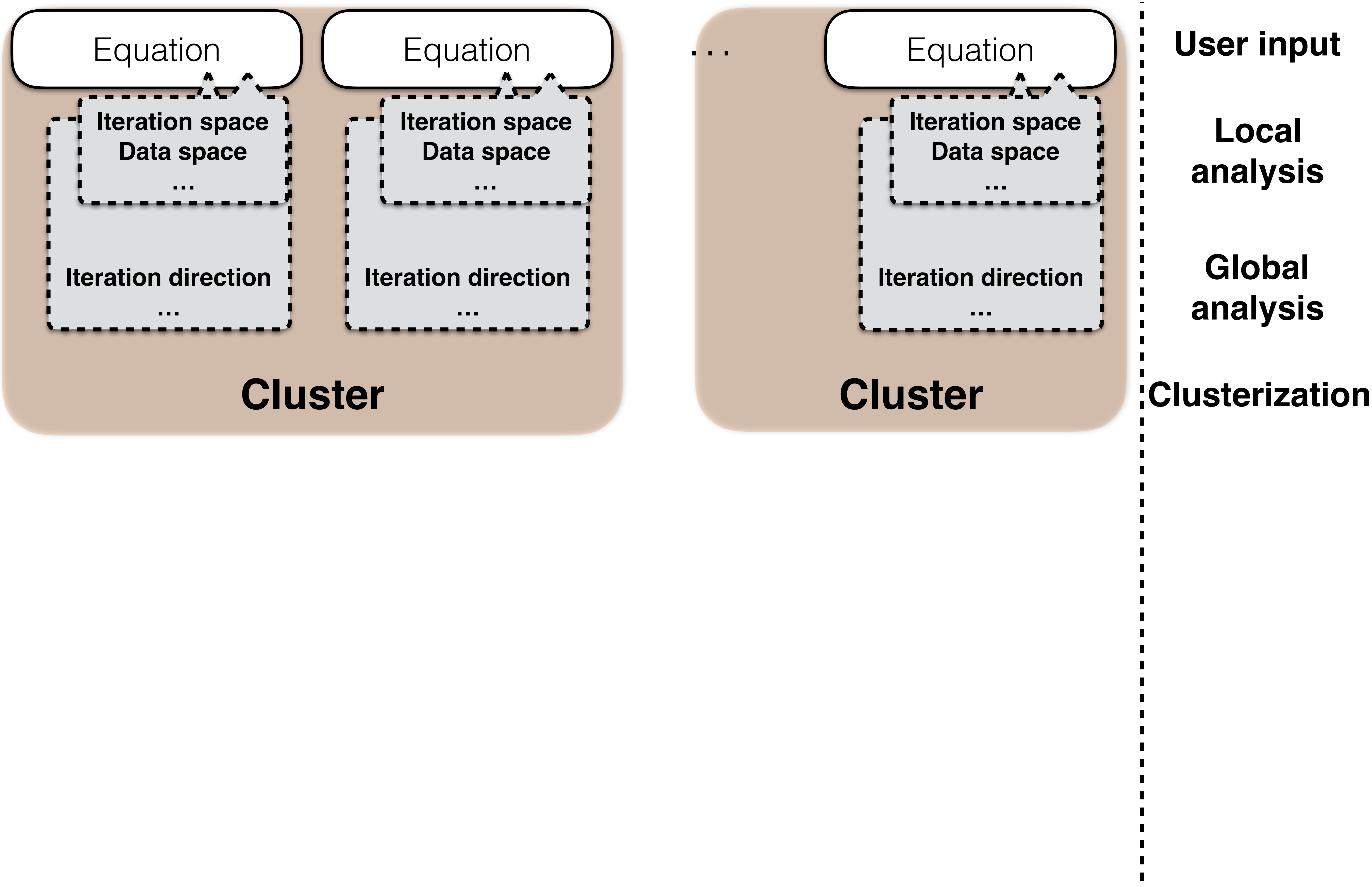
Devito: compilation passes and IRs overview



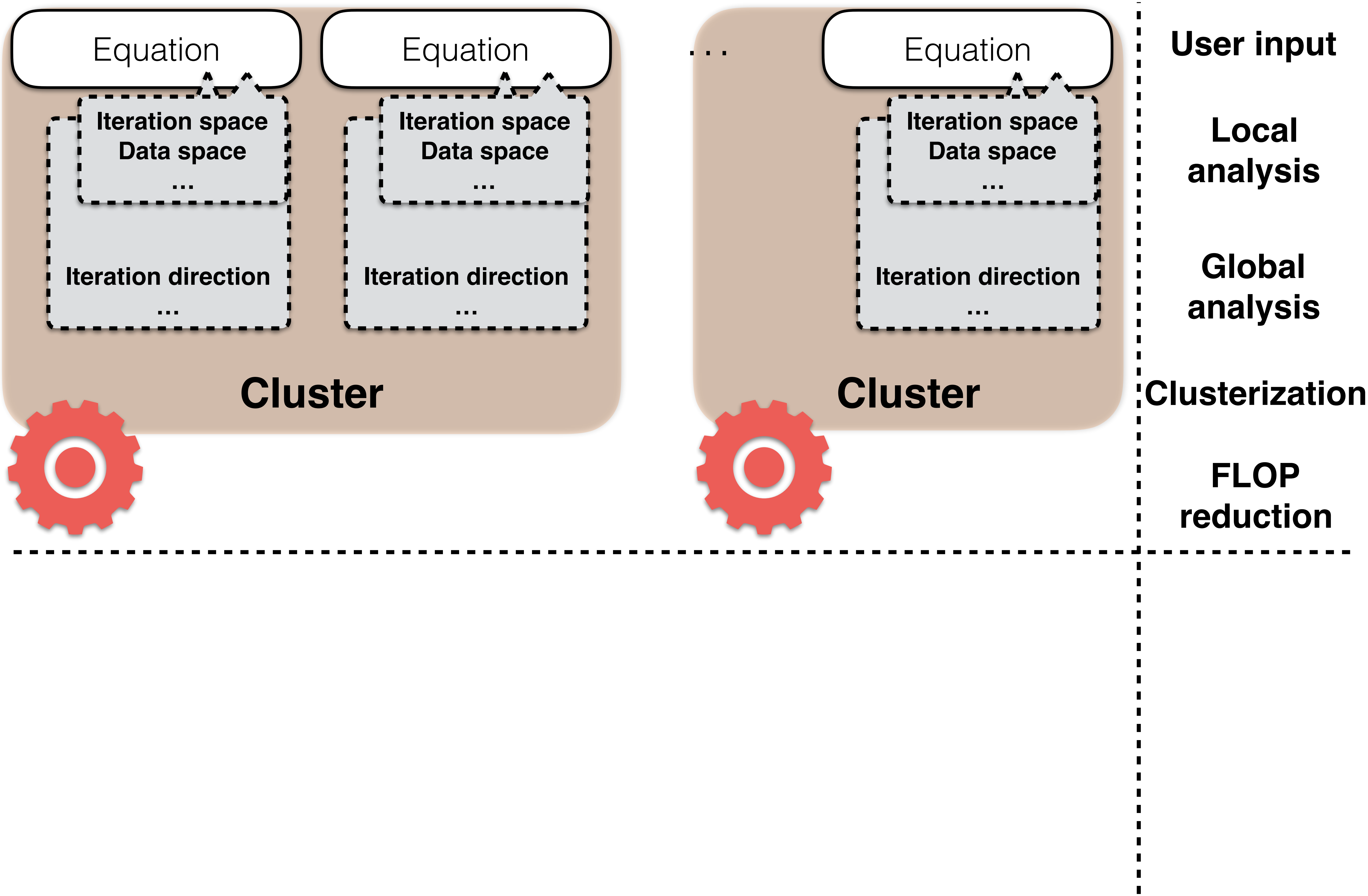
Devito: compilation passes and IRs overview



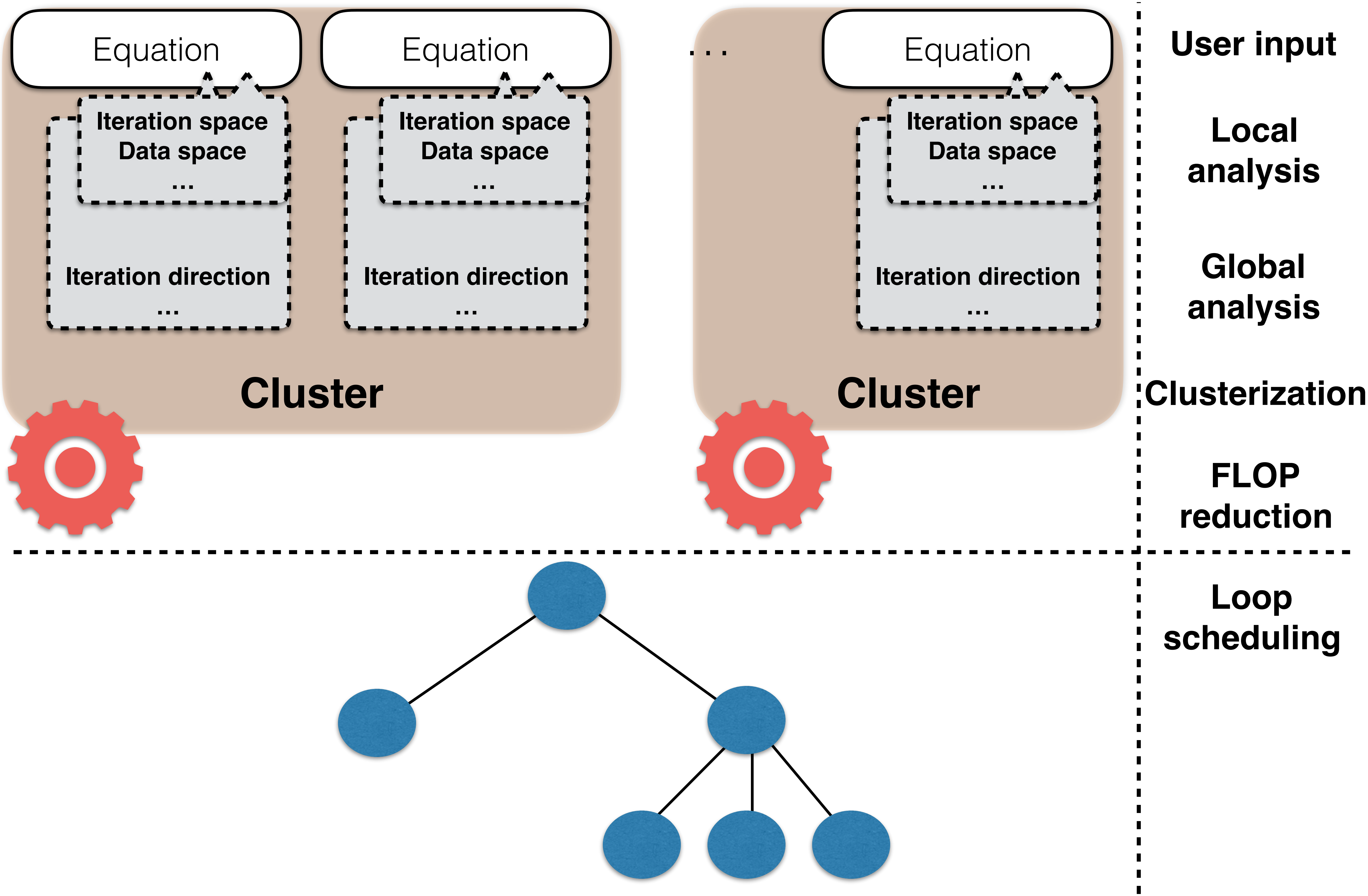
Devito: compilation passes and IRs overview



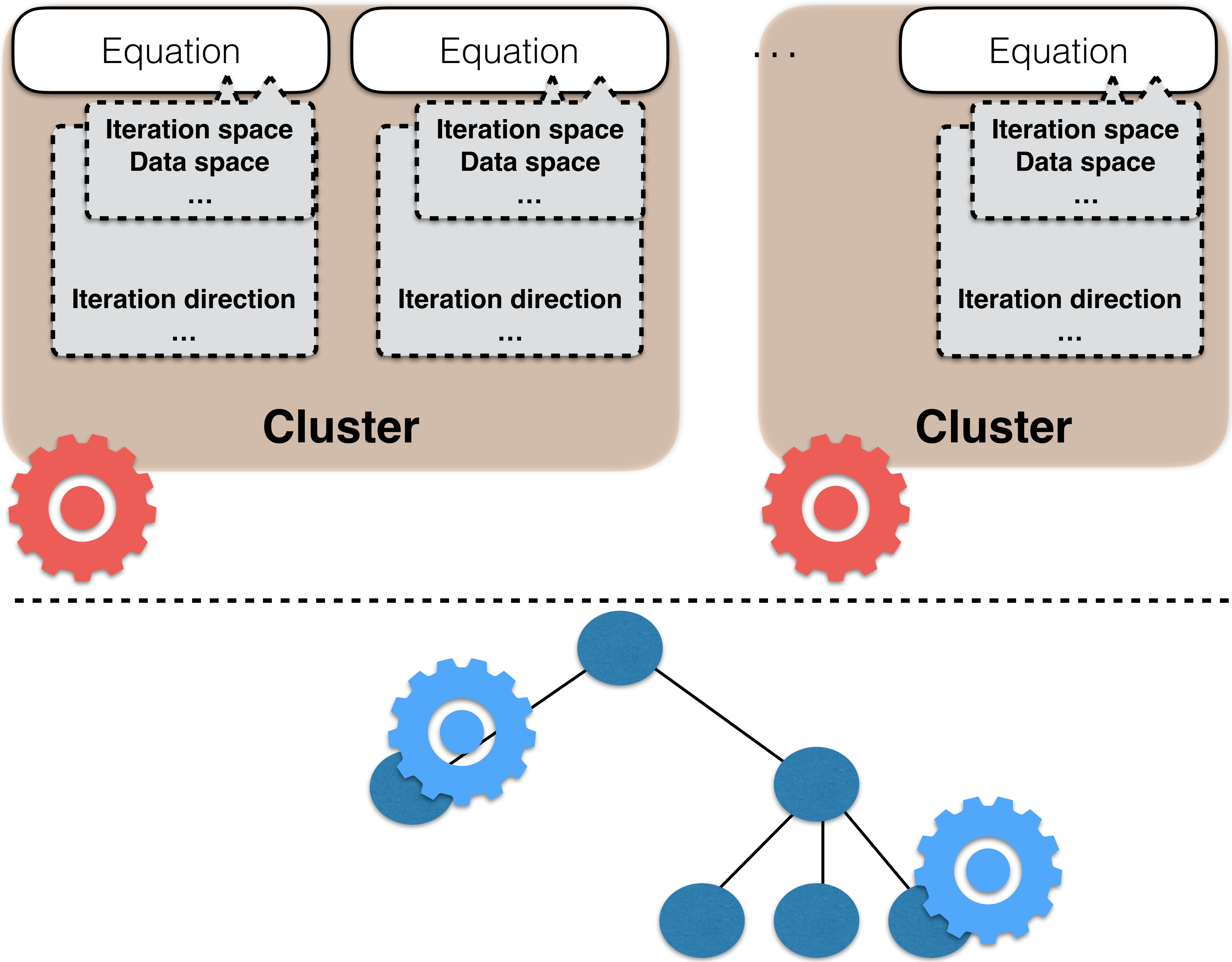
Devito: compilation passes and IRs overview



Devito: compilation passes and IRs overview



Devito: compilation passes and IRs overview



User input

Local analysis

Global analysis

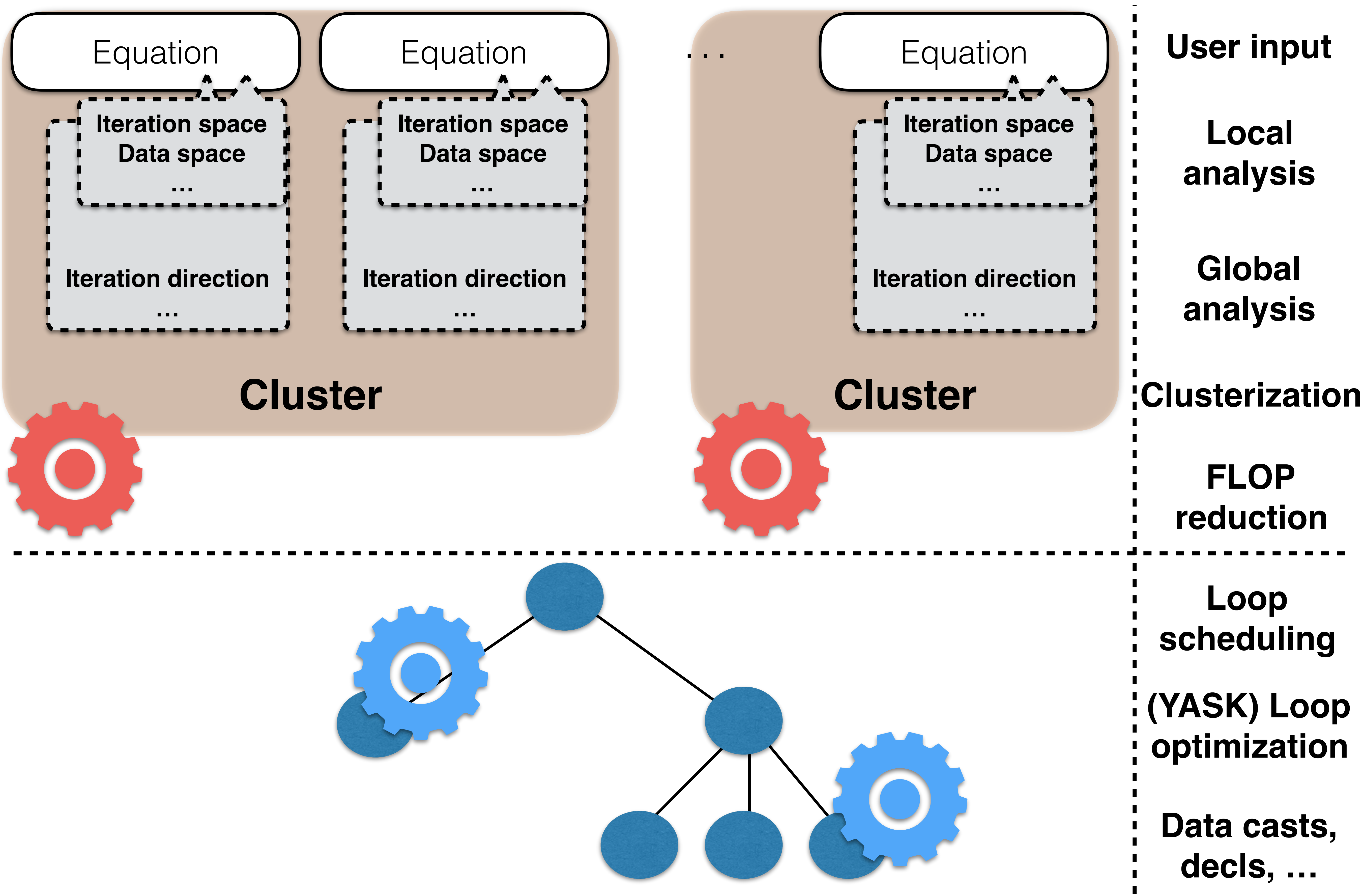
Clusterization

FLOP reduction

Loop scheduling

(YASK) Loop optimization

Devito: compilation passes and IRs overview



FLOPs reduction by symbolic transformations

- Common sub-expressions elimination, factorization, …

FLOPs reduction by symbolic transformations

- Common sub-expressions elimination, factorization, …
- **Cross-iteration redundancies elimination**

```
for i, for j, …
  sin(phi[i,j]) + sin(phi[i-1,j-1]) + sin(phi[i+2,j+2])
```

Observations:

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

```
for i, for j
  B[i,j] = sin(phi[i,j])
for i, for j, …
  B[i,j] + B[i-1,j-1] + B[i+2,j+2]
```

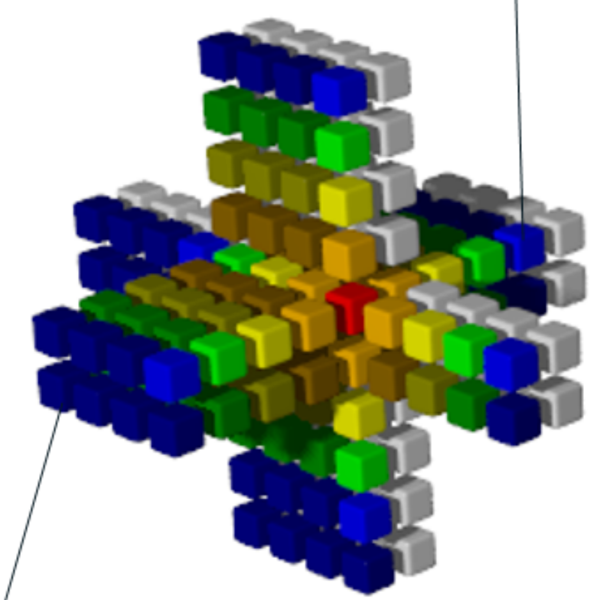
Trading FLOPs for storage?

Vector folding via YASK (a Devito backend)

Data layout transformation + cross-loop vectorization to optimize bandwith usage

25-point 3D stencil input vectorized using 8-element vectors, *each containing a 4x2 grid in the x-y plane*

Inner 3D loop iterates in z direction, i.e., *perpendicular* to 2D vector



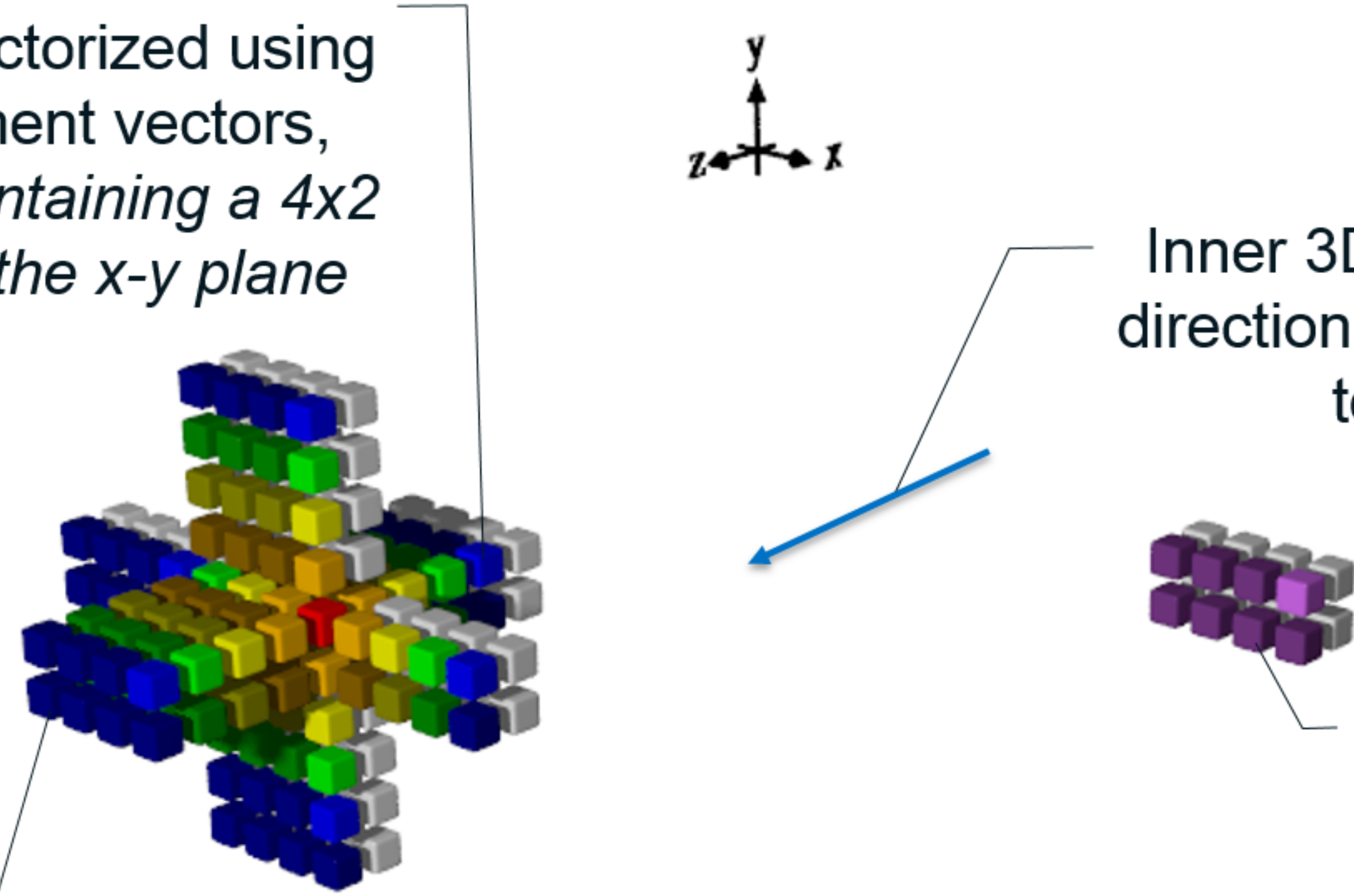
One 8-element (4x2) vector output per iteration

Need to read only 7 new cache lines for each iteration (vectors overlap in x-y dimensions within an iteration and in z dimension between iterations)

Steady-state memory BW = **7** new cache lines input to calculate each vector of output: **2.4x lower** than in-line

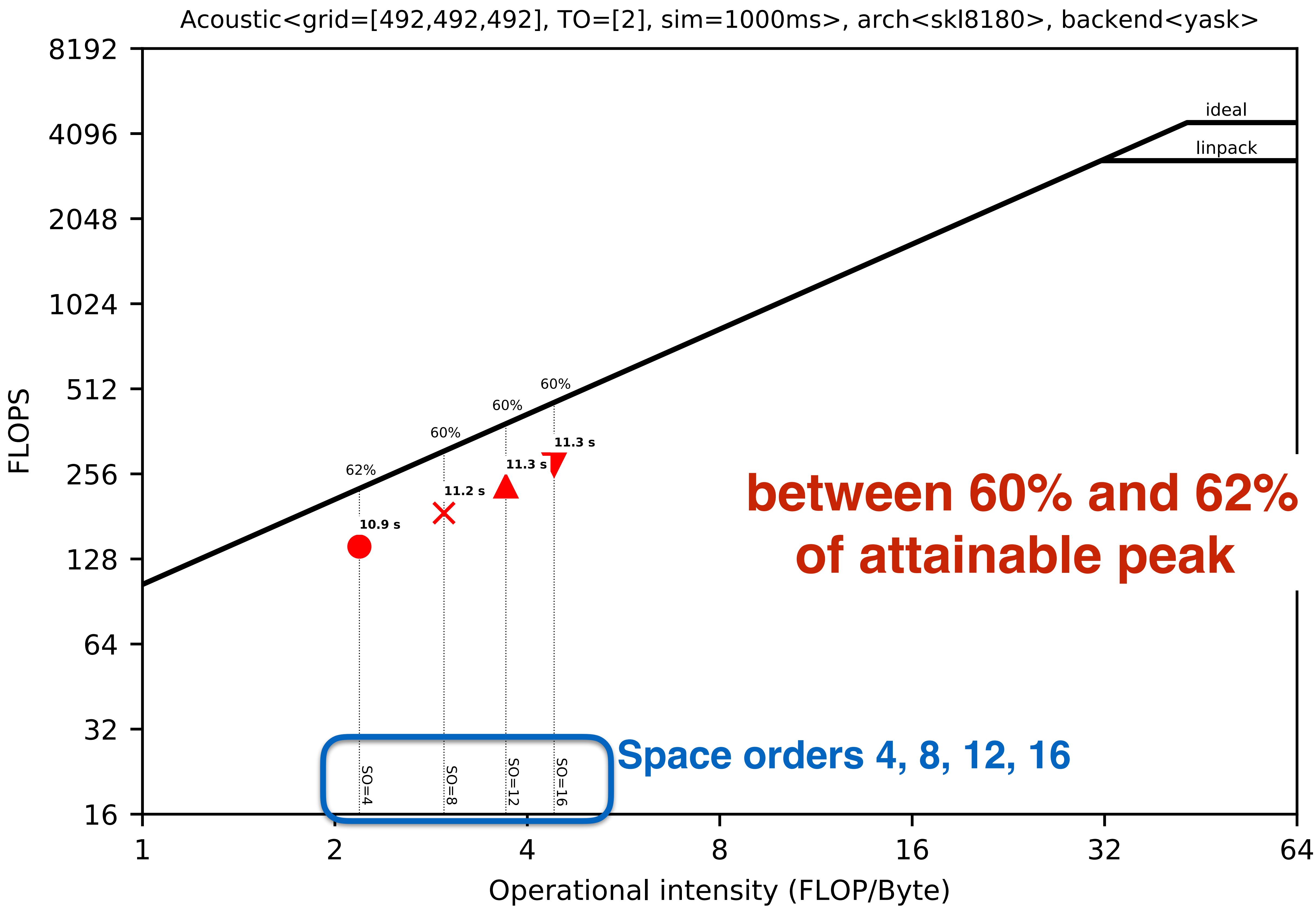
Vector folding via YASK (a Devito backend)

Data layout transformation + cross-loop vectorization to optimize bandwith usage

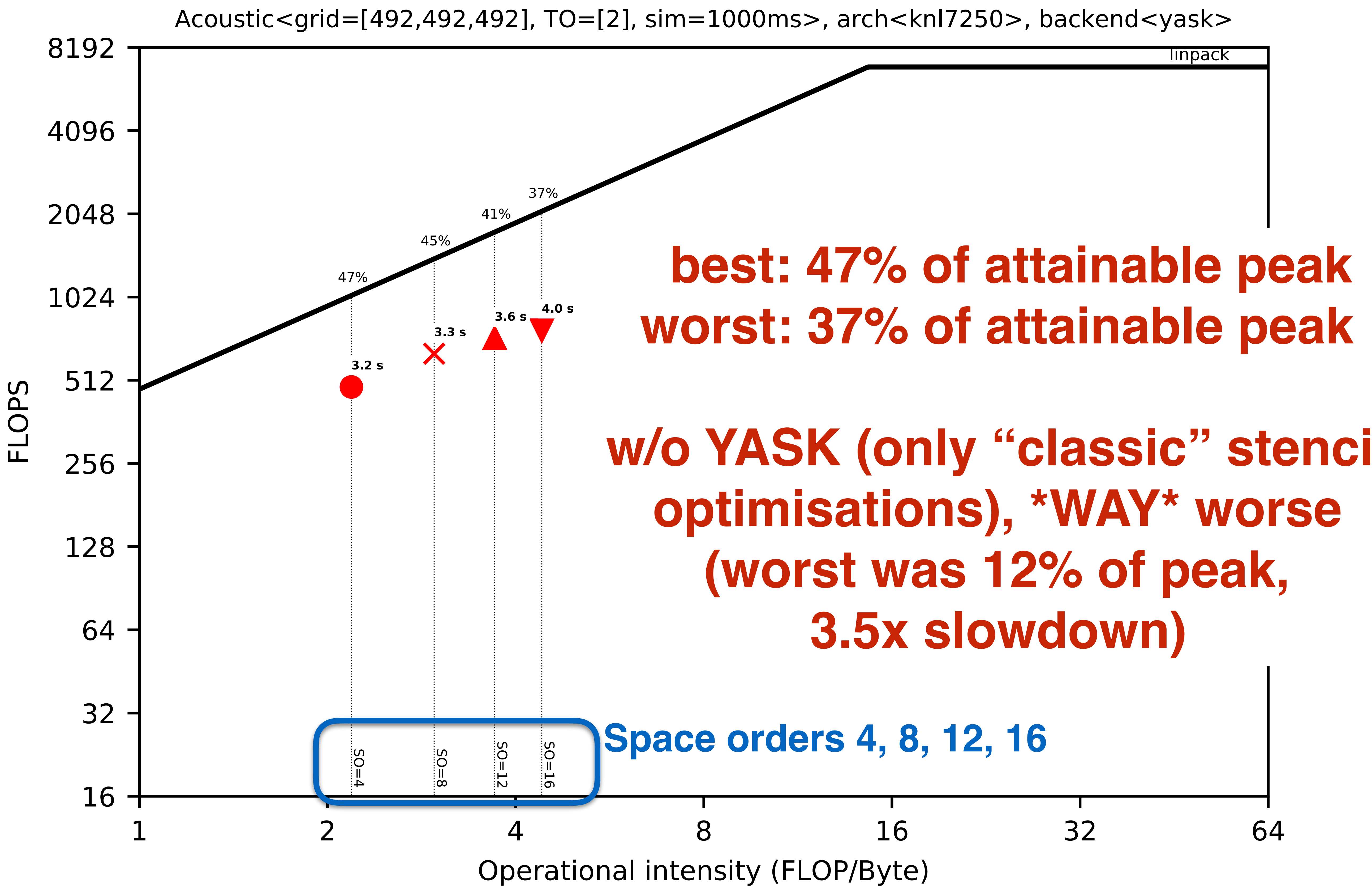


There's actually much more:
<u>multi-level tiling</u>
<u>software prefetching</u>
<u>temporal wavefront blocking</u>

Acoustic on Skylake 8180 with YASK



Acoustic on Xeon Phi 7250 with YASK



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Conclusions and resources

- Devito: an efficient and sustainable ~~finite difference DSL~~ system to express and execute "numerical kernels"
- Driven by real-world seismic imaging, inspired by projects such as FEniCS/Firedrake
- Based on actual compiler technology
- Interdisciplinary, interinstitutional research effort

Useful links

- **Website: http://www.devitoproject.org**
- **GitHub: https://github.com/opesci/devito**
- **Slack: https://opesci-slackin.now.sh**

Imperial College London

EPSRC Engineering and Physical Sciences Research Council

intel

POLYHEDRAL??

Appendix

Experimentation details

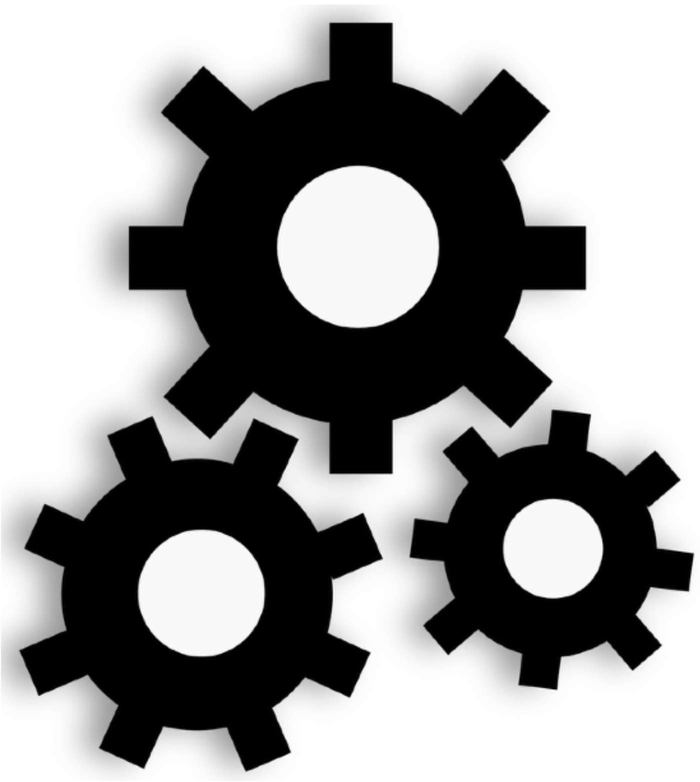
- Architectures
  - Intel® Xeon® Platinum 8180 Processor (“Skylake”, 28 cores)
  - Intel® XeonPhi® 7250 (68 cores)
    - Quadrant mode (still no support for NUMA)
    - Tried 1, 2, 4 threads per core. Shown best.

- Compiler
  - ICC 18 -xHost -O3
  - -xMIC-AVX512 on Xeon Phi
  - -qopt-zmm-usage=high on Skylake

- Runs
  - Single socket
  - Pinning via Numactl
  - On the XeonPhi®, data fits in MCDRAM

- Roofline calculations:
  - Memory bandwidth: STREAM
  - CPU peak: pen & paper
  - Operational intensity: source-level analysis (automated through Devito)

Philosophy: optimizations at the RIGHT level of abstraction



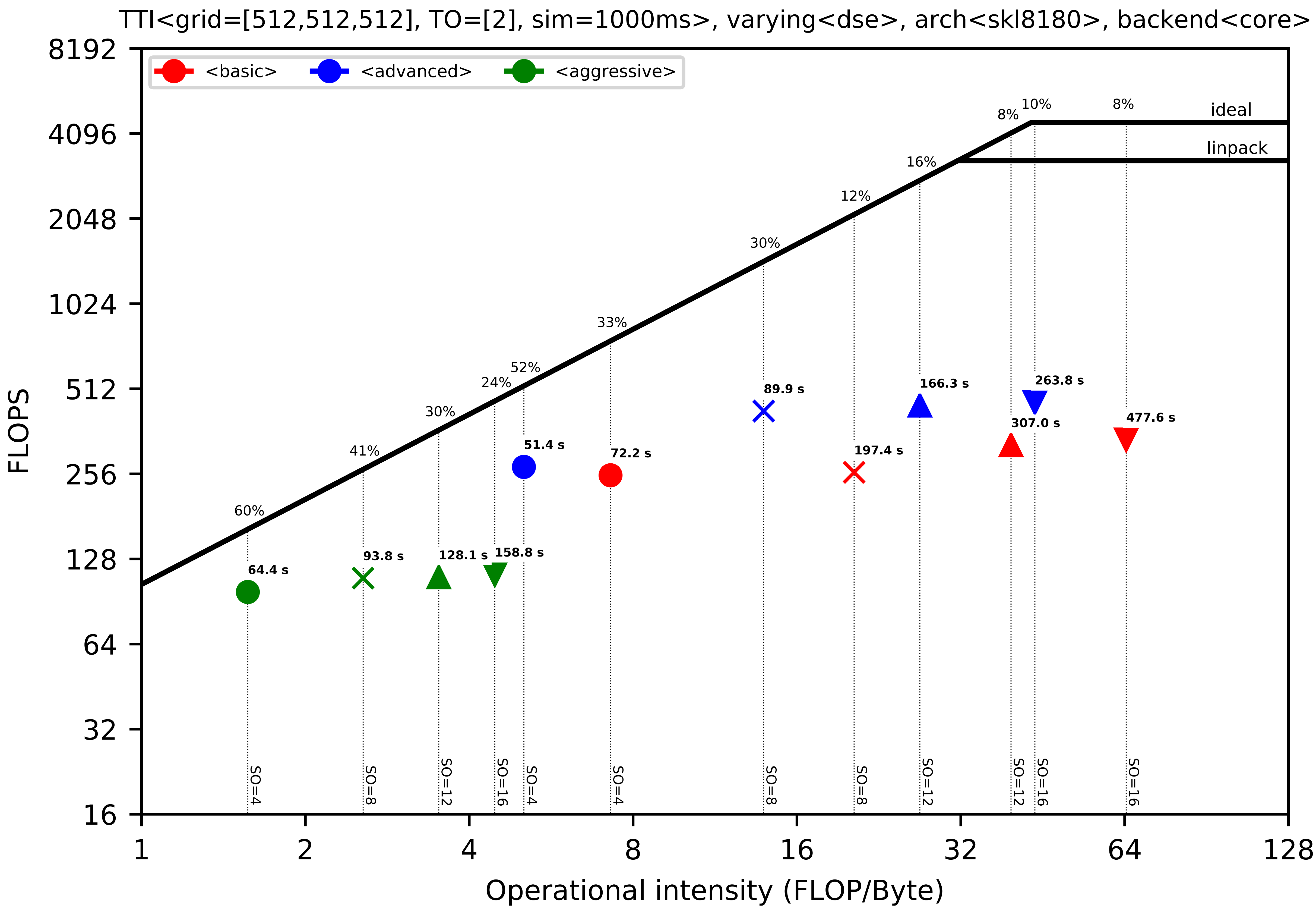
Example: optimizations for FLOPs reduction

```
Operator([eqn1, eqn2, …, eqn3])
```

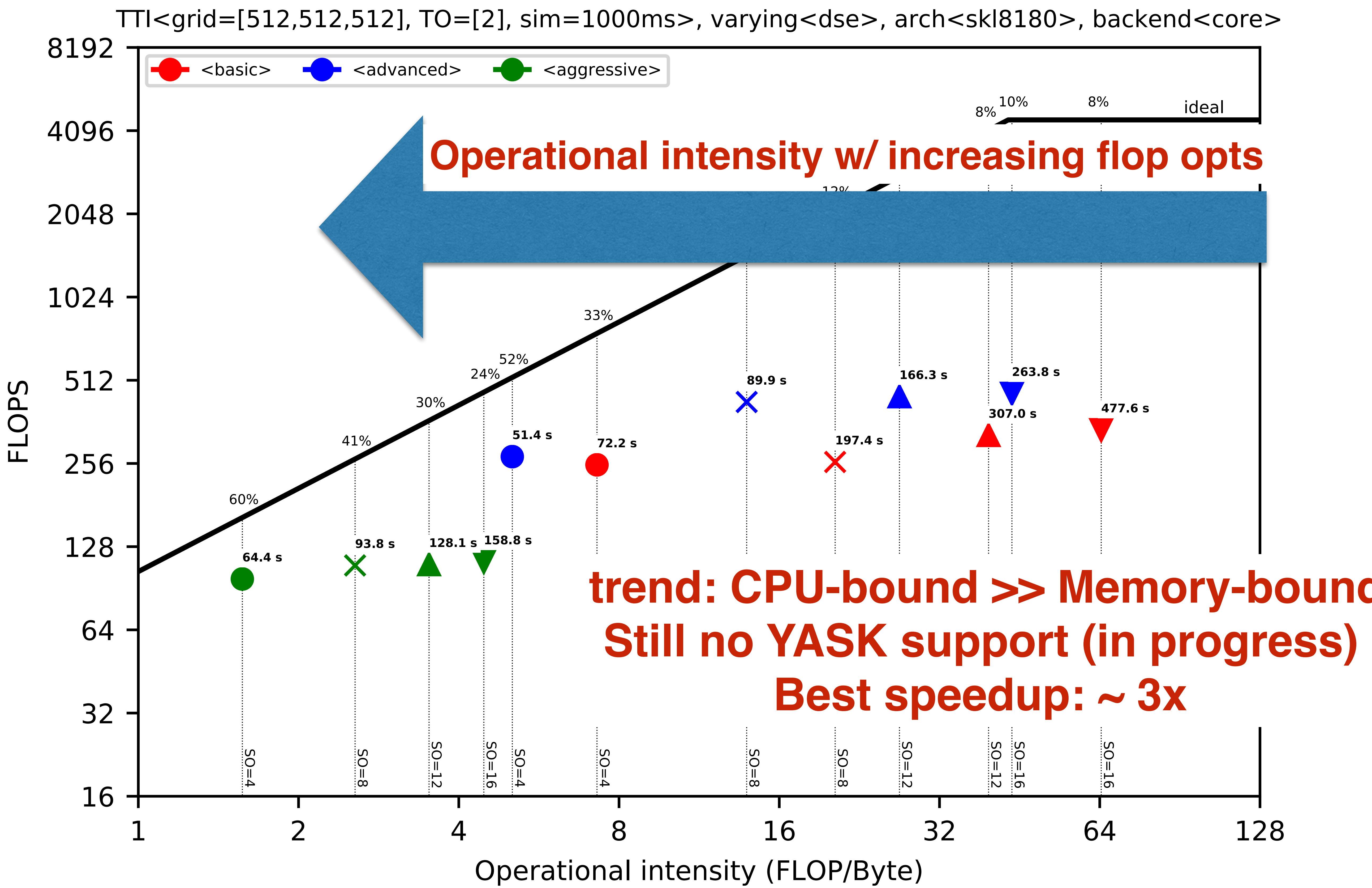
- Runtime constant propagation
- Equation clustering, **NOT** loop fusion
- Symbolic transformations to minimize the operation count of the equations

all based on Python and SymPy; no trace of loops yet!

More aggressive FLOP reduction strategies



More aggressive FLOP reduction strategies

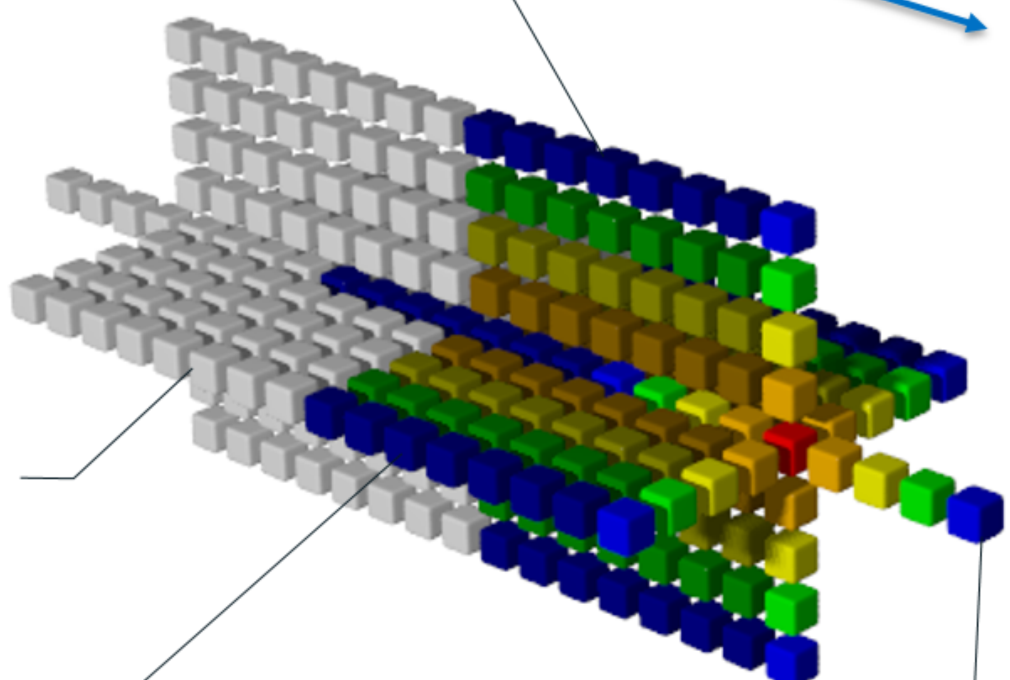


Beyond 1D vectorization …

Traditional "1D" vectorization requires lots of bandwidth

25-point 3D stencil input vectorized using 8-element vectors, each parallel to x-axis

Inner 3D loop iterates in x direction, i.e., *same dimension* as vectorization



Previous iteration

Current iteration

One 8-element vector output per iteration

Need to read 17 new cache lines* for each iteration (8 of the 25 vectors overlap in x dimension)

Steady-state memory BW = **17** new cache lines input to calculate each vector of output

*Assuming cache line size = vector size.