Imperial College London

Temporal blocking of finite-difference stencil operators with sparse off-the-grid sources

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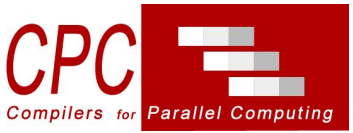

21st Workshop on Compilers for Parallel Computing

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Talk outline

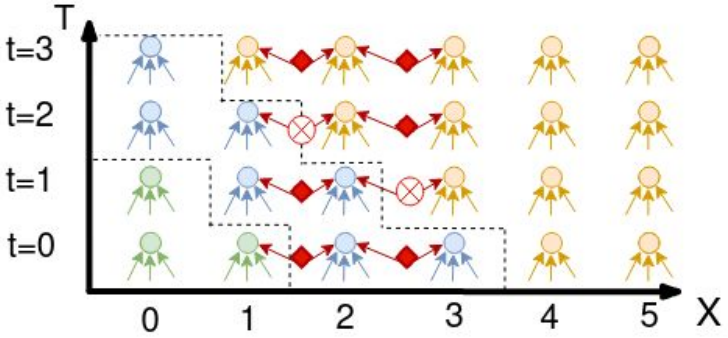
- Motivation: speed up computationally expensive scientific simulations involving the solution of PDEs modelling wave equations through explicit FD methods (seismic and medical imaging)

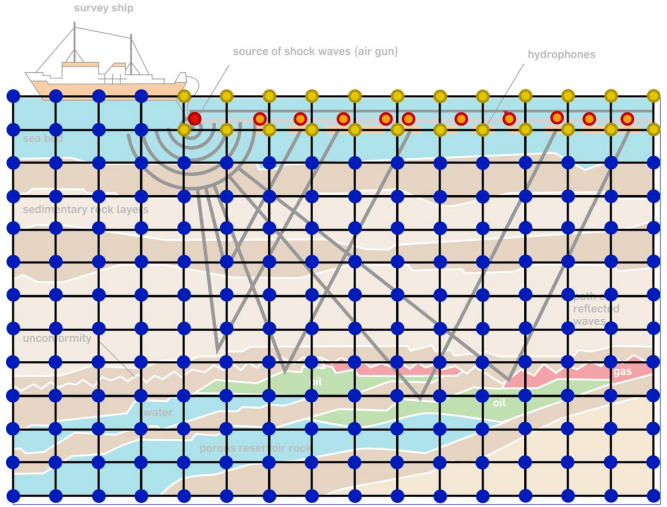
- Accelerating through cache optimizations, more **specifically through temporal blocking**

- Enabling **temporal blocking** on practical wave-propagation simulations is complicated as they consist of **sparse "off-the-grid"** operators (**Not** a typical stencil benchmark!) => **Applicability issues**

- We present **an approach to overcome limitations** and enable TB

- Experimental results show **improved** performance





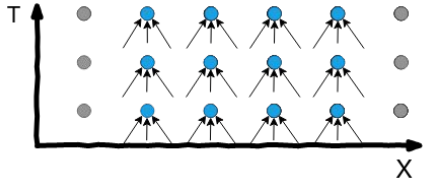
Modelling practical applications

- Stencils everywhere, not only though.
  What else?

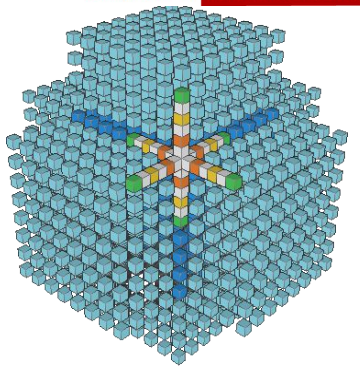
- Remarkable amount of work in the past on optimizing stencils...
  (Parallelism, cache optimizations, accelerators)

- Sources injecting and receivers interpolating at sparse off-the-grid coordinates.
  Non-conventional update patterns.

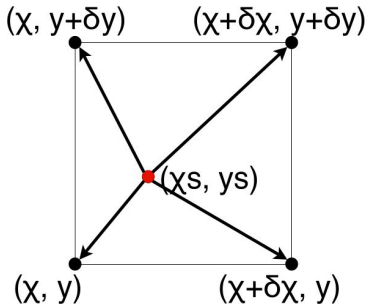
- Usually their coordinates are not aligned with the computational grid. How do we iterate over them?

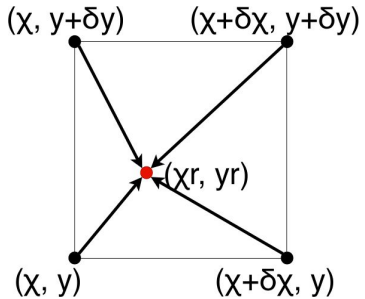


A 1d 3pt stencil update



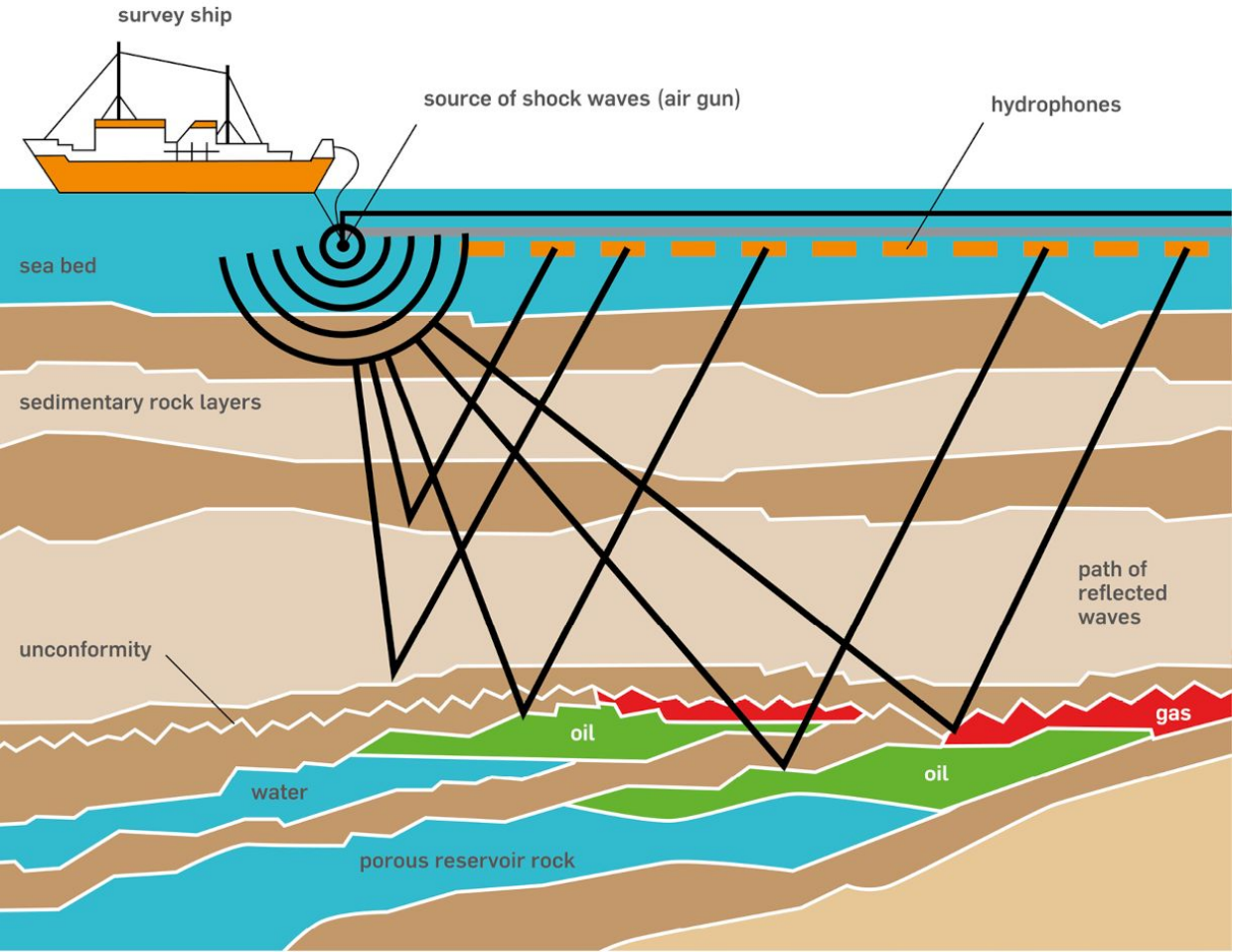
A 3d-19pt stencil update





Off-the-grid operators (Source injection/Receiver interpolation)

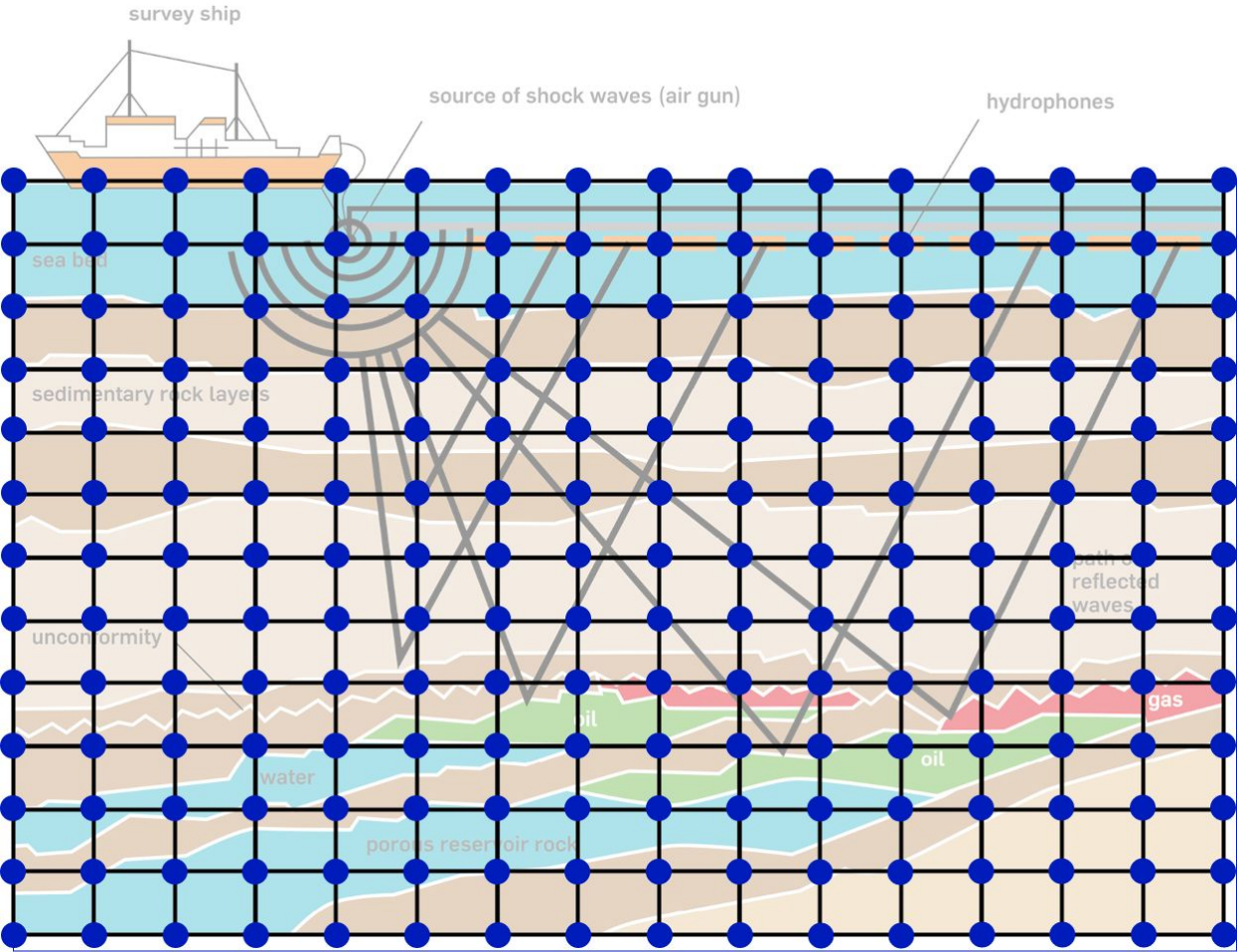
Sparse off-the-grid operators



- How a seismic survey looks like

Source: KrisEnergy 2021

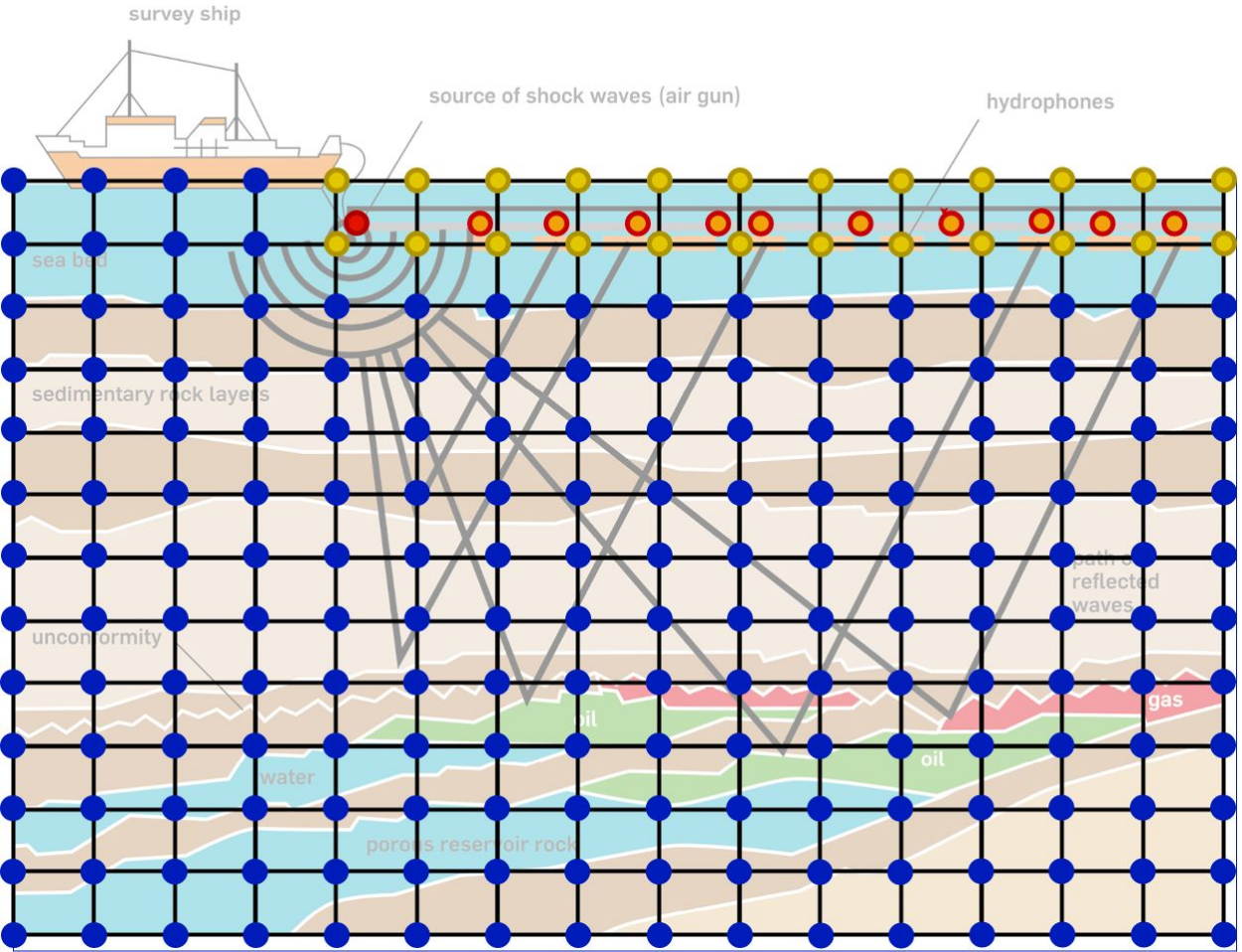
Sparse off-the-grid operators



- How a seismic survey looks like
- Discretizing the computational domain (the FD-grid). Solution computed on the points

Source: KrisEnergy 2021

Sparse off-the-grid operators



- How a seismic survey looks like
- Discretizing the computational domain (the FD-grid). Solution computed on the points
- Not-aligned “off-the-grid” operators exist (source injection/receiver interpolation)

Source: KrisEnergy 2021

A typical time-stepping loop with source injection

- Stencil computation, points on the domain are updated as a weighted function of neighbouring points
- Then we update the points that are affected from sources
- Each source has 3D coordinates
- Indirect accesses are used to scatter injection to neighbouring points
- Sources are aligned in time, same time index with points
- Sources are NOT aligned in space, off-the grid discretization

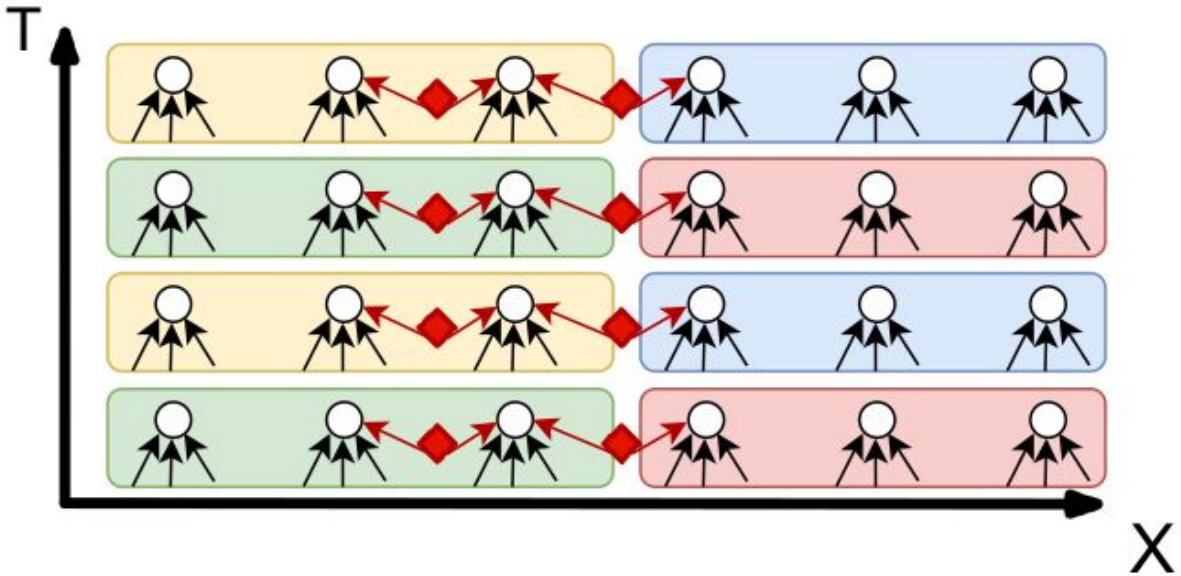
Listing 1: A typical time-stepping loop nest structure for a stencil update with source injection. This stencil has one temporal and three spatial dimensions.

```
1 for t = 1 to nt do
2   for x = 1 to nx do
3     for y = 1 to ny do
4       for z = 1 to nz do
5         A(t, x, y, z) ≡ u[t, x, y, z] = u[t-1, x, y, z] + Σ_{r=1}^{r=so/2} w_r (
            u[t-1, x - r, y, z] + u[t-1, x + r, y, z] + u[t-1, x, y - r, z] +
            u[t-1, x, y + r, z] + u[t-1, x, y, z - r] + u[t-1, x, y, z + r] );
6   foreach s in sources do // For every source
7     for i = 1 to np do // Get the points affected
8       xs, ys, zs = map(s, i) // through indirection
9       u[t, xs, ys, zs] + = f(src(t, s)) // add their impact
          on the field
```

Applying loop-blocking

Loop blocking (aka space blocking, loop tiling):

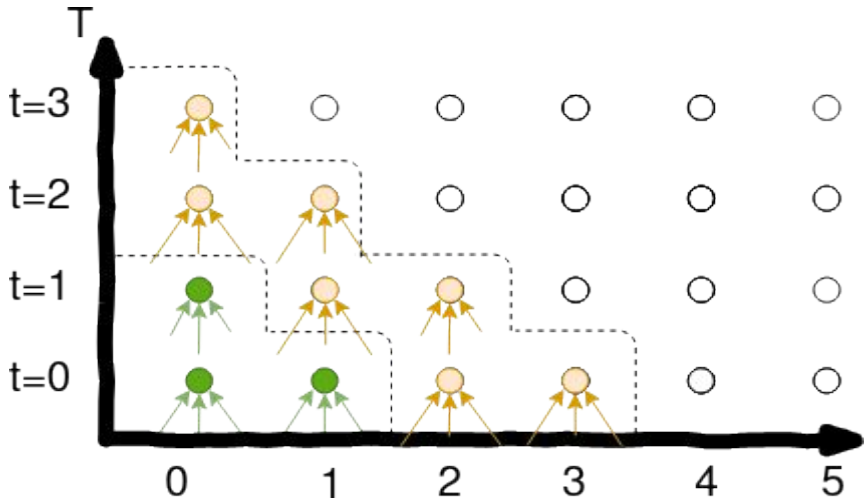
- Decompose grids into blocks/tiles. Iteration space partitioned to smaller chunks/blocks
- Improved data locality ⇛ Increased performance (Rich literature)
- Sparse off-the-grid operators are iterated as without blocking

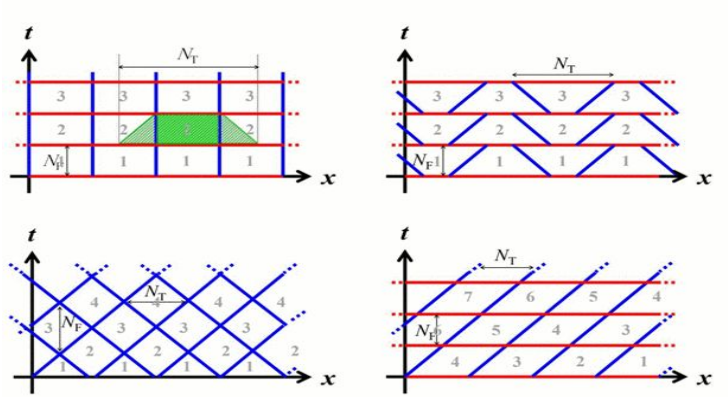


Applying temporal-blocking

Temporal blocking (Time-Tiling):

- Space blocking but data reuse is extended to time-dimension.
- Update grid points in future where (space) and when (time) possible
- Rich literature, several variants of temporal blocking, shapes, schemes
  - **Wave-front / Skewed** (Approach followed in the paper)
  - Diamonds, Trapezoids, Overlapped, Hybrid models

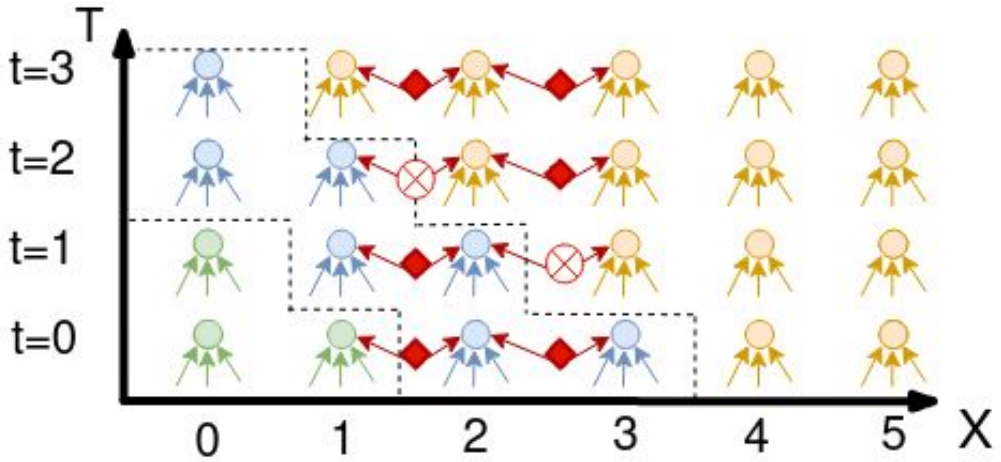




Tanaka et.al. (2018)

Off-the-grid operators: the issue

- Data dependences violations happen while a temporal update
- Source injection is in a different iteration space
- When a sparse operator exists in the boundary between space-time blocks, the order of updates is not preserved
- **Solution**: Need to align off-the-grid operators



Off-the-grid operators: the issue

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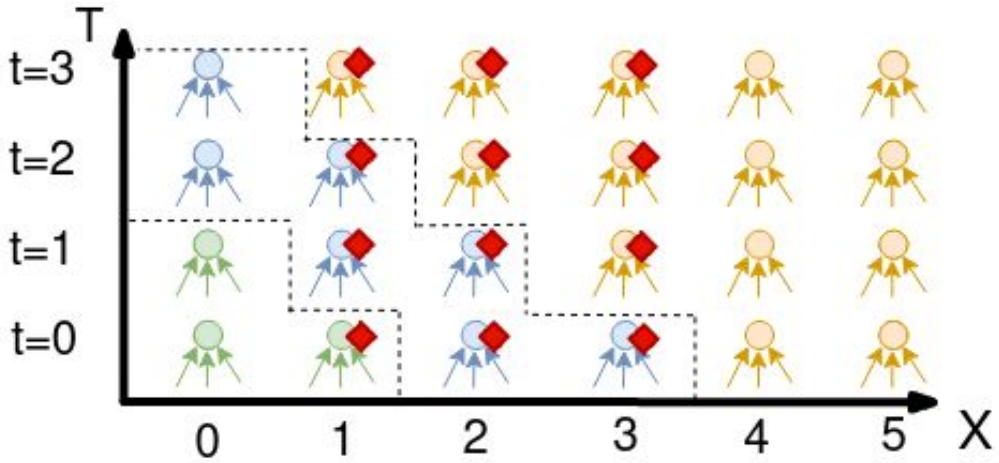


Methodology

- A negligible-cost scheme to precompute the source injection contribution.
- Align source injection data dependences to the grid
- This scheme is applicable to other fields as well (e.g. medical imaging)

Iterate over sources and store indices of affected points

- Inject to a **zero-valued initialized grid** for one (or a few more) timesteps
- **Hypothesis:** non-zero source-injection values at the first time-steps
- **Independent** of the injection and interpolation type (e.g. non-linear injection)

Listing 2: Source injection over an empty grid. No PDE stencil update is happening.

```
1 for t = 1 to 2 do
2     foreach s in sources do
3         for i = 1 to np do
4             xs, ys, zs = map(s, i);
5             u[t, xs, ys, zs] += f(src(t, s))
```

- Then, we **store the non-zero** grid point coordinates

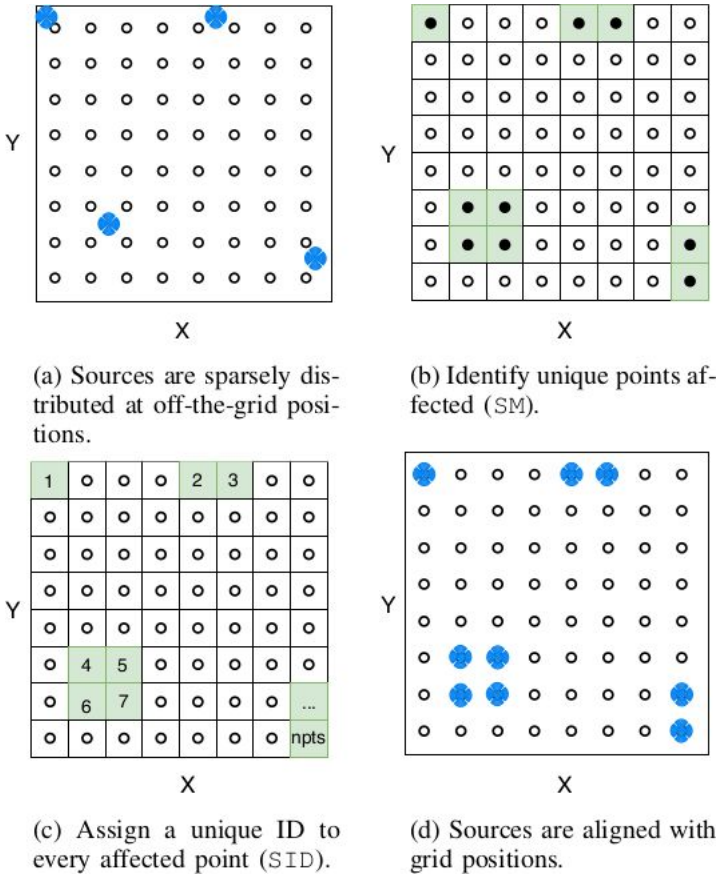
Generate sparse binary mask, unique IDs and decompose wavefields

- Perform source injection to decompose the off-the-grid wavefields to on-the-grid per point wavefields.
- Inject sources to sources

	Off-the-grid	Aligned
len(sources)	n_src	n_aff_pts
len(sources.coords)	(n_src, 3)	(n_aff_pts, 3)
len(sources.data)	(n_src, nt)	(n_aff_pts, nt)

Listing 3: Decomposing the source injection wavefields.

```
1 for t = 1 to nt do
2     foreach s in sources do
3         for i = 1 to np do
4             xs, ys, zs = map(s, i);
5             src_dcmp[t, SID[xs, ys, zs]] += f(src(t, s));
```



(a) Sources are sparsely distributed at off-the-grid positions.

(b) Identify unique points affected (SM).

(c) Assign a unique ID to every affected point (SID).

(d) Sources are aligned with grid positions.

Fuse iteration spaces

- Indirection mapping has changed. We still use indirections but now they are on the point.
- By using the aligned structure, we fuse the source injection loop inside the kernel update iteration space.
- The source mask SM is used to add (if 1) or not (if 0) the impact and SID is used to indirect to the impact values using the traversed grid coordinates.

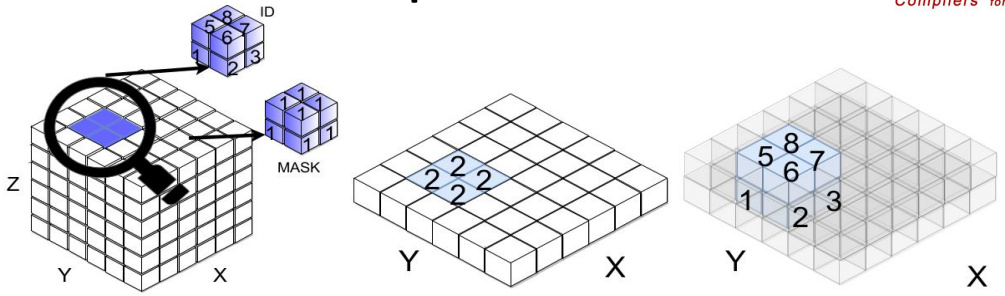
Listing 4: Stencil kernel update with fused source injection.

```
1 for t = 1 to nt do
2   for x = 1 to nx do
3     for y = 1 to ny do
4       for z = 1 to nz do
5         A(t, x, y, z, s);
6       for z2 = 1 to nz do
7         u[t, x, y, z2] += SM[x, y, z2] * src_dcmp[t, SID[x, y, z2]];
```

SIMD? (AVX512)

Reducing the iteration space size

- Lots of redundant ops due to sparsity
- A schedule to perform only necessary operations
- Aggregate NZ along the z-axis keeping count of them in a reduced-size structure named ***nnz_mask***
- Reduce the size of SID by cutting off zero z-slices



(a) `SID` and `SM` are very sparse in the general case.

(b) `nnz_mask` Aggregating non-zero values along z-axis.

(c) `Sp_SID`, a reduced size `SID`.

Listing 5: Stencil kernel update with reduced size iteration space for source injection.

```
1 for t = 1 to nt do
2   for x = 1 to nx do
3     for y = 1 to ny do
4       for z = 1 to nz do
5         A(t, x, y, z, s);
6       for z2 = 1 to nnz_mask[x][y] do
7         I(t, x, y, z, s) ≡{ zind = Sp_SID[x, y, z2];
8         u[t, x, y, z2] += src_dcmp[t, SID[x, y, zind]]; }
```

Listing 1: A typical time-stepping loop nest structure for a stencil update with source injection. This stencil has one temporal and three spatial dimensions.

```
1 for t = 1 to nt do
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6     foreach s in sources do // For every source
7       for i = 1 to np do // Get the points affected
8         xs, ys, zs = map(s, i) // through indirection
9         u[t, xs, ys, zs] + = f(src(t, s)) // add their impact
            on the field
```

Non-aligned

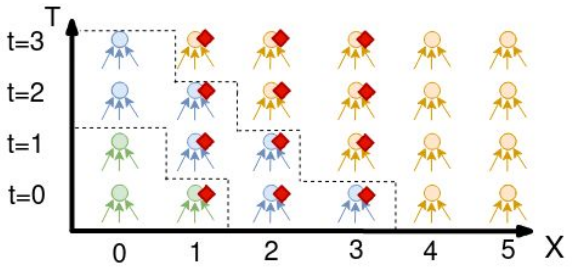
Listing 5: Stencil kernel update with fused - reduced size iteration space - source injection.

```
for t = 1 to nt do
  for x = 1 to nx do
    for y = 1 to ny do
      for z = 1 to nz do
        A(t, x, y, z, s);
      for z2 = 1 to nnz_mask[x][y] do
        I(t, x, y, z, s) ≡{ zind = Sp_SM[x, y, z2];
        u[t, x, y, z2] +=
        SM[x, y, zind] * src_dcmp[t, SID[x, y, zind]]; }
```

Aligned

- ✅ Aligned to grid
- ✅ Same OPS
- ✅ Parallelism
- ✅ SIMD
- ⏭ Apply TB

Everything so far, automated in Devito DSL



Applying wave-front temporal blocking

- TB with manually editing the Devito generated code
- Skewing factor depends on data dependency distances (higher for higher SO, multigrid)

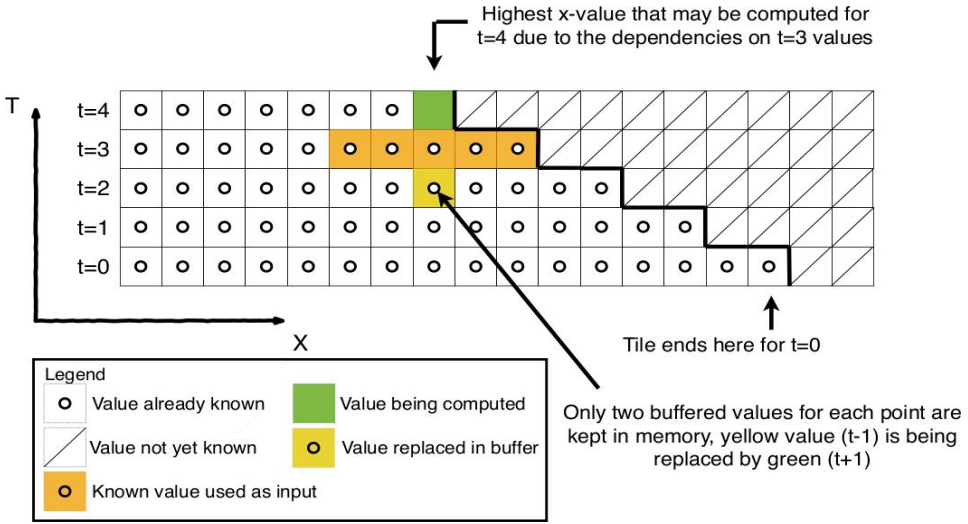
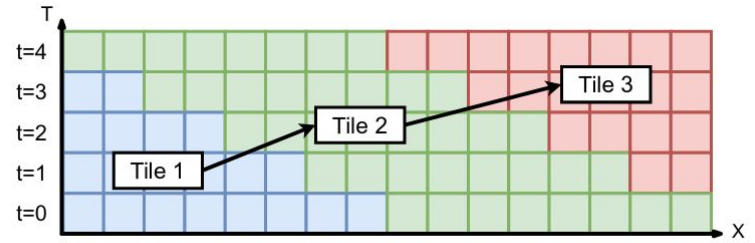
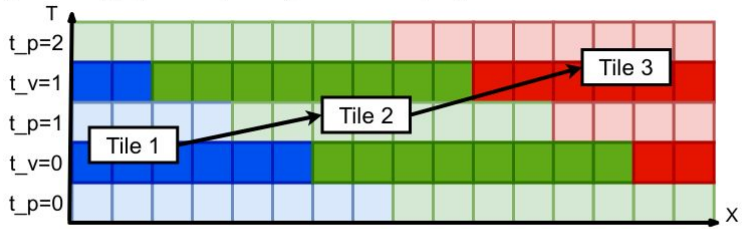


Figure from YASK, Yount et. al (2016)



(a) The figure shows multiple wave-front tiles evaluated sequentially, partially adapted from [15].



(b) The figure shows multiple wave-front tiles evaluated sequentially in multigrid stencil codes.

Listing 6: The figure shows the loop structure after applying our proposed scheme.

```
for t_tile in time_tiles do
    for xtile in xtiles do
        for ytile in ytiles do
            for t in t_tile do
                OpenMP parallelism
                for xblk in xtile do
                    for yblk in ytile do
                        for x in xblk do
                            for y in yblk do
                                SIMD vectorization
                                for z = 1 to nz do
                                    A(t, x − time, y − time, z, s);
                                for z2 = 1 to nnz_mask[x][y] do
                                    I(t, x − time, y − time, z2, s);
```

Iterate space-time tiles

Time-stepping in the tile and loop-blocking within the tile. Collapse outer loops that are loop-blocked

No loop blocking on z-dim, full stride for max-vectorization performance

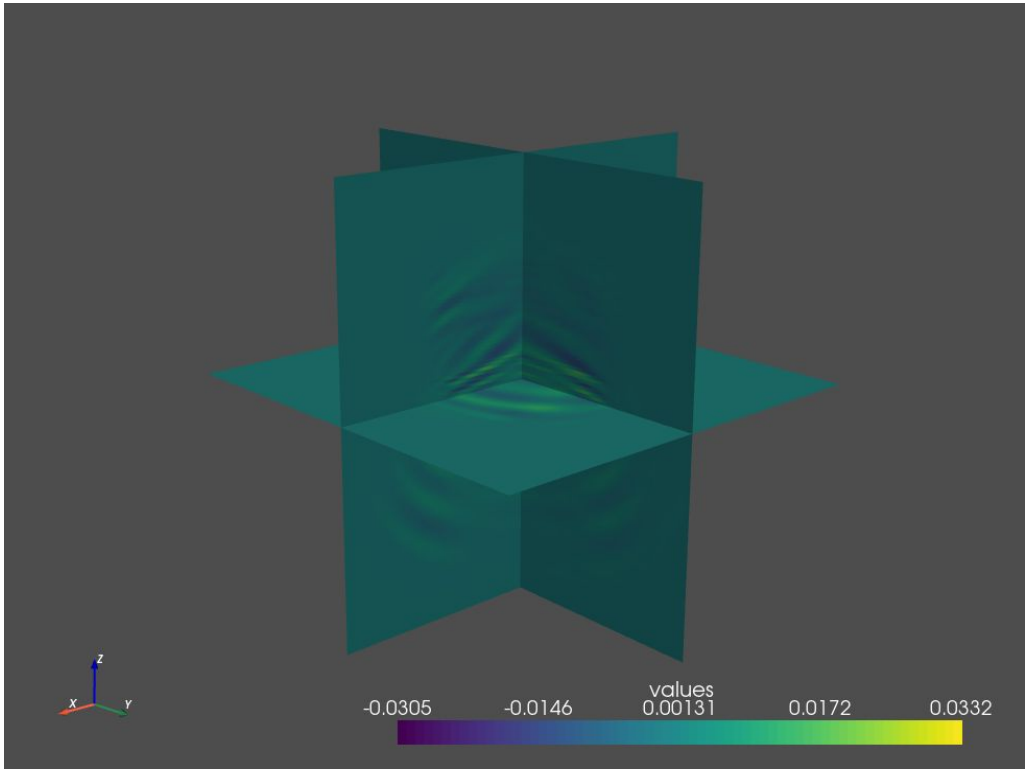
Experimental evaluation: the models

- **Isotropic Acoustic**
  Generally known, single scalar PDE, laplacian like, low cost

- **Isotropic Elastic**
  Coupled system of a vectorial and tensorial PDE, explosive source, increased data movement, first order in time, cross-loop data dependencies

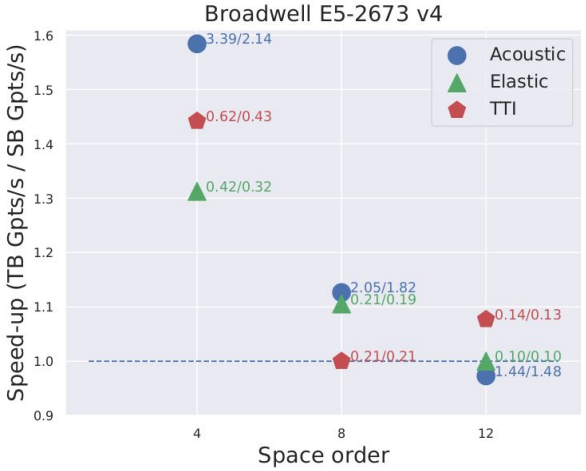
- **Anisotropic Acoustic (aka TTI)**
  Industrial applications, rotated laplacian, coupled system of two scalar PDEs

Industrial-level, 512^3 grid points, 512ms simulation time, damping fields ABCs

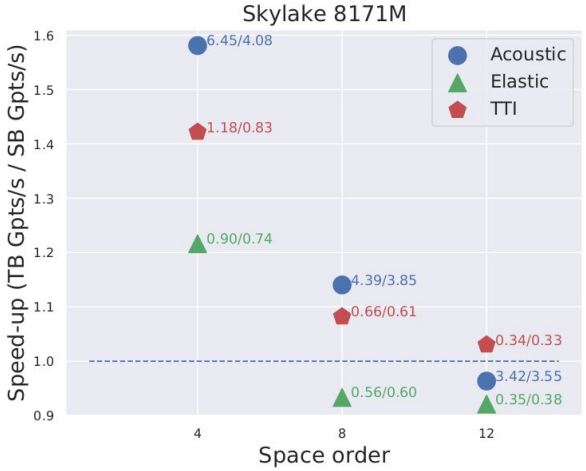


Velocity field, TTI wave propagation after 512ms

Experimental evaluation: the results



(a) Throughput speed-up of kernels for Broadwell.



(b) Throughput speed-up of kernels for Skylake.

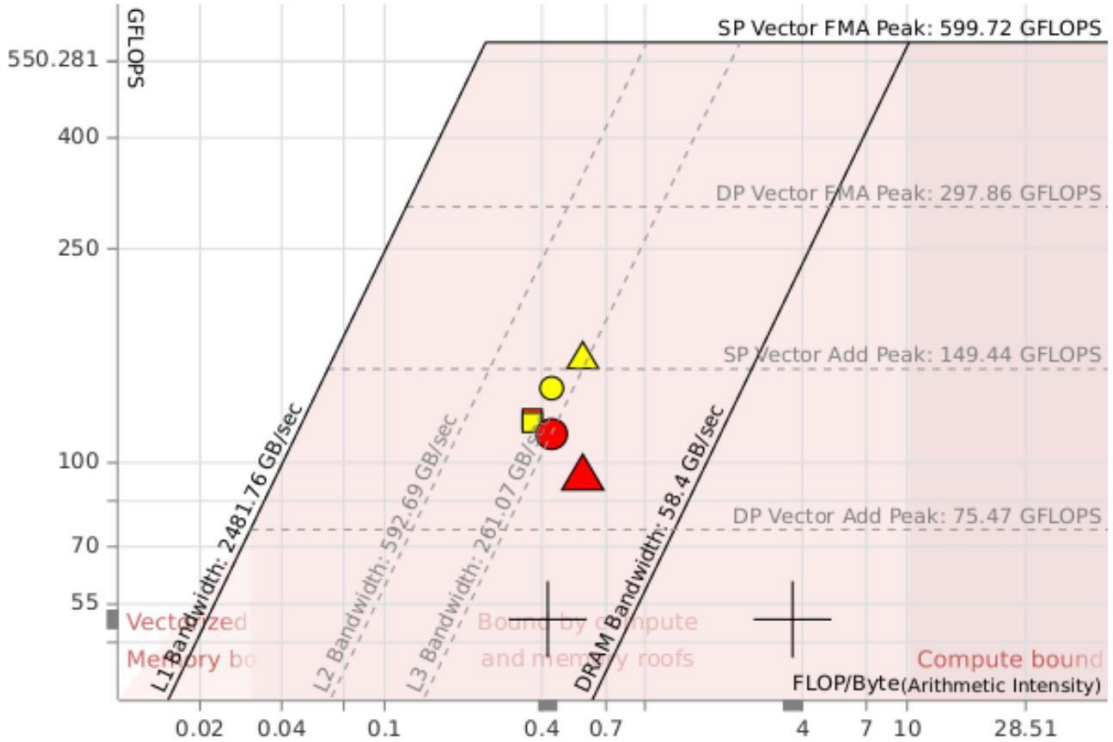
Azure model Architecture	**E16s v3** **Broadwell**	**E32s v3** **Skylake**
vCPUs	16	32
GiB memory	128	256
Model name	E5-2673 v4	8171M
CPUs	16	32
Thread(s) per core	2	2
Core(s) per socket	8	16
Socket(s)	1	1
NUMA node(s)	1	1
Model	79	85
CPU MHz	2300	2100
L1d cache	32K	32K
L1i cache	32K	32K
L2 cache	256K	1024K
L3 cache	51200K	36608K

TABLE I: VM specification

- Benchmark on Azure VMs
- GCC, ICC
- Thread pinning
- OpenMP, SIMD
- Aggressive auto-tuning

- Kernels are flop-optimized through Devito.
- Gpts/s aka Gcells/s: time to solution metric in stencil computations
- (!) High Gflops/s do not guarantee a faster solution.

Cache-aware roofline model



Space order:

- △ 4
- ○ 8
- □ 12

Temporal Blocking

Spatial Blocking

Broadwell, isotropic acoustic, 512^3 grid points, 512ms

Conclusions

- We presented an approach to apply temporal blocking to stencil kernels with sparse off-the-grid operators.
- The additional cost is negligible compared to the achieved gains.
- Solution built on top of Devito-DSL
- Performance gains of up to 1.6x on low order (4) and 1.15x on medium order (8).

Current WIP

- Integration to DSL
- User will get out-of the box time tiled code for all PDEs!

Future plans

- MPI-aware scheme
- GPUs
- High-order stencils

- Open-source, on top of Devito v4.2.3 - https://github.com/georgebisbas/devito

http://www.devitoproject.org

https://github.com/devitocodes/devito

https://opesci-slackin.now.sh

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- Navjot Kukreja (Imperial College)
- John Washbourne (Chevron)
- Edward Caunt (Imperial College)

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