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Towards automatic code generation for high-order compact schemes

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Motivation

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Separation of concerns (and domain specific language approach)
The algorithms that encapsulate the mathematics and physics of the problem are separated from the computational science of their implementation.
Exascale computer - The UK plans to have such a supercomputer by 2025

9K IBM POWER9 and 27K NVIDIA GPU

9K AMD EPYC and 37K AMD (Instinct) GPU

Motivation

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Separation of concerns (and domain specific language approach)
The algorithms that encapsulate the mathematics and physics of the problem are separated from the computational science of their implementation.
Complex mathematics?

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \tfrac{1}{3}\mu \nabla(\nabla \cdot \mathbf{u}) + \rho \mathbf{g}.$$

OpenSBLI: a domain-specific langauge type modelling framework that is capable of expanding a set of differential equations written in Einstein notation, and automatically generating C/C++ code that performs the finite difference approximation to obtain a solution**. Currently with the OP-DSL backend.**

Compact scheme

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From computational point of view, it is a type of relatively complicated finite-difference scheme, which requires:

- Prepare matrix (a,b,c,d)
- Linear solver
- Extra treatments for (periodic) boundary condition

$$\frac{1}{4}f'_{i-1} + f'_i + \frac{1}{4}f'_{i+1} = \frac{3}{2}\frac{f_{i+1} - f_{i-1}}{2\Delta}$$

Using the OP-DSL, we need following lines

```
ops_par_loop(preprocessX, "preprocessX", compact3d, 3, iterRange,
             ops_arg_dat(u, 1, S3D_7PT, "double", OPS_READ),
             ops_arg_dat(a, 1, S3D_000, "double", OPS_WRITE),
             ops_arg_dat(b, 1, S3D_000, "double", OPS_WRITE),
             ops_arg_dat(c, 1, S3D_000, "double", OPS_WRITE),
             ops_arg_dat(d, 1, S3D_000, "double", OPS_WRITE),
ops_arg_idx());
ops_tridMultiDimBatch_Inc(3, 0, size, a, b, c, d, ux, trid_ctx);
```

- It is better not to repeat all these sentence and arguments for each terms

Design and implementation

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- Combine the power of Python and a little more abstraction from C/C++ and OPS

In this case, we propose a general C/C++ function template to make codes more concise. Otherswise, it will leads to much longer codes than typical explicit schemes

- No interference on existing codes following OOP principle

  The existing applications should be run without problem

- Consider future requirements while implementing using simple problems

Linear solver class

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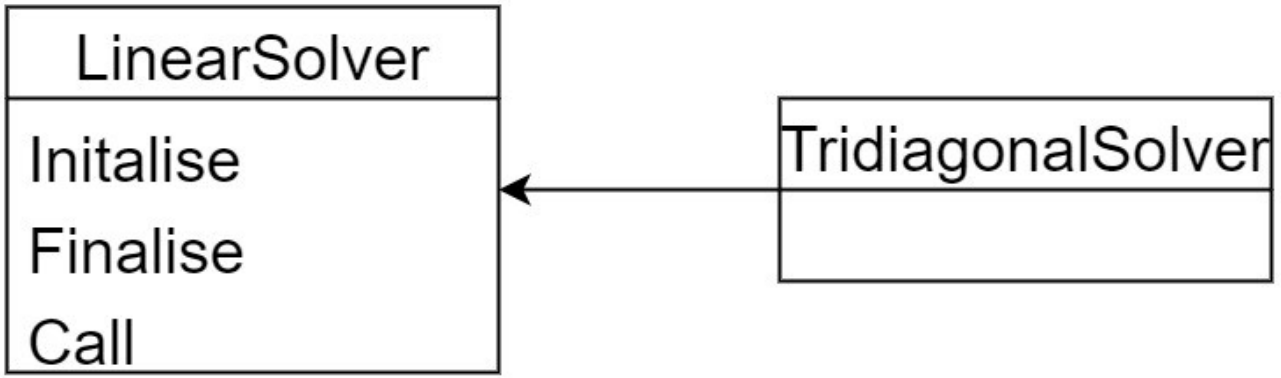

For generating code to initialise, finalise and call linear algebra solver

Compact class

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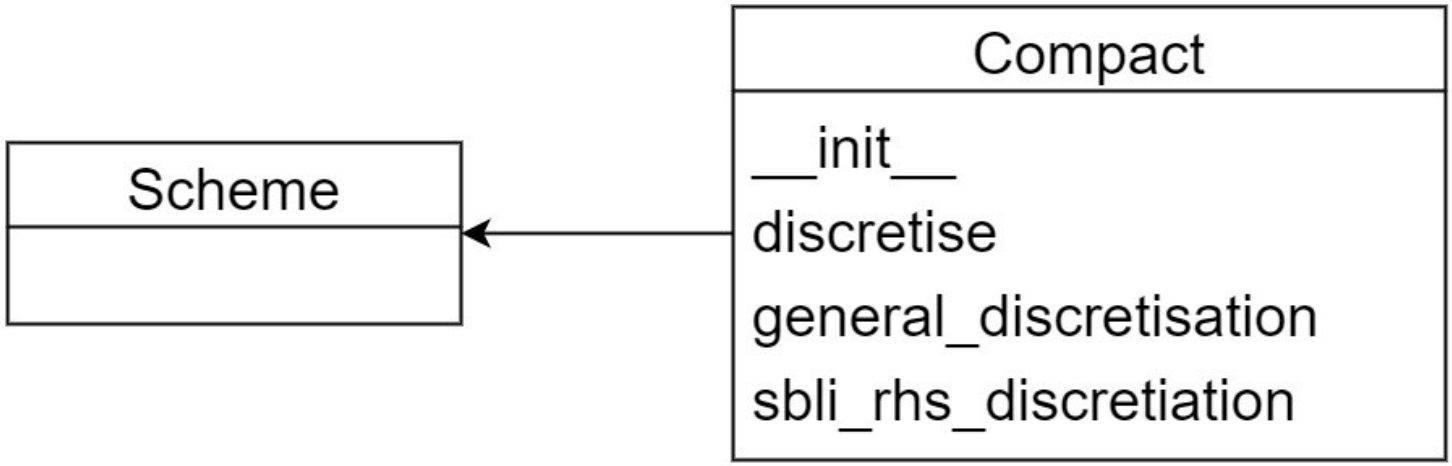

To use the compact scheme to discrete derivatives.

OPSCCompact class

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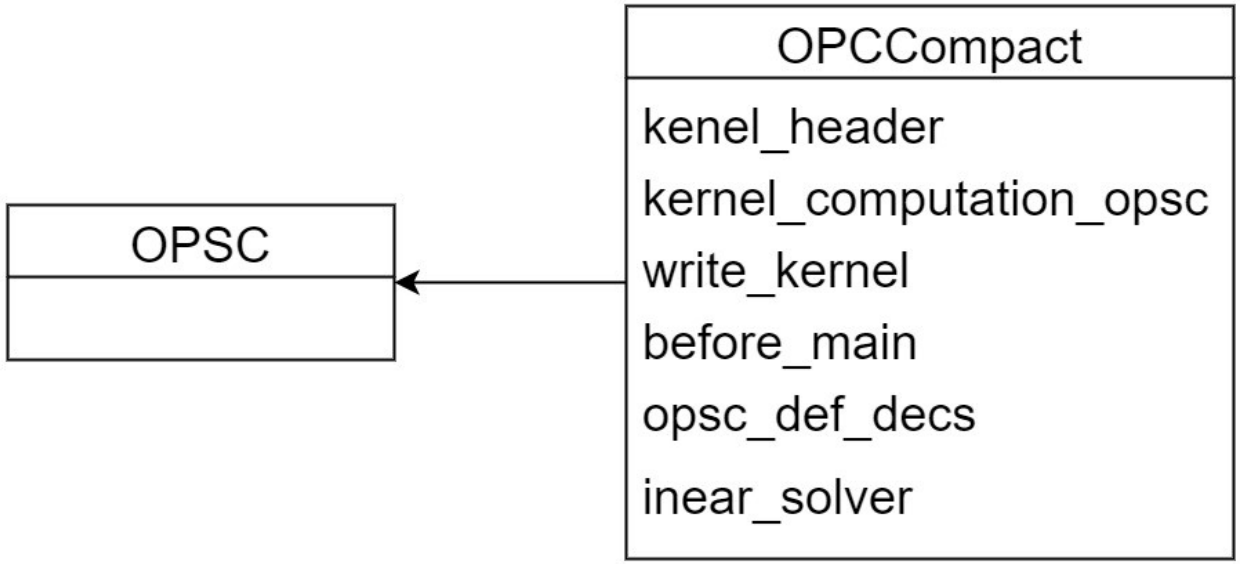

To geneate the framework of the main source file

Implicit kernel, CR, and algorithm

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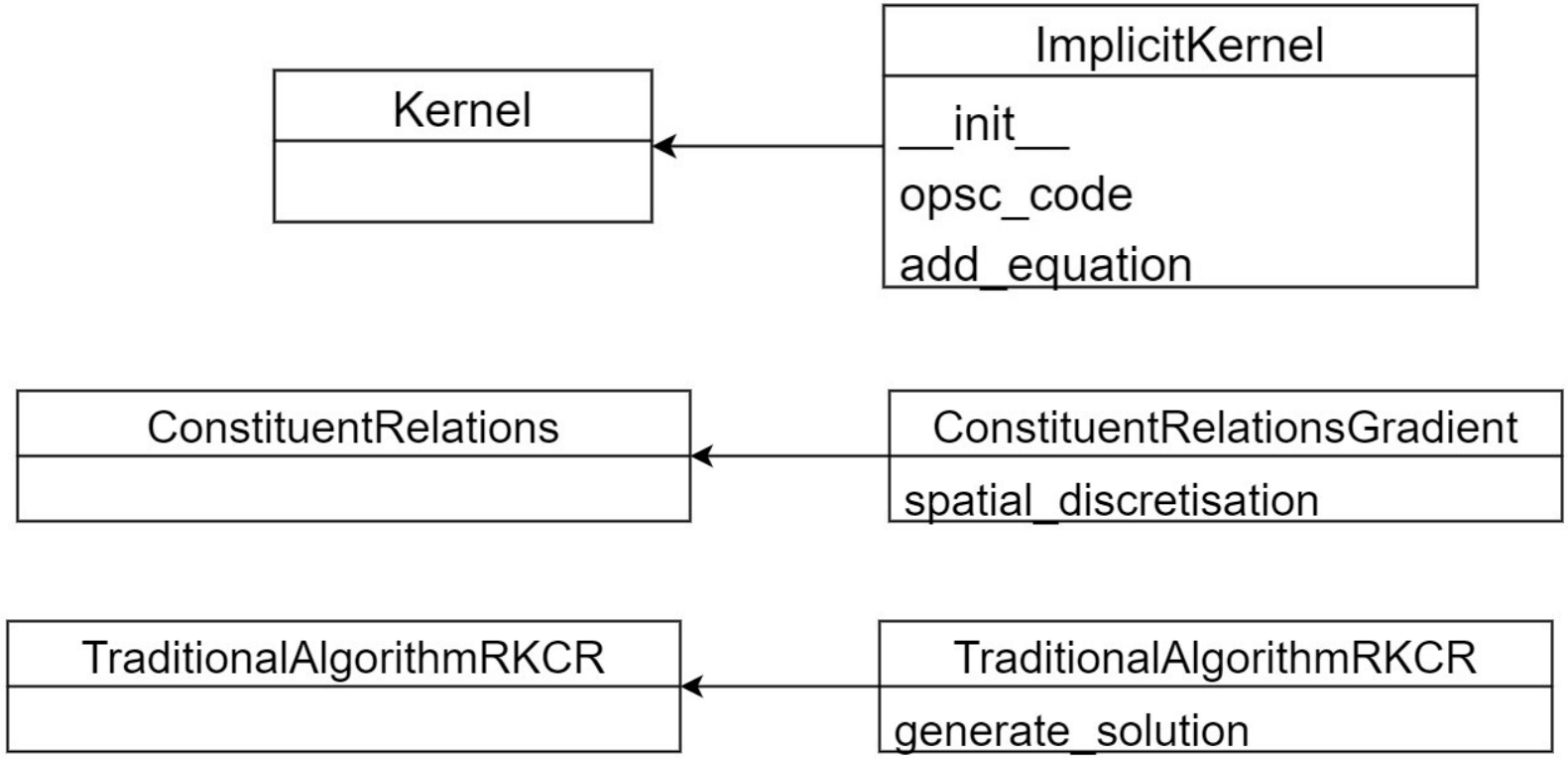

One-dimensional wave equation

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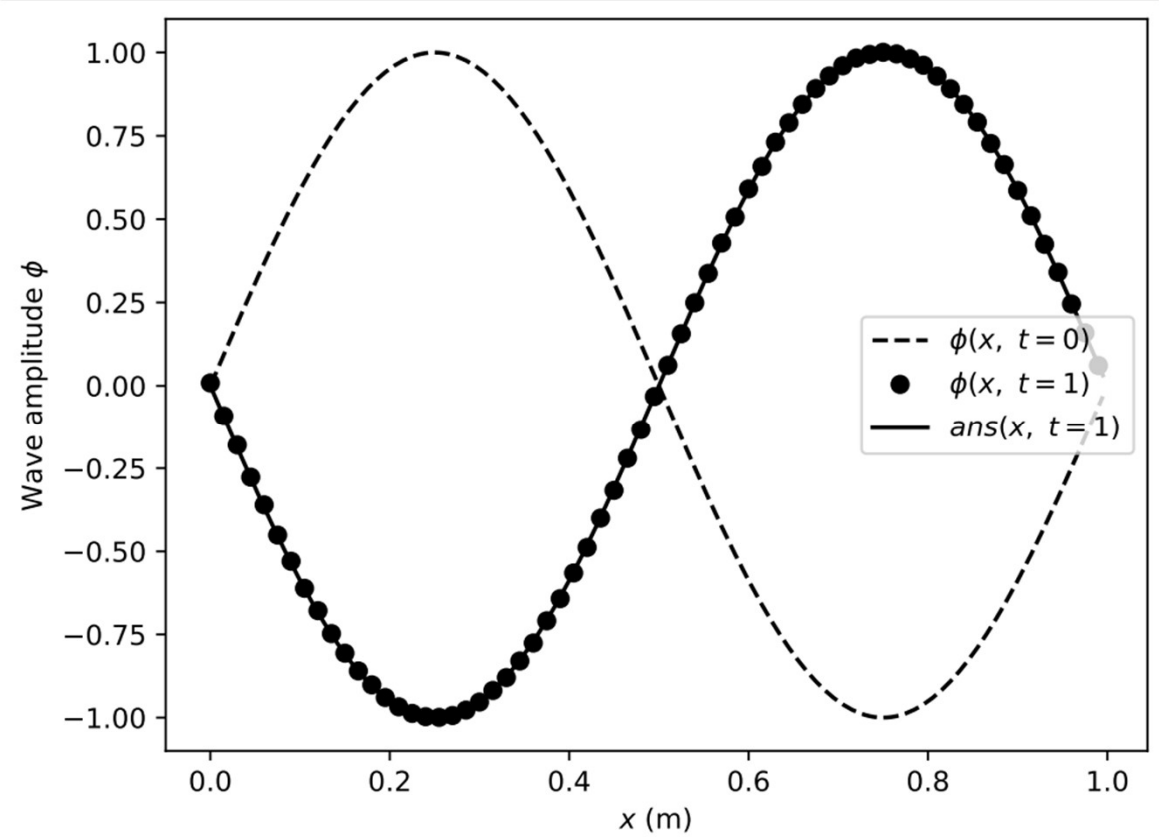
$$\frac{\partial \phi}{\partial t} = -c\frac{\partial \phi}{\partial x}$$

$$\phi|_{t=0} = \sin(2\pi x)$$

Generated code successfully run on both GPU and CPU



Taylor - Green vortex

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- Lead to shorter source code
- The source code looks correct by comparing with those of the central differencing schemes
- The codes compiles without problem.
- Further numerical tests are under way (after we investigate the proper periodic boundary or other alternatives.)

	Main	kernel
Central	651	727
Compact	798	461

```
void CompactDifference4thX1st(ops_block& block, ops_dat& u, ops_dat& a,
                              ops_dat& b, ops_dat& c, ops_dat& d, ops_dat& ux,
                              ops_tridsolver_params* trid, double delta,
                              int layer = 0) {
  int* size{u->size};
  int* dm{u->d_m};
  int* dp{u->d_p};
  int spaceDim{block->dims};
  int* tridSize{new int[spaceDim]};
  for (int i = 0; i < spaceDim; i++) {
    tridSize[i] = size[i] - dp[i] + dm[i];
  };
  int* iterRange{new int[2 * spaceDim]};
  for (int i = 0; i < spaceDim; i++) {
    iterRange[2 * i] = -layer;
    iterRange[2 * i + 1] = size[0] + layer;
  };
  ops_par_loop(PreprocessX4thCompact1st, "preprocessX", block, 1, iterRange,
               ops_arg_dat(u, 1, neighbor_stencil, "double", OPS_READ),
               ops_arg_dat(a, 1, local_stencil, "double", OPS_WRITE),
               ops_arg_dat(b, 1, local_stencil, "double", OPS_WRITE),
               ops_arg_dat(c, 1, local_stencil, "double", OPS_WRITE),
               ops_arg_dat(d, 1, local_stencil, "double", OPS_WRITE),
               ops_arg_dat(ux, 1, local_stencil, "double", OPS_WRITE),
               ops_arg_idx(), ops_arg_gbl(&size[0], 1, "int", OPS_READ),
               ops_arg_gbl(&layer, 1, "int", OPS_READ),
               ops_arg_gbl(&delta, 1, "double", OPS_READ));
  ops_tridMultiDimBatch_Inc(spaceDim, 0, tridSize, a, b, c, d, ux, trid);
  delete[] iterRange;
  delete[] tridSize;
}
```

```
for (int stage = 0; stage <= 2; stage++) {
    CompactDifference4thX1st(opensbliblock00, phi_B0, a, b, c, d, wk0_B0,
                             trid_at_opensbliblock000, Delta0block0, 0);
    int iteration_range_4_block0[] = {0, block0np0};
    ops_par_loop(opensbliblock00Kernel004, "Convective residual ",
                 opensbliblock00, 1, iteration_range_4_block0,
                 ops_arg_dat(wk0_B0, 1, stencil_0_00, "double", OPS_READ),
                 ops_arg_dat(Residual_TimeDer_phi_B0_t_B0, 1, stencil_0_00,
                             "double", OPS_WRITE));

    int iteration_range_9_block0[] = {0, block0np0};
    ops_par_loop(
        opensbliblock00Kernel009, "Sub stage advancement", opensbliblock00, 1,
        iteration_range_9_block0,
        ops_arg_dat(Residual_TimeDer_phi_B0_t_B0, 1, stencil_0_00, "double",
                    OPS_READ),
        ops_arg_dat(phi_RKold_B0, 1, stencil_0_00, "double", OPS_READ),
        ops_arg_dat(phi_B0, 1, stencil_0_00, "double", OPS_WRITE),
        ops_arg_gbl(&rknew[stage], 1, "double", OPS_READ));

    int iteration_range_8_block0[] = {0, block0np0};
    ops_par_loop(opensbliblock00Kernel008, "Temporal solution advancement",
                 opensbliblock00, 1, iteration_range_8_block0,
                 ops_arg_dat(Residual_TimeDer_phi_B0_t_B0, 1, stencil_0_00,
                             "double", OPS_READ),
                 ops_arg_dat(phi_RKold_B0, 1, stencil_0_00, "double", OPS_RW),
                 ops_arg_gbl(&rkold[stage], 1, "double", OPS_READ));

    ops_halo_transfer(exchange5_block0);
    ops_halo_transfer(exchange6_block0);
  }
```

Slice capability for OPS and OpenSBLI

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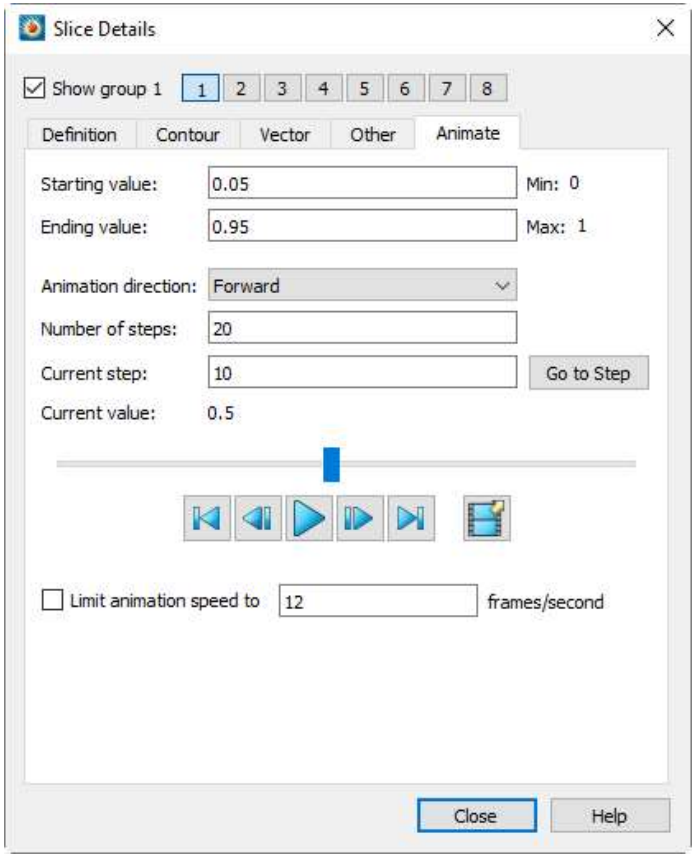
Motivation

- Always writing out 3D data is very expensive
- Often we would like to focus at a few planes
- Users from NASA, JAXA… requested

Desired capabilities

- Writing out a plane (say I=20)
- Writing out arbitrary selection of data
- Organised the slices in a specified structure

HDF5 files can be directly imported into Matlab, Python (h5py), Julia(HDF5), TecPlot, Visit and Paraview with a little more works (or convert to VTK)



Slice capability for OPS and OpenSBLI

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```
void ops_write_plane_hdf5(const ops_dat dat, const int cross_section_dir,
                          const int pos, char const *file_name,
                          const char *data_name);
```

Writ data of a plane specified by cross_section_dir, pos
data_name="block/time/rho" – HDF5 convention for making data structure where data are stored under block and time group
data_name="block_time_rho" – data stored at the root
Data dimension will be reduced by one

```
void ops_write_data_slab_hdf5(const ops_dat dat, const int
                              const char *file_name, const
```

Write data of an arbitrary slab specified by the range array

```
void ops_write_plane_group_hdf5(
    const std::vector<std::pair<int, int>> &planes, const s
    const std::vector<std::vector<ops_dat>> &data_list);

ops_write_plane_group_hdf5({{1, 16}, {0, 1}, {2, 16}}, "2",
                           {{u, v}, {u, v}, {u, v}});
```

```
1  I1=h5open("I1.h5","r")
[6]  0.3s
HDF5.File: (read-only) I1.h5
slice3Du
  1
    u
  2
    u
slice3Dv
  1
    v
  2
    v
```

Slice capability for OPS and OpenSBLI

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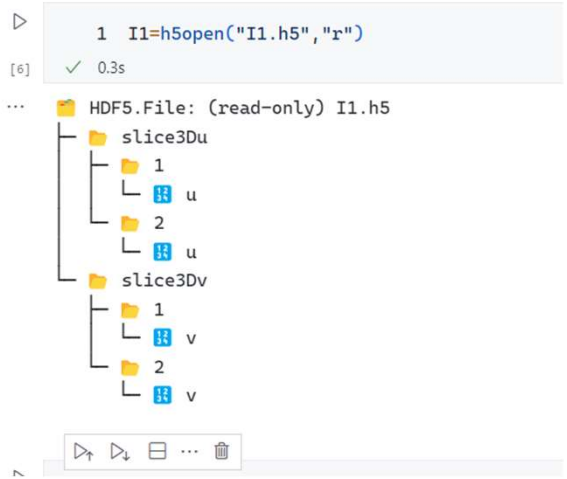
Archer2
Two-block mini-application
1024^3
Block 1: slice3Du
Block 2: slice3Dv

	128	256	512
1	8.94	14.49	21.87
2	9.6	17.97	20.56
3	12.06	14.74	21.29
avg	10.2	15.73	21.24

	128	256	512
1	2.7	5.42	3.63
2	2.9	3.23	4.17
3	2.68	3.78	7.78
avg	2.76	4.14	5.19

Bede2
Two-block mini-application
512^3
Block 1: slice3Du
Block 2: slice3Dv

4 nodes with 16 GPUS (NVIDIA V100)
First: 0.78
Second: 0.52



Concluding remarks

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- Lead to shorter source code for the TGV case
- The source code for the TGV case looks correct by comparing with the central differencing one.
- The implementation of slice HDF5 output
- Testing more cases and looking at performance including the ARM system

Thanks and Questions?