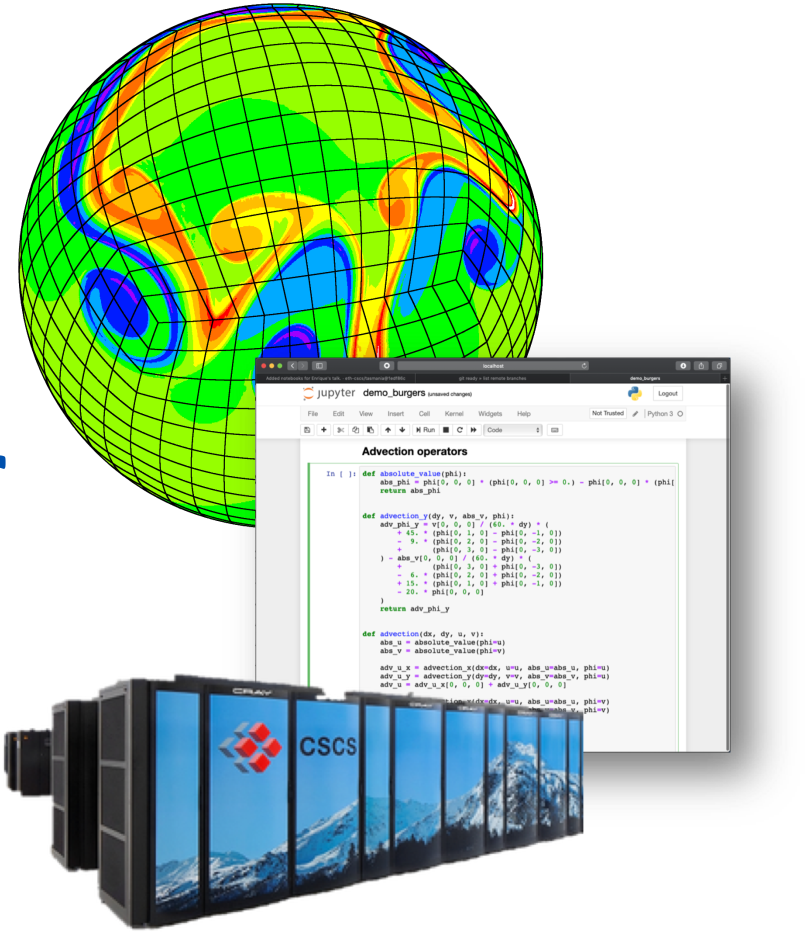
High Performance Computing for Weather and Climate (HPC4WC)

Content: High-Level Programming
Lecturer: Stefano Ubbiali
Block course 701-1270-00L
Summer 2020



Learning Goals

- Learning what a domain-specific language (DSL) is.
- Understanding how a DSL helps in writing hardware-agnostic, maintainable code without sacrificing performance.
- Be able to apply a DSL to a stencil program from a weather and climate model.

Typical Workflow

solver.py

```
import numpy as np
```

Fast prototyping in Python (or MATLAB)

solver.cpp

```
#include <vector>
```

Naïve implementation in a compiled language (e.g. C++)

solver_omp.cpp

```
#pragma omp parallel
```

Multi-threaded version using OpenMP

solver_mpi.cpp

```
MPI_Init(&argc, &argv);
```

Going multi-node with MPI (possibly blended with OpenMP)

solver.cu

```
cudaMalloc(&d_x, …));
```

CUDA version for impressive single-node performance

solver_mpi.cu

```
MPI_Recv(d_x, …);
```

CUDA-aware MPI: getting the best out of Piz Daint

Why is this approach problematic?

Possible Scenarios

What if …

1. … we want to introduce a modification at the algorithmic/numerical level?

2. … our application has a broad user community and it must run efficiently on a variety of platforms?

3. … our code consists of thousands (if not millions) LOC?

The explosion of hardware architectures made this development model obsolete!

A Real-Case Example : COSMO

- Limited-area model developed by the **Co**nsortium for **S**mall-Scale **Mo**deling.
- Run operationally by 7 national weather services and used by several academic institutions as a research tool.
- Two target architectures: CPUs and GPUs.
- Around 330K lines of F90 code and 90K lines of C/C++ code.
- Cost of porting the full code base to GPU: approx. 20-30 Man-Years!

Separation of Concerns

Domain expert	Performance expert
Answer scientific research questions	Write optimized code for target platform
Declarative programming style: Focus on **what** you want to do	Imperative programming style: Focus on **how** to do it
Common data access interface: e.g. `data[i, j, k]`	Storage and memory allocation: e.g. C-layout vs F-layout
Computation kernels: Calculations for a single grid point	Control structure (e.g. for loops): Optimized data traversal
Individual operators (“grains”)	Final computation: Detect and exploit parallelism b/w grains

Overarching Goals

- Single **hardware-agnostic** application code.
- Easy to implement.
- Easy to **read**.
- Easy to **maintain**.
- **Performance portable**.

Domain Specific Languages (DSLs)

- Programming language tailored for a specific class of problems.
- Higher level of abstraction w.r.t. a general purpose language.
- Intended to be used by domain experts, who may not be fluent in programming.
- Abstractions and notations much aligned to concepts and rules from the domain.
- Some examples:
  - Machine Learning: TensorFlow (Keras)
  - Scientific Computing: Kokkos, FEniCS, FreeFEM
  - Fluid Dynamics: OpenFOAM
  - Image Processing: Halide
  - Stencils: Ebb, Taichi, GT4Py

GT4Py

- High-performance implementation of a stencil kernel from a high-level definition.
- GT4Py is a domain specific **library** which exposes a domain specific **language** (GTScript) to express the stencil logic.
- GTScript is embedded in Python (**eDSL**).
  - Legal Python syntax and (almost) legal Python semantics.
- GT4Py = **G**rid**T**ools **For P**ython
  - Harnessing the C++ GridTools ecosystem to generate native implementations of the stencils.
- Emphasis on tight integration with scientific Python stack.

Definitions Function

```python
import gt4py as gt
from gt4py.gtscript import Field, PARALLEL, computation, interval
import numpy as np

f64 = np.float64

def laplacian_defs(in_field: Field[f64], out_field: Field[f64]):
    with computation(PARALLEL), interval(...):
        out_field = (
            - 4. * in_field[ 0,  0, 0]
            +      in_field[-1,  0, 0]
            +      in_field[+1,  0, 0]
            +      in_field[ 0, -1, 0]
            +      in_field[ 0, +1, 0] )
```

Regular (named) function

Definitions Function

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```

Input and output fields
(object-oriented interface)

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            +      in_field[ 0, +1, 0] )
```

Field descriptors
as type annotations

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```

Any computation must be wrapped in a `with` construct which can be thought of as being a k-loop

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```

Iteration order in the vertical direction : PARALLEL, FORWARD, BACKWARD

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            +      in_field[+1,  0, 0]
            +      in_field[ 0, -1, 0]
            +      in_field[ 0, +1, 0] )
```

Vertical region of application:
... = full column

Definitions Function

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```

Each statement (or **stage**) can be thought of as an ij-loop

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            +      in_field[ 0, +1, 0] )
```

Neighboring points accessed through offsets

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            +      in_field[ 0, -1, 0]
            +      in_field[ 0, +1, 0] )
```

1st horizontal dimension

2nd horizontal dimension

Vertical dimension

Neighboring points accessed through offsets

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import gt4py as gt
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def laplacian_defs(in_field: Field[f64], out_field: Field[f64]):
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            +      in_field[ 0, -1, 0]
            +      in_field[ 0, +1, 0] )
```

No for loops!
No return statement!

Compilation

- A stencil needs to be compiled for a given **backend**:

```
backend = "gtx86"
laplacian = gt.stencil(backend, laplacian_defs)
```

- Available backends:
  - Python: `"debug"` (for loops), `"numpy"` (vectorized syntax);
  - C++: `"gtx86"` (x86), `"gtmc"` (MIC), `"gtcuda"` (NVIDIA GPU).

- For GT-based backends, compilation consists of three steps:
  1) Generate optimized code for the target architecture.
  2) Compile the automatically generated code.
  3) Build Python bindings to that code.

Storages

- The compilation returns a callable object which can be invoked on GT4Py storages.
- Storages have optimal memory **strides**, **alignment** and **padding**.
- `gt.storage` provides functionalities to allocate storages …

```
nx, ny, nz = 128, 128, 64
def_orig = (1, 1, 0)
out_field = gt.storage.zeros(
    backend, def_orig, (nx, ny, nz), dtype=f64 )
```

… and convert NumPy arrays into valid storages:

```
in_field = gt.storage.from_array(
    np.randon.rand(nx, ny, nz), backend, def_orig, dtype=f64 )
```

Storages

- Storages can be accessed as NumPy arrays:

```
in_field[0, 0, 0] = 4.
print(in_field[0, 0, 0])
```

Running

- Running computations is as simple as a function call:

```
laplacian(
    in_field=in_field,
    out_field=out_field,
    origin=(1, 1, 0),
    domain=(nx - 2, ny - 2, nz)
)
```

Bindings b/w the symbols used within the definitions fct. and the arrays holding the data

Running

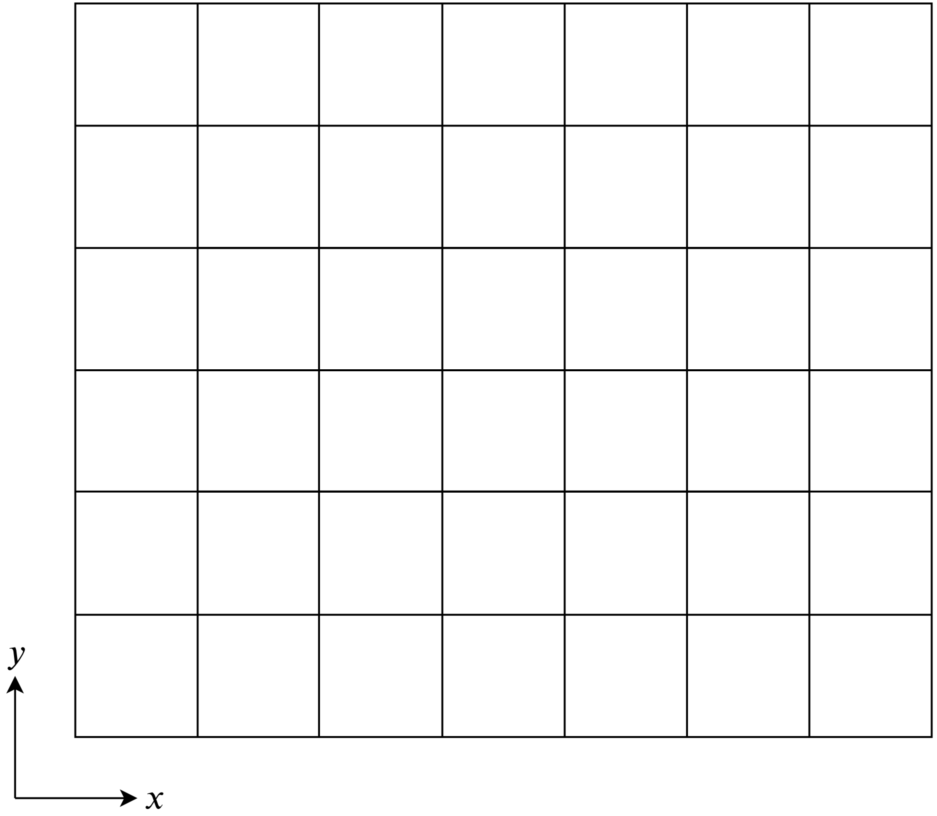
- Running computations is as simple as a function call:

```
laplacian(
    in_field=in_field,
    out_field=out_field,
    origin=(1, 1, 0),
    domain=(nx - 2, ny - 2, nz)
)
```

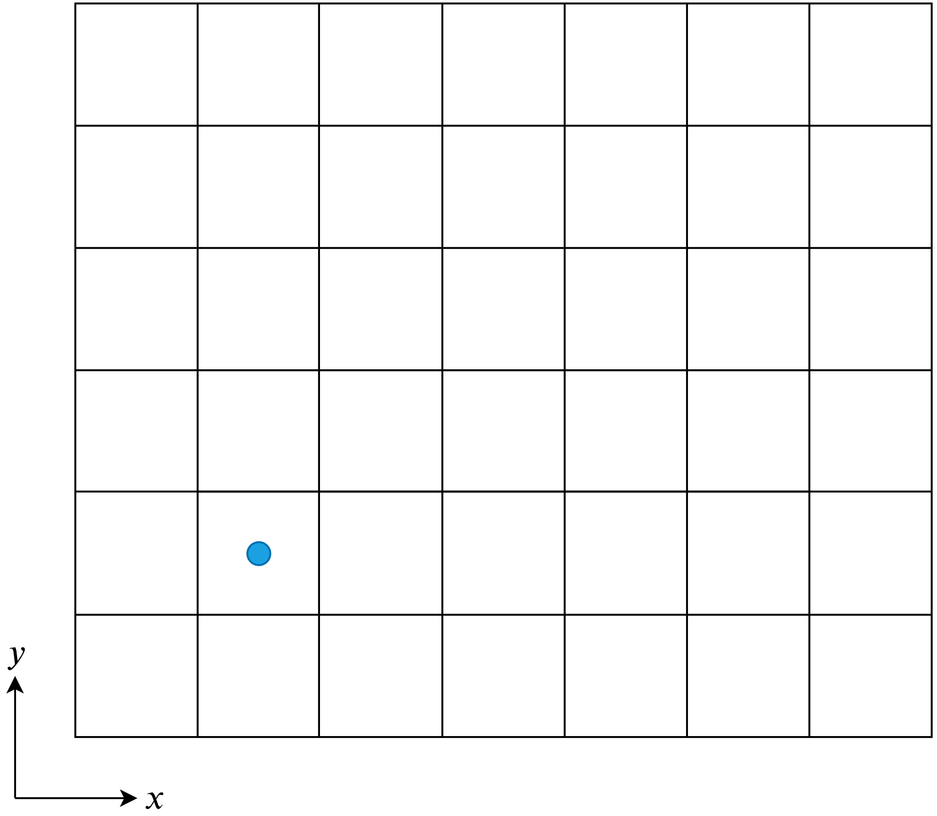
Origin and extent of the computation domain

- `out_field` now contains the results of the computation.

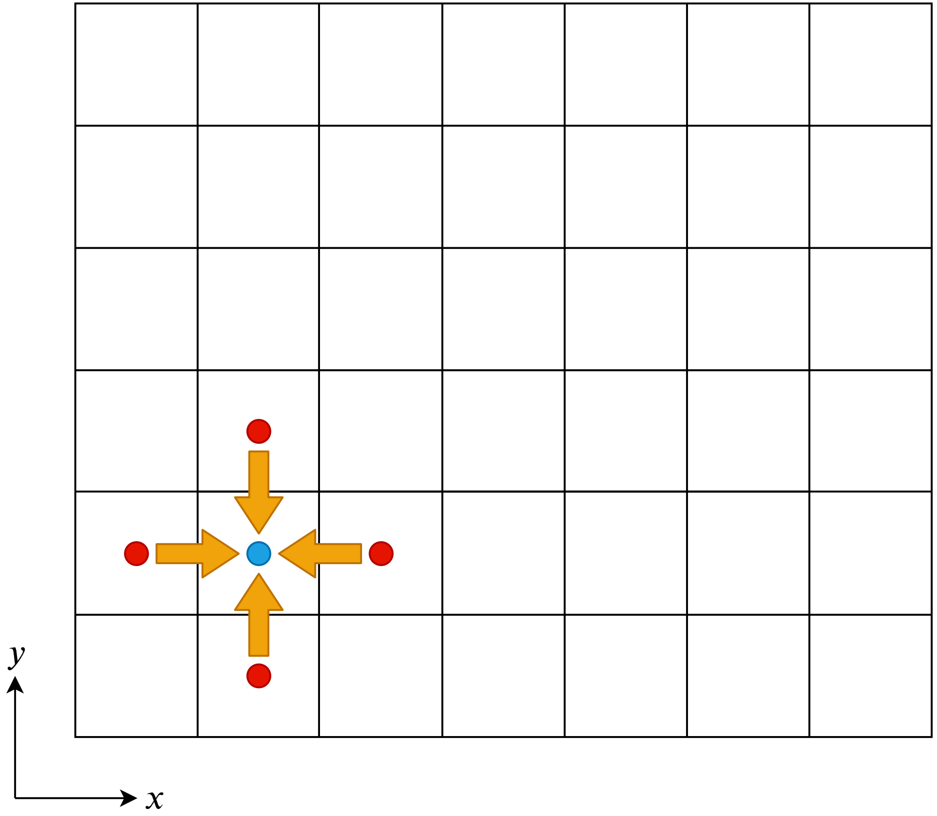
Region of application



Region of application



Region of application



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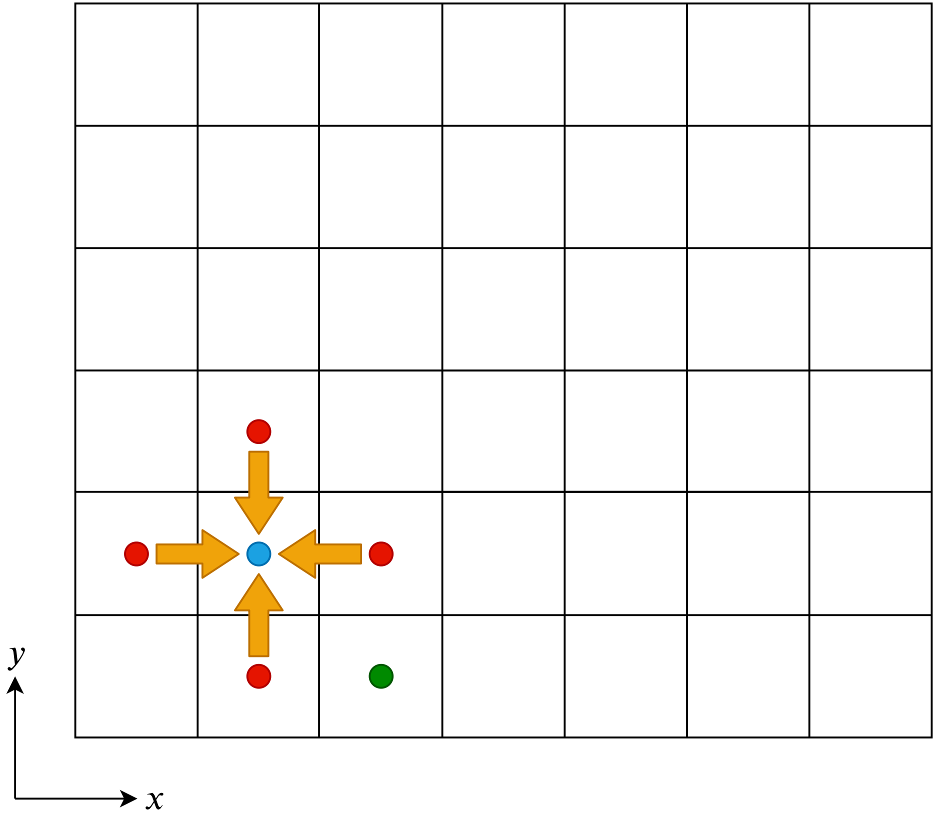
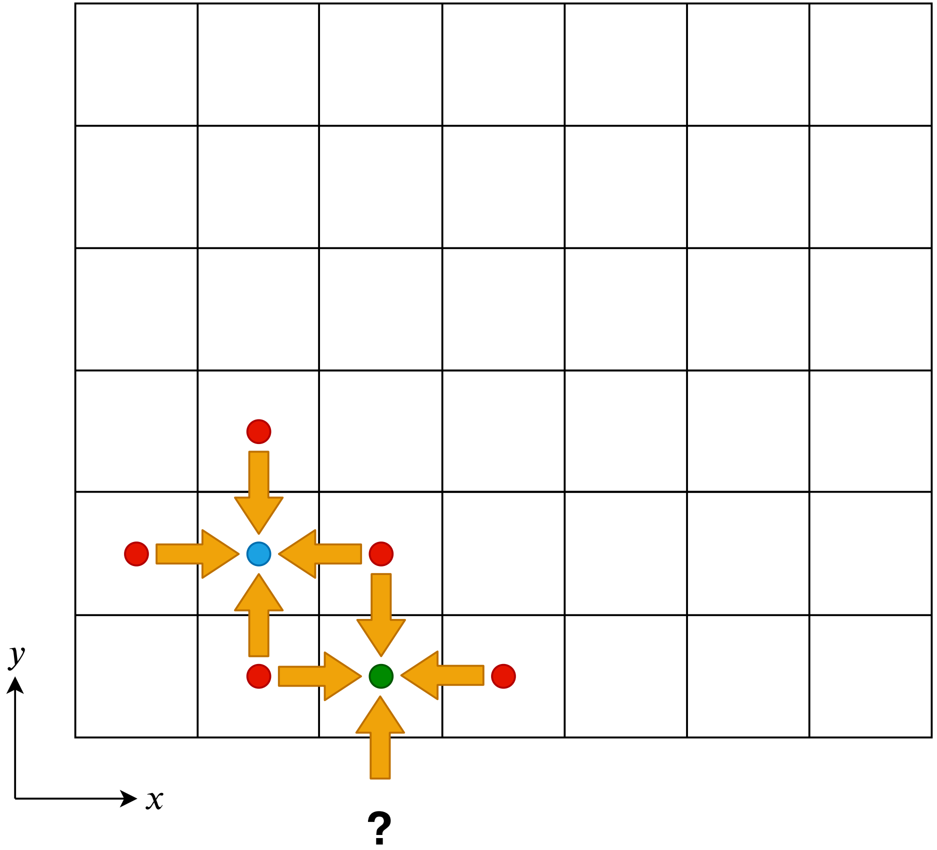
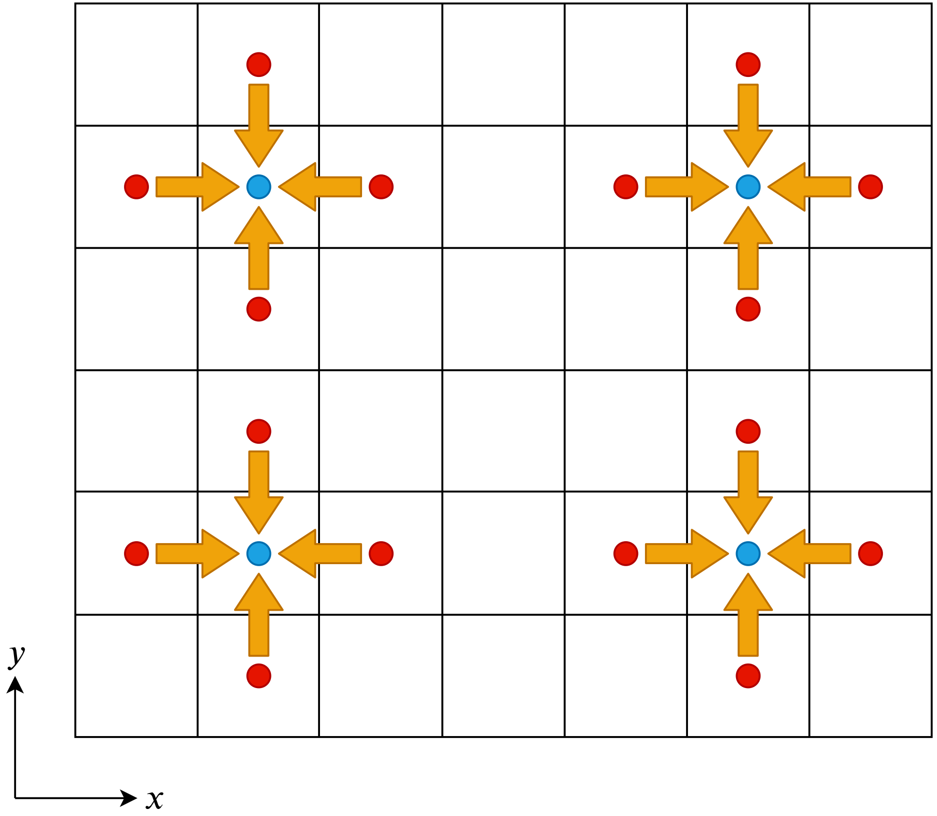


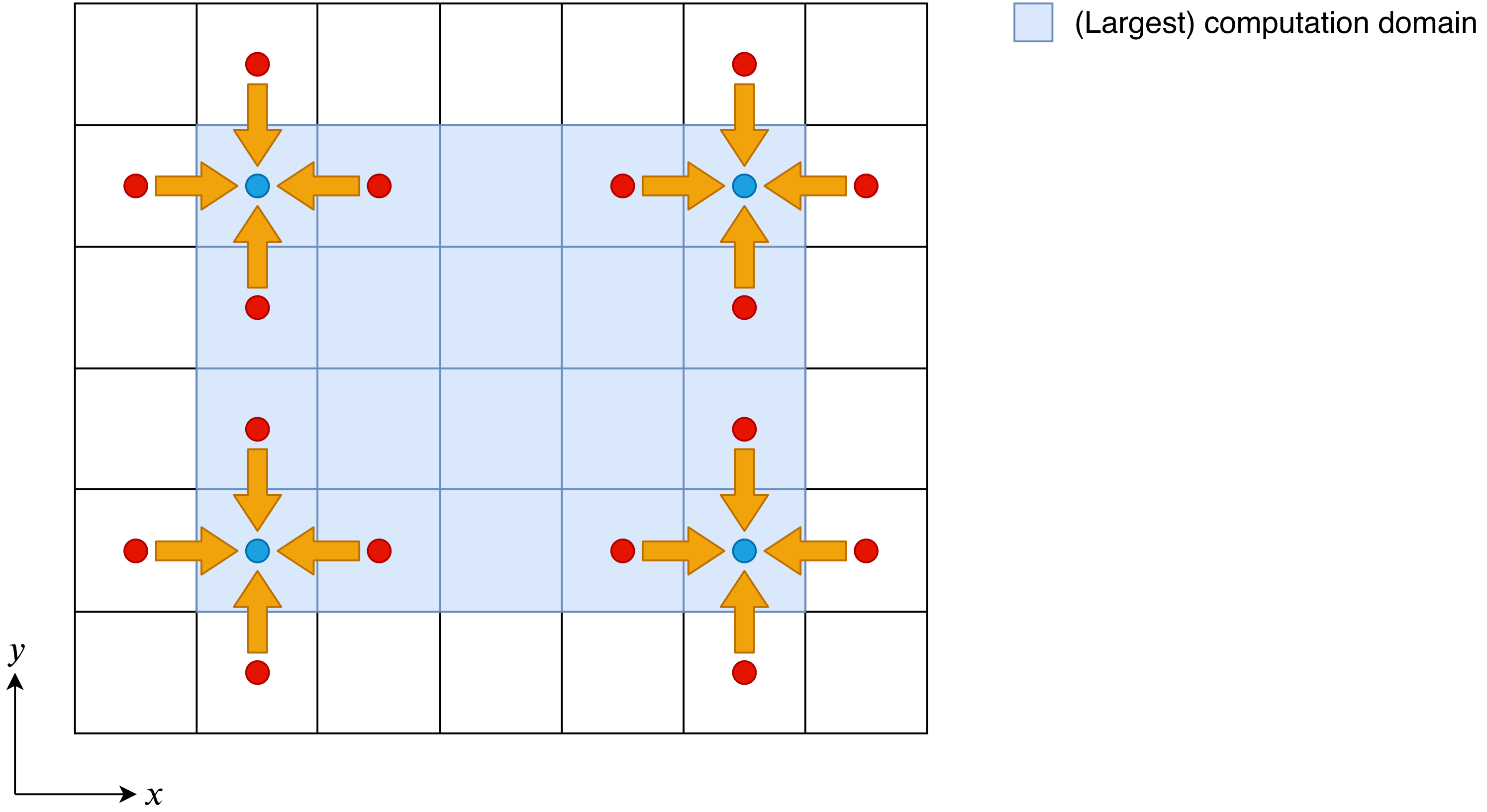
Region of application



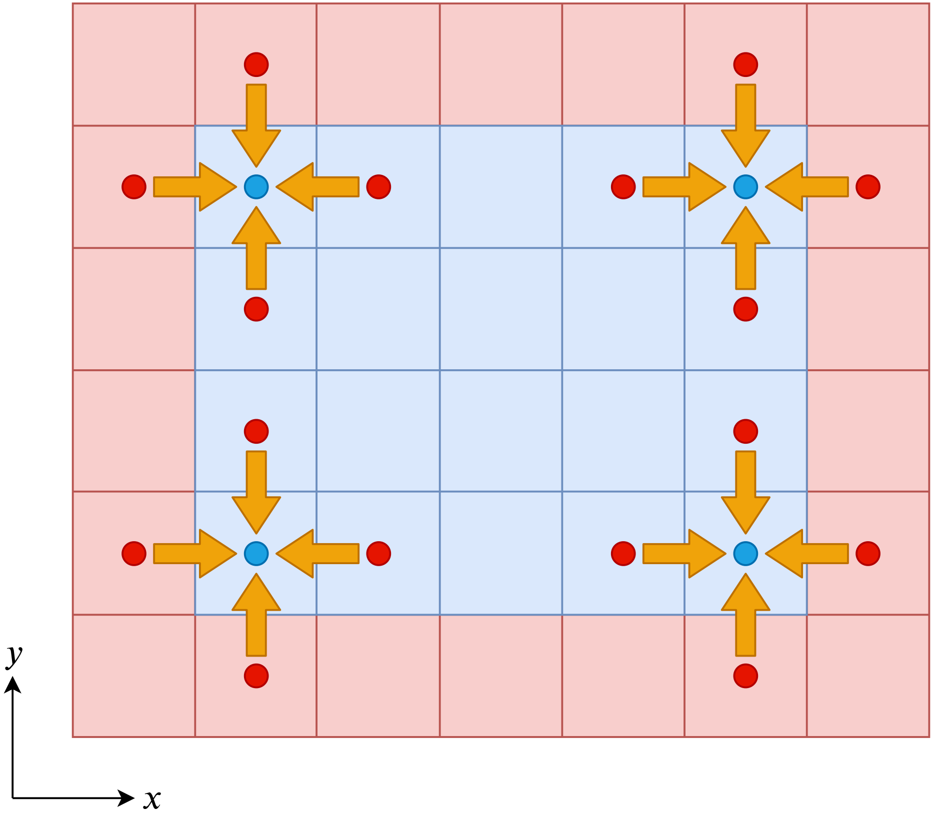
Region of application



Region of application



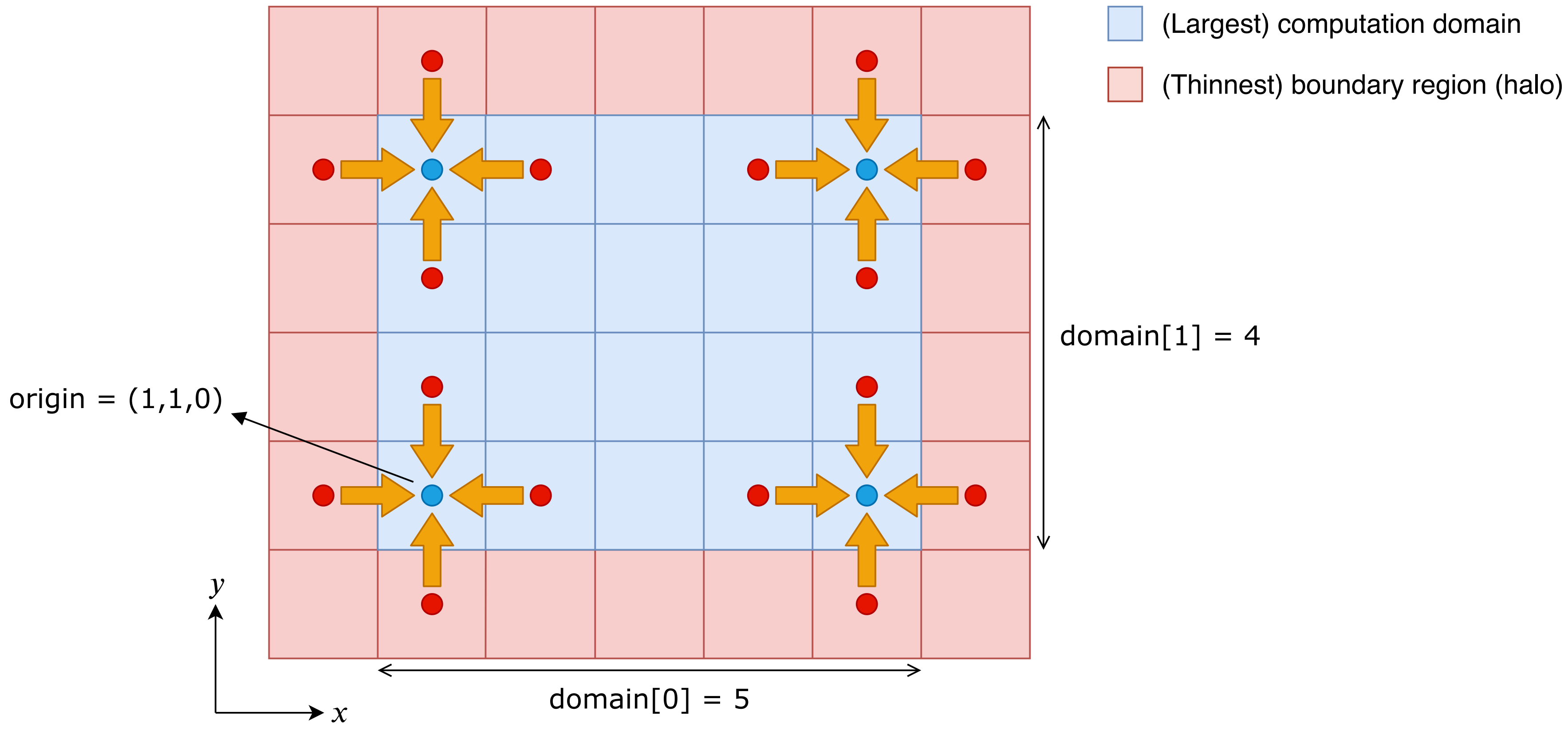
Region of application



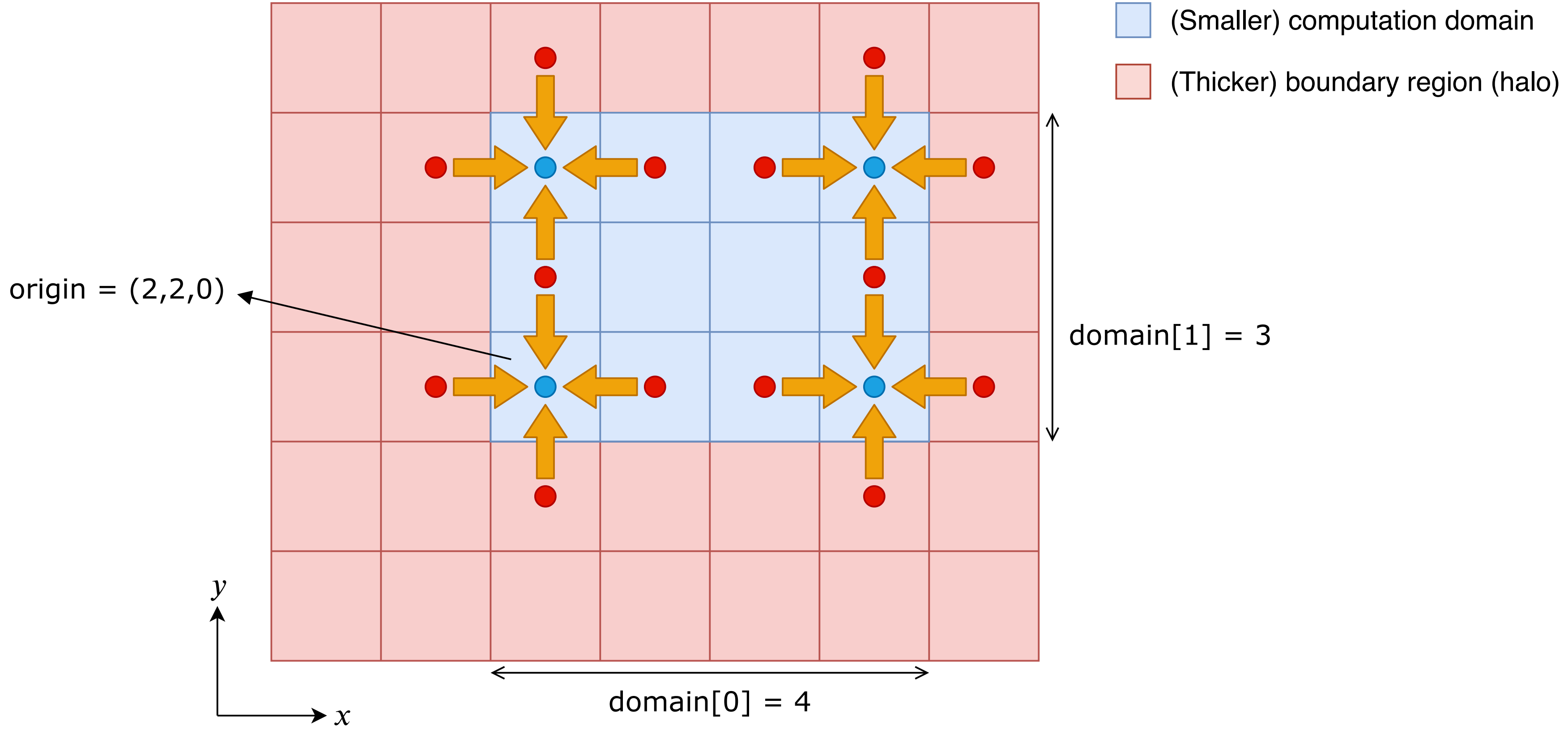
(Largest) computation domain

(Thinnest) boundary region (halo)

Region of application



Region of application



Disadvantages of a DSL

- Lack of generality: A DSL is not a complete ontology!
- Debugging on the generated code.
- Cost of developing and maintaining the DSL compiler toolchain.

Conclusions

- High-level programming techniques hide the complexities of the underlying architecture to the end user.
- DSL allows to target multiple platforms without polluting the application code with hardware-specific boilerplate code.
- GT4Py is a Python framework to write performance portable applications in the weather and climate area. It ships with a DSL to write stencil computations.

Lab Exercises

01-GT4Py-sumdiff.ipynb

- Compare NumPy, CuPy and GT4Py on the sum-diff stencil (demo).

02-GT4Py-laplacian.ipynb

- Compare NumPy, CuPy and GT4Py on the Laplacian stencil (demo).

03-GT4Py-concepts.ipynb

- Digest the main concepts of GT4Py.
- Get familiar with writing, compiling and running stencils.
- Get insights on the internal data-layout of the storages.

04-GT4Py-stencil2d.ipynb

- Step-by-step porting of stencil2d.py to GT4Py.
- Write two alternative versions of stencil2d-gt4py-v0.py

Before Starting

1. Pull the latest commit from the Github repo.

2. Make sure that your `.jupyterhub.env` contains the following lines:

```
module load Boost
module load cudatoolkit
NVCC_PATH=$(which nvcc)
CUDA_PATH=$(echo $NVCC_PATH | sed -e "s/\/bin\/nvcc//g")
export CUDA_HOME=$CUDA_PATH
export LD_LIBRARY_PATH=$CUDA_PATH/lib64:$LD_LIBRARY_PATH
```

After updating your `.jupyterhub.env` from a terminal (see Oli's post in #general): terminate the JupyterLab session and fire up a new one.

Have fun with GT4Py!

References

Broad introduction to DSLs:
https://www.jetbrains.com/mps/concepts/domain-specific-languages/

Designing APIs - The Case of GridTools (M. Bianco):
https://www.youtube.com/watch?v=IzWxgFcJFdk&list=PL1tk5lGm7zvQOXi24s586pwDF_yseZ-80&index=7
https://www.youtube.com/watch?v=2tCVOkbediU&list=PL1tk5lGm7zvQOXi24s586pwDF_yseZ-80&index=9

GT repo: https://github.com/GridTools

GT4Py repo: https://github.com/GridTools/gt4py