# High Performance Computing for Weather and Climate (HPC4WC)

Content: High-Level Programming
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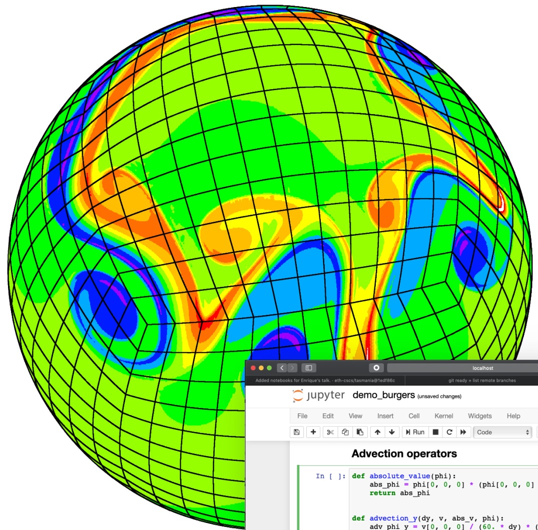
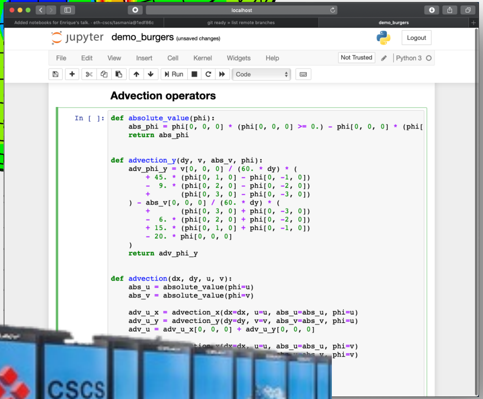
Block course 701-1270-00L
Summer 2024



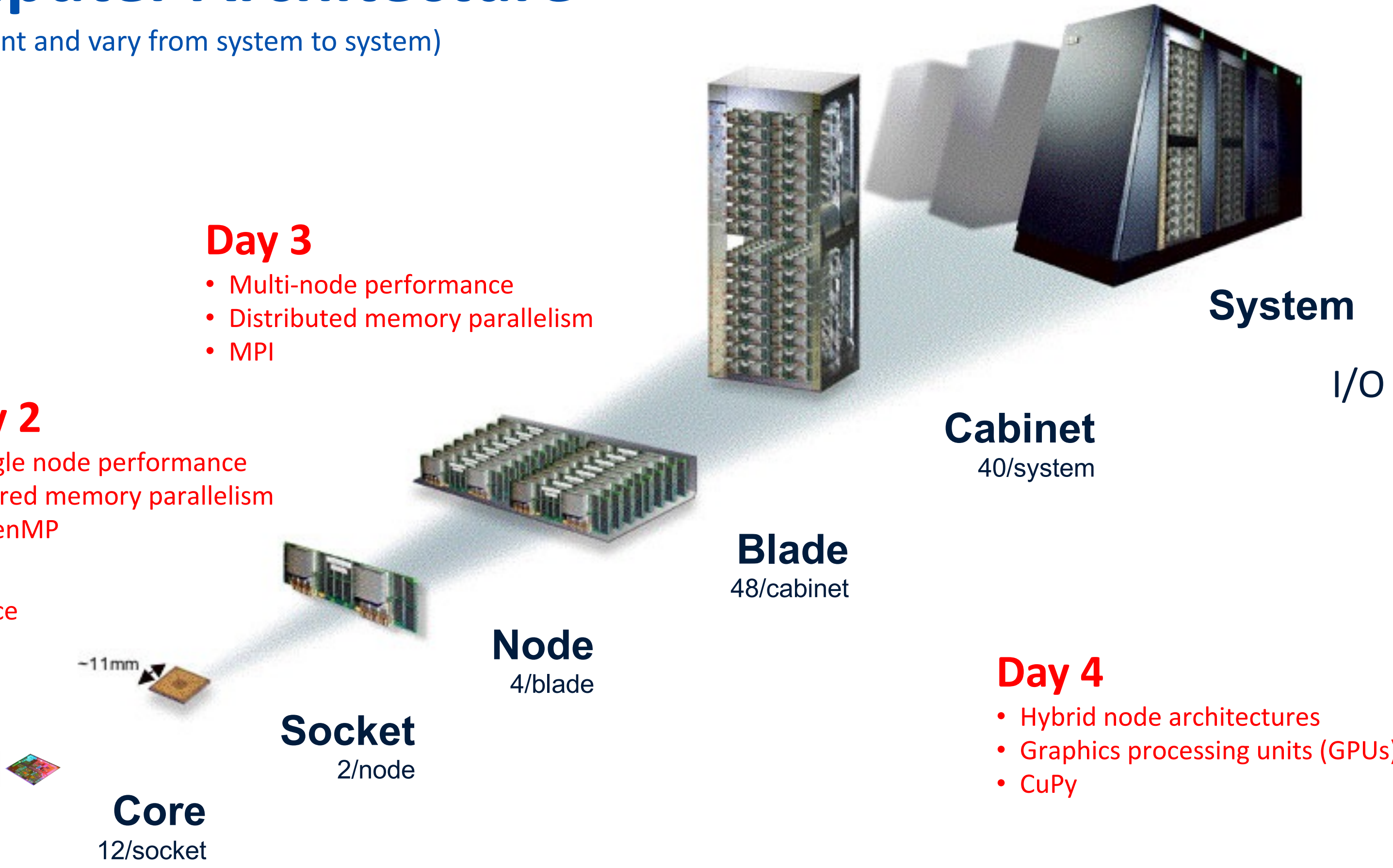

jupyter demo_burgers (unsaved changes)
Logout
File Edit View Insert Cell Kernel Widgets Help
Not Trusted
Python 3
Run
Code

Advection operators

```
In [ ]: def absolute_value(phi):
            abs_phi = phi[0, 0, 0] * (phi[0, 0, 0] >= 0.) - phi[0, 0, 0] * (phi[
            return abs_phi


        def advection_y(dy, v, abs_v, phi):
            adv_phi_y = v[0, 0, 0] / (60. * dy) * (
                + 45. * (phi[0, 1, 0] - phi[0, -1, 0])
                -  9. * (phi[0, 2, 0] - phi[0, -2, 0])
                +       (phi[0, 3, 0] - phi[0, -3, 0])
            ) - abs_v[0, 0, 0] / (60. * dy) * (
                +       (phi[0, 3, 0] + phi[0, -3, 0])
                -  6. * (phi[0, 2, 0] + phi[0, -2, 0])
                + 15. * (phi[0, 1, 0] + phi[0, -1, 0])
                - 20. * phi[0, 0, 0]
            )
            return adv_phi_y


        def advection(dx, dy, u, v):
            abs_u = absolute_value(phi=u)
            abs_v = absolute_value(phi=v)

            adv_u_x = advection_x(dx=dx, u=u, abs_u=abs_u, phi=u)
            adv_u_y = advection_y(dy=dy, v=v, abs_v=abs_v, phi=u)
            adv_u = adv_u_x[0, 0, 0] + adv_u_y[0, 0, 0]

                       tion_x(dx=dx, u=u, abs_u=abs_u, phi=v)
                                                      phi=v)
```

# Supercomputer Architecture

(Numbers are for Piz Daint and vary from system to system)



**Day 3**
- Multi-node performance
- Distributed memory parallelism
- MPI

**Day 2**
- Single node performance
- Shared memory parallelism
- OpenMP

**Day 1**
- Single core performance
- Caches

**Day 4**
- Hybrid node architectures
- Graphics processing units (GPUs)
- CuPy

# Future of HPC in Weather and Climate?

## Yesterday

x86 CPU

MPI

Fortran

OpenMP

## Today

GPU

C++

Python

mpi4py

CuPy

## Tomorrow

Specialized hardware?

ASIC?

FPGA?

ML?

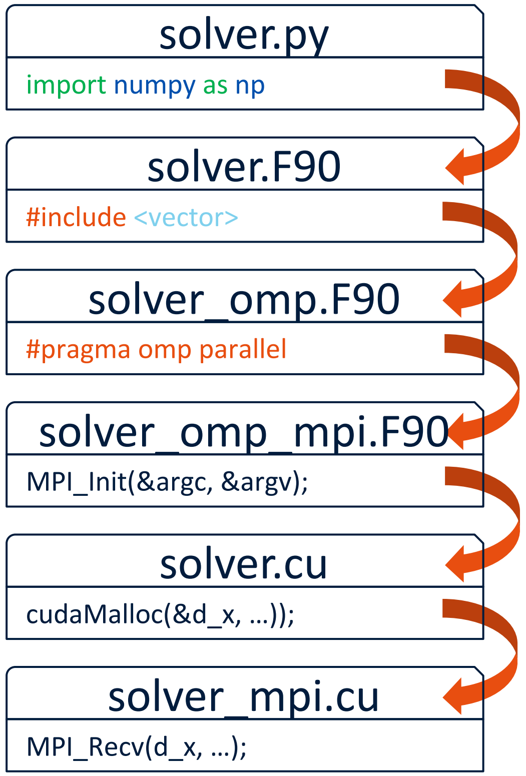
Domain-specific languages?

GT4Py?

## Learning Goals

- Understand what a domain-specific language (DSL) is.
- Understand how a DSL helps in writing hardware-agnostic and 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
```

solver.F90
```
#include <vector>
```

solver_omp.F90
```
#pragma omp parallel
```

solver_omp_mpi.F90
```
MPI_Init(&argc, &argv);
```

solver.cu
```
cudaMalloc(&d_x, …));
```

solver_mpi.cu
```
MPI_Recv(d_x, …);
```

Fast prototyping in Python (or MATLAB)

Naïve implementation in a compiled language (e.g. F90, C++)

Multi-threaded version using OpenMP

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

CUDA version for impressive single-node performance

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

## Possible Scenarios

**What if…**

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

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

…our code consists of thousands (if not millions) lines of code?

**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 8 national weather services and used by several academic institutions as a research tool.
- Three target architectures: x86 CPUs, NVIDIA GPUs and NEC vector CPUs
- Around 400K lines of F90 code and 90K lines of C/C++ code.
- Cost of porting the full code base to GPU: approx. 20-30 programmer-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 (The 3 P’s)

- **Productivity**
  Easy to implement.
  Easy to **read**.
  Easy to **maintain**.

- **Performance**
  Is **fast**.

- **Portability**
  Single **hardware-agnostic** application code.
  Runs efficiently on **different hardware** targets.

## 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.

# 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:
  - Typesetting: LaTeX
  - Machine Learning: PyTorch, TensorFlow (Keras)
  - Scientific Computing: Kokkos, FEniCS, FreeFEM
  - Fluid Dynamics: OpenFOAM
  - Image Processing: Halide, Taichi
  - Stencils: Devito, Ebb, 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.

# What Does The GT4Py DSL Need?

```
import numpy as np

def laplacian_np(in_field):
    out_field = np.zeros_like(in_field)
    nx, ny, nz = in_field.shape
        for i in range(1, nx - 1):
            for j in range(1, ny - 1):
                for k in range(0, nz):
                    out_field[i, j, k] = (
                        - 4 * in_field[i, j, k]
                        + in_field[i - 1, j, k]
                        + in_field[i + 1, j, k]
                        + in_field[i, j - 1, k]
                        + in_field[i, j + 1, k] )
        return out_field
```

Input, output, and possibly temporary 3D fields

Nested loops iterating along both horizontal and vertical directions

Math operations

Indices and offsets

## Definitions Function

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

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

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

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] )
```

Input and output fields
(with type annotations)

## Definitions Function

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

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] )
```

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

## Definitions Function

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

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] )
```

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

# Definitions Function

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

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

Vertical region of application:
... = full column

## Definitions Function

```
import numpy as np
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    with computation(PARALLEL), interval(...):
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            +      in_field[-1,  0, 0]
            +      in_field[+1,  0, 0]
            +      in_field[ 0, -1, 0]
            +      in_field[ 0, +1, 0] )
```

Each statement can be thought of as being an ij-loop

## Definitions Function

```
import numpy as np
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f64 = np.float64

def laplacian_defs(in_field: Field[f64], out_field: Field[f64]):
    with computation(PARALLEL), interval(...):
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            - 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] )
```

Neighboring points accessed through offsets

## Definitions Function

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

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] )
```

1st horizontal dimension

2nd horizontal dimension

Vertical dimension

Neighboring points accessed through offsets

## Definitions Function

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

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] )
```

No for loops!
No return statement!

# Compilation

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

```
backend = “gt:cpu_ifirst”
laplacian = gt.stencil(backend, laplacian_defs)
```

- Backends target different purposes, needs, and computer architectures:
  - Python: “numpy” (vectorized syntax);
  - C++: “gt:cpu_ifirst” (x86), “gt:cpu_kfirst” (MIC), “gt:gpu” and “cuda” (NVIDIA GPU).

- For non-Python backends, compilation consists of three steps:
  1) Generate optimized code for the target architecture (cached in .gt_cache).
  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])
# Output: 4.0
```

## 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

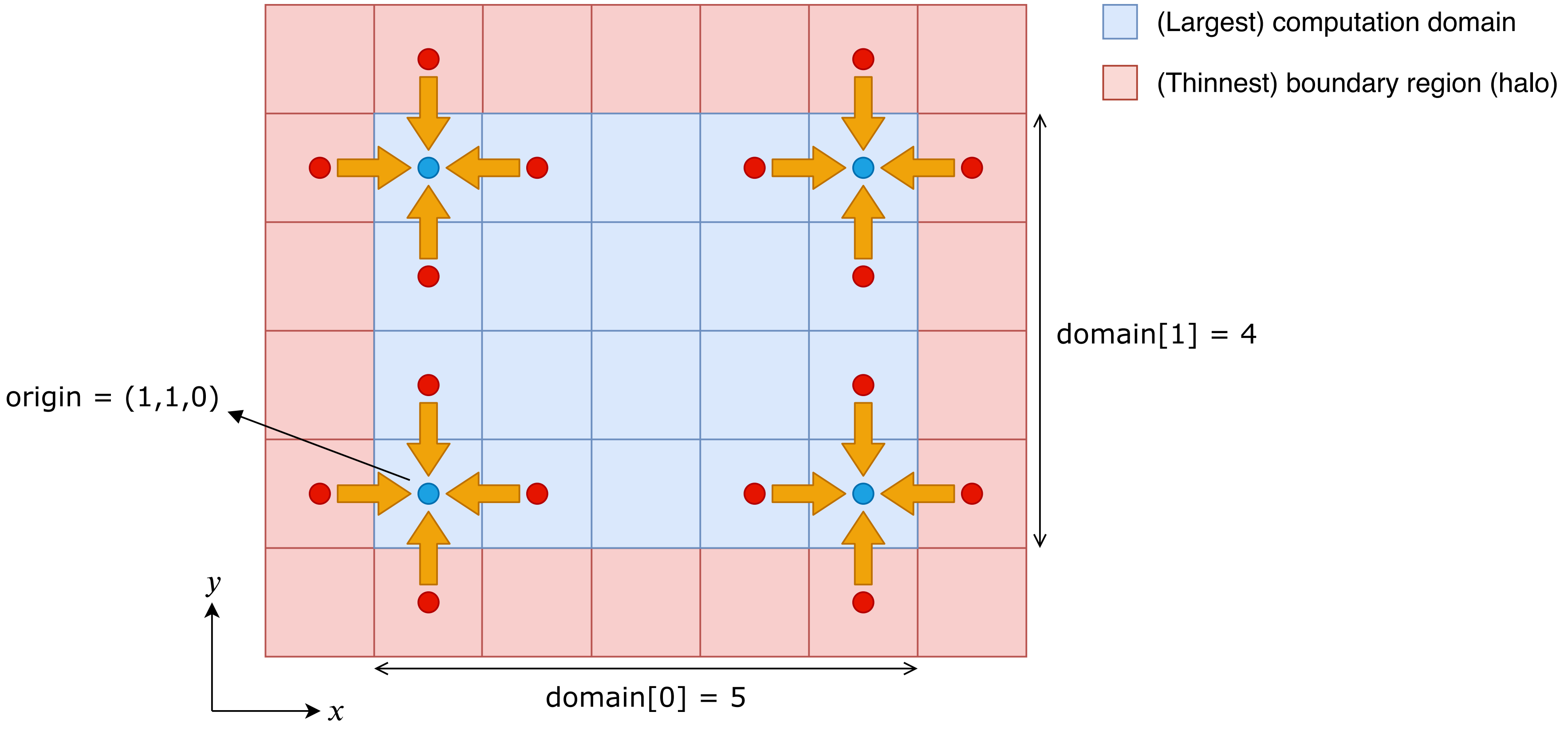
- Running computations is as simple as a function call:

```
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

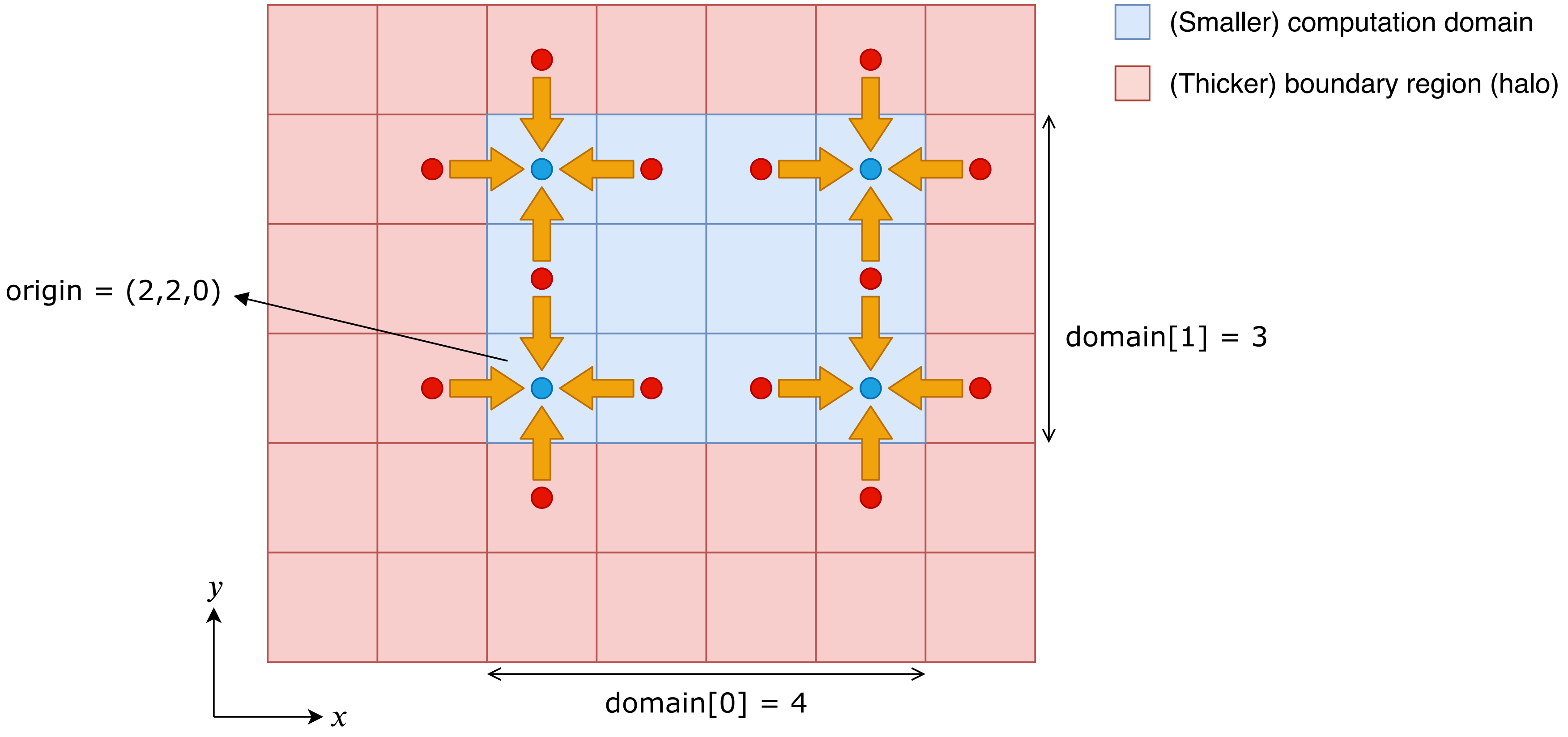
- out_field now contains the results of the computation.

## Region of application



🟦 (Largest) computation domain
🟥 (Thinnest) boundary region (halo)
domain[1] = 4
origin = (1,1,0)
domain[0] = 5
y
x

# Region of application



🟦 (Smaller) computation domain
🟥 (Thicker) boundary region (halo)
origin = (2,2,0)
domain[1] = 3
domain[0] = 4
y
x

## Weather and Climate on DSLs

- Several models (FV3, FVM and ICON) being ported to GT4Py
- Other approaches
  - COSMO (MeteoSwiss) dynamical was re-written in C++ using GridTools library.
  - E3SM (US DOE) using the Kokkos library for on-node parallelism.
  - LFric (UK MetOffice)
- Who knows what the future will bring…

## 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-motivation.ipynb**

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

**02-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

## References

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

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

More in-depth introduction to GT4Py:
https://github.com/ai2cm/dsl_workshop