Atlas, a library for NWP and climate modelling

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ECMWF

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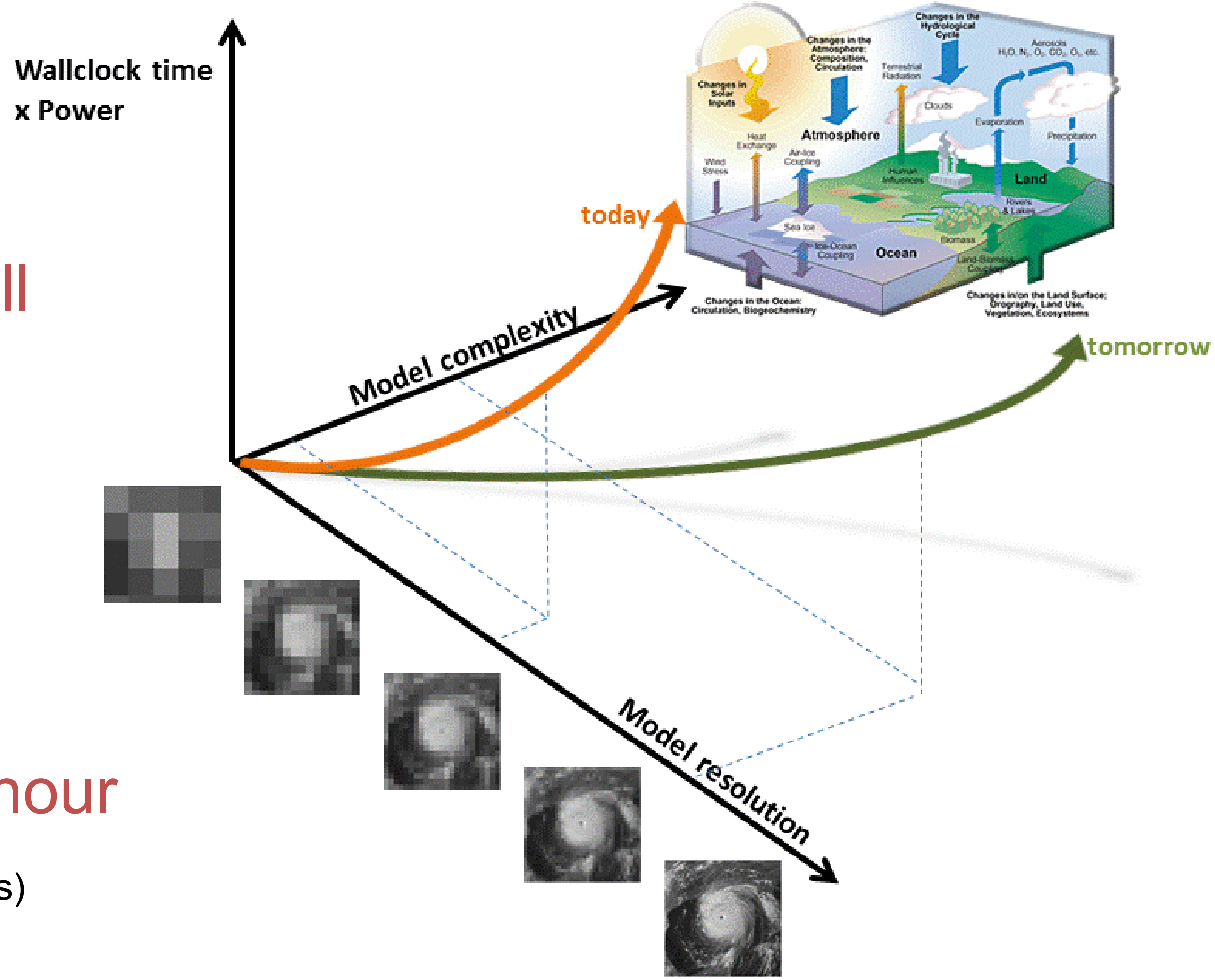
Growth in model resolution and model complexity

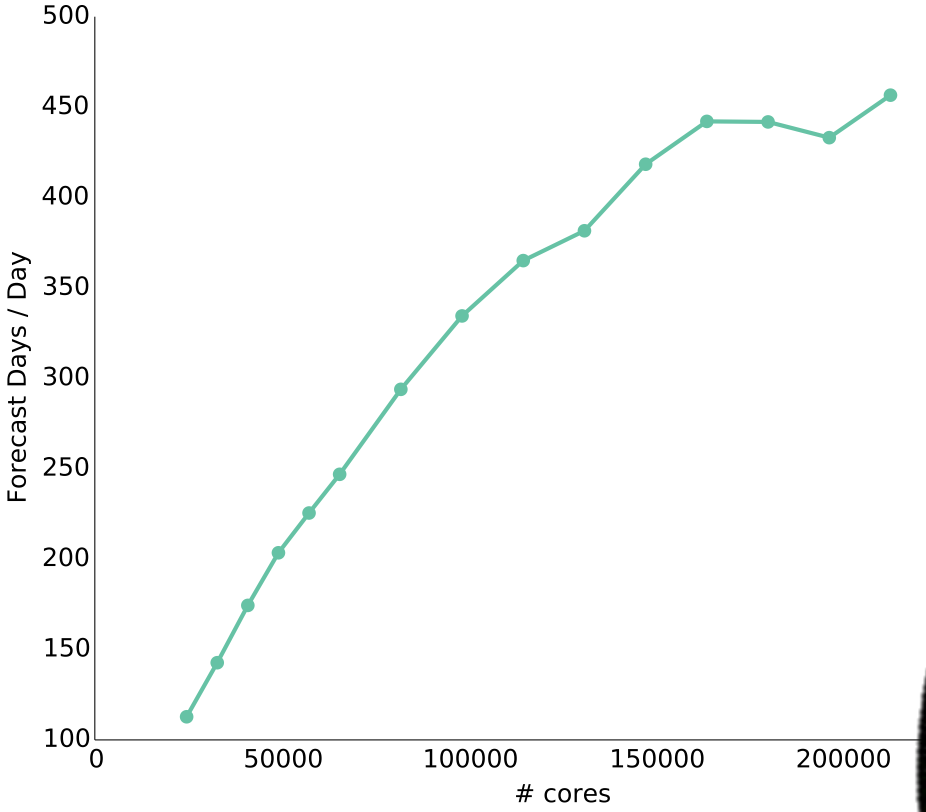
Improving forecast skill

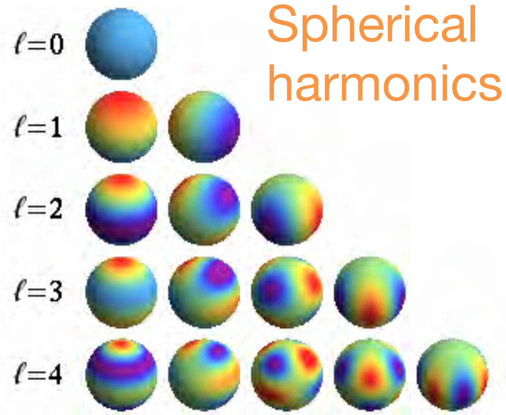


Limited by ability to forecast 10 days in 1 hour

(currently with 360 Cray XC40 nodes)

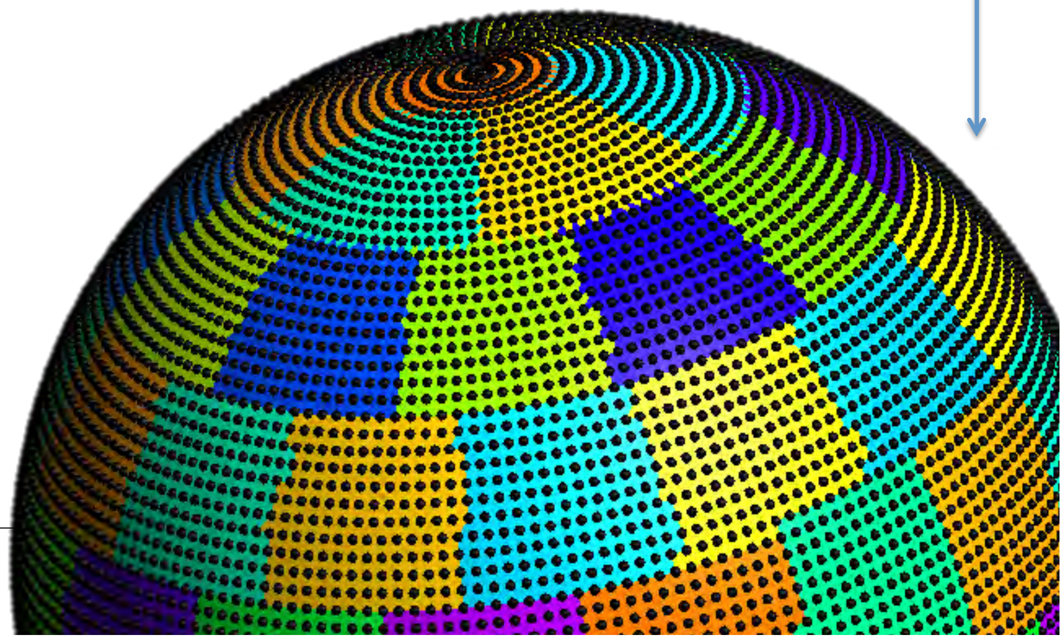
IFS faces a (long-term) scalability problem





transform

global all-to-all communications



Atlas, a library for NWP and climate modelling – *Deconinck et al. 2017, J-CPC*

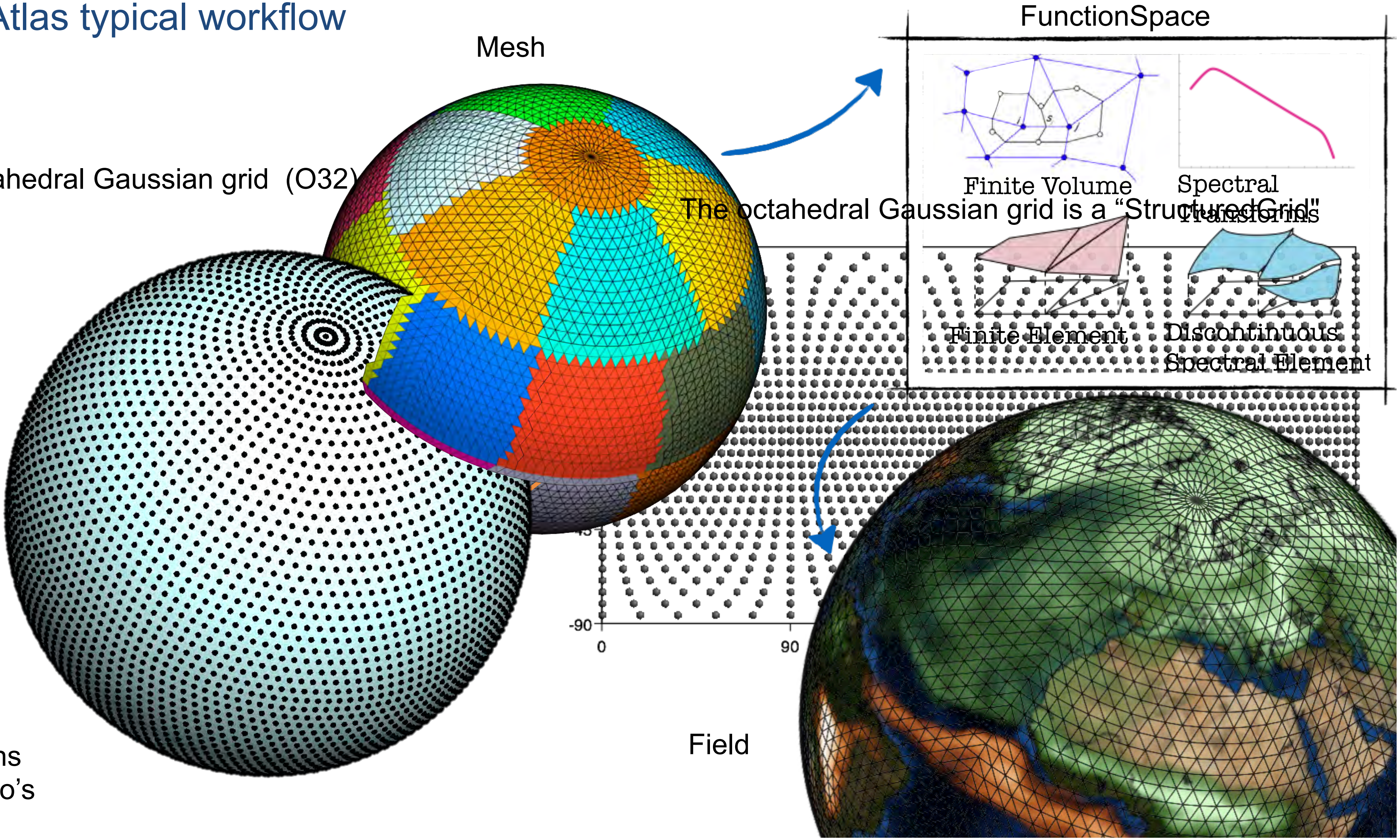
- A new foundation built with future challenges for HPC in mind
- Modern C++ library implementation with modern Fortran 2008 (OOP) interfaces → integration in existing models
- Open-source (Apache 2.0), http://github.com/ecmwf/atlas
- Data structures to enable new numerical algorithms, e.g. based on unstructured meshes
- Separation of concerns:
  - Parallelisation
  - Accelerator-awareness (GPU/CPU/…)
- Readily available operators
  - Remapping and interpolation
  - Gradient, divergence, laplacian
  - Spherical Harmonics transforms
- Support structured and unstructured grids (**global** as well as **regional**)

Atlas typical workflow

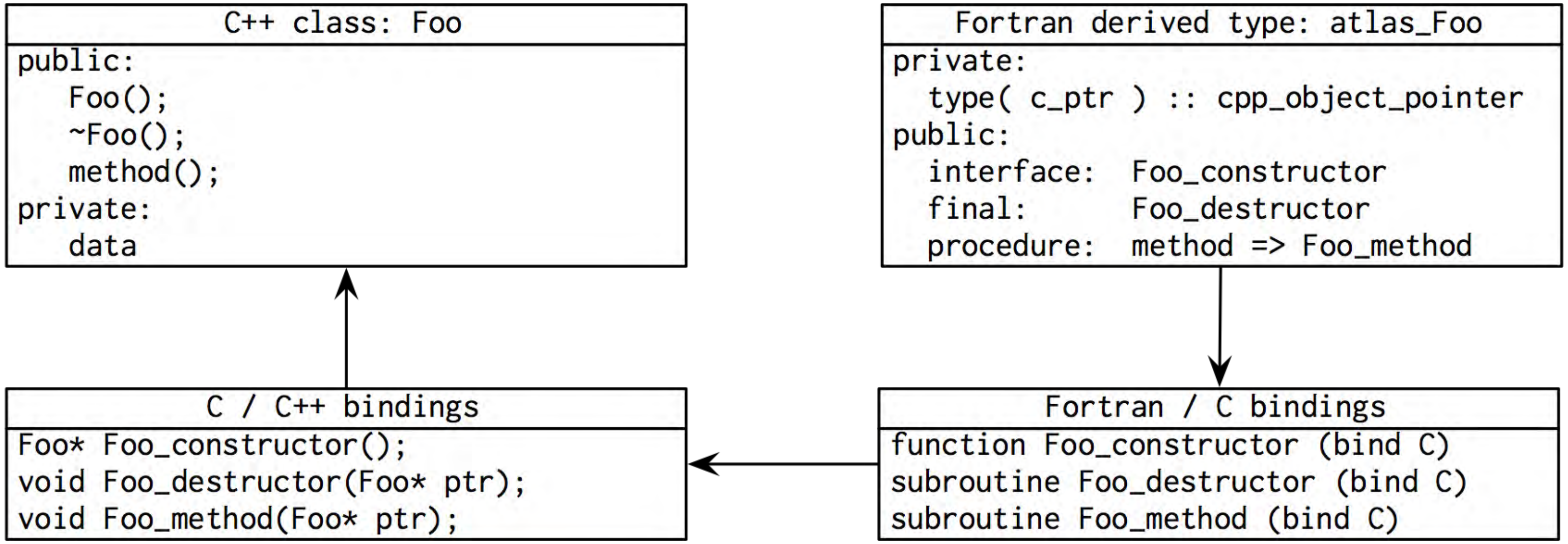
Octahedral Gaussian grid (O32)

Grid

Partitions
with halo's



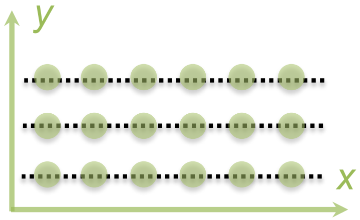
Object oriented design C++ / Modern Fortran

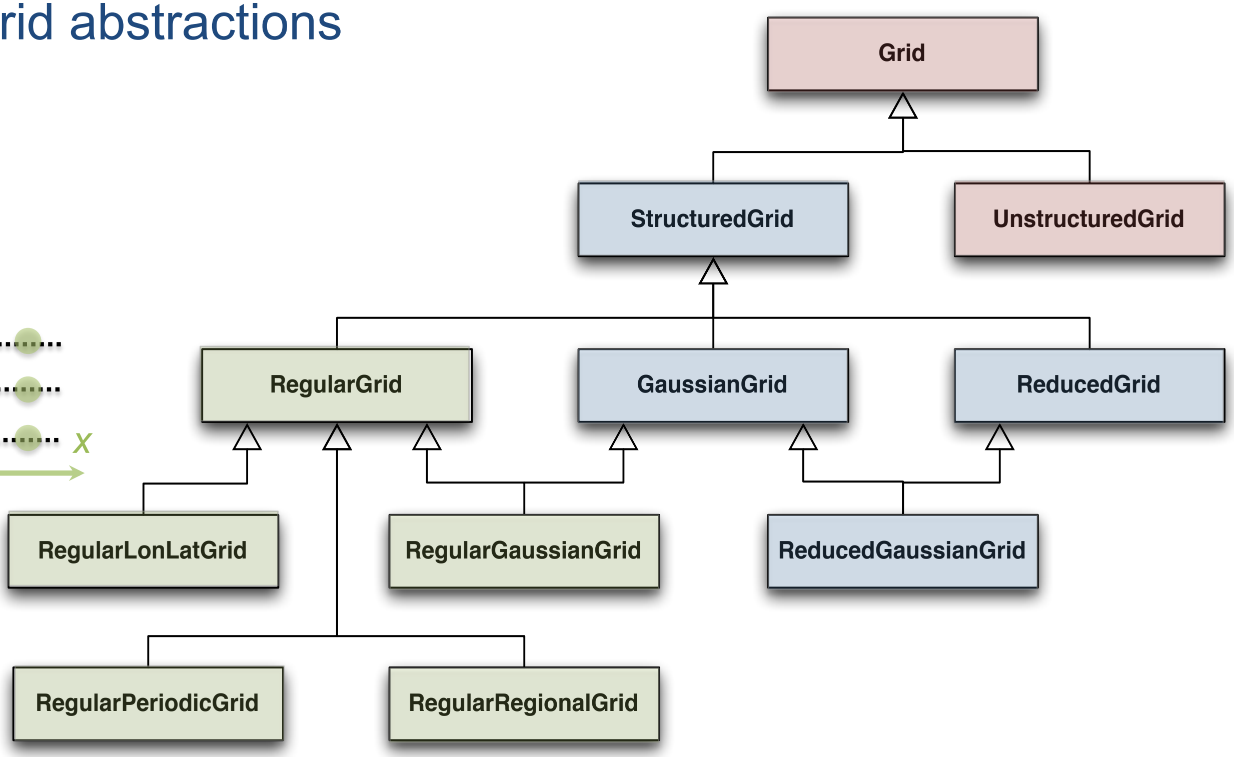


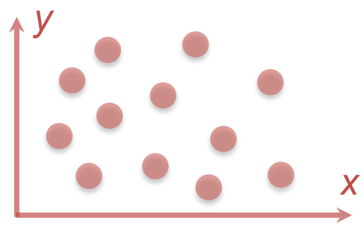

```cpp
Foo foo;
foo.method();
```

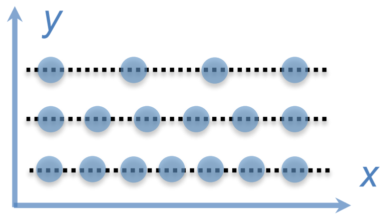
```fortran
type(atlas_Foo) :: foo
foo = atlas_Foo()
call foo%method()
```

A library of grid abstractions









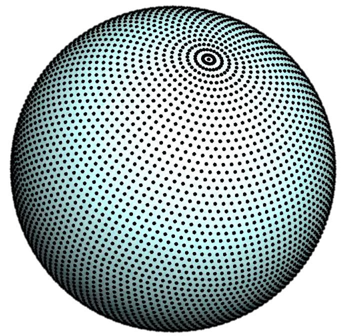
Example creation of operational octahedral reduced Gaussian grid using unique identifier

C++

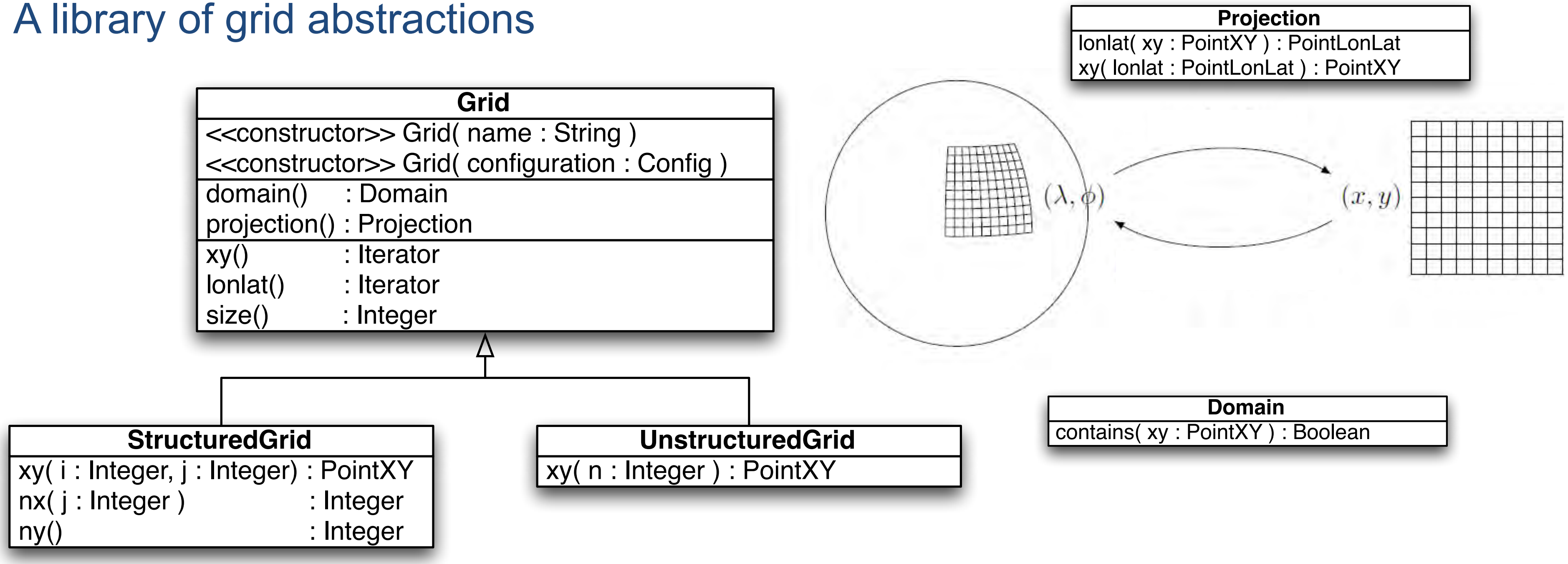
```
atlas::Grid grid;
grid = atlas::Grid ( “O1280” )
```

Fortran

```
type(atlas_Grid) :: grid
grid = atlas_Grid( “O1280” )
```



A library of grid abstractions



Iterating over all grid points, regardless of used projection, structure, domain

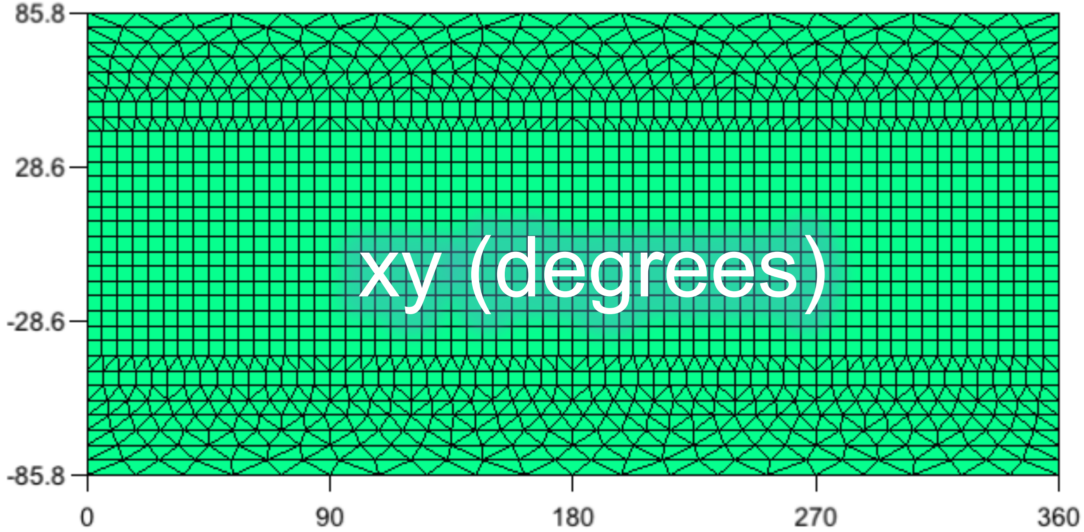
Grid coordinates (x,y)

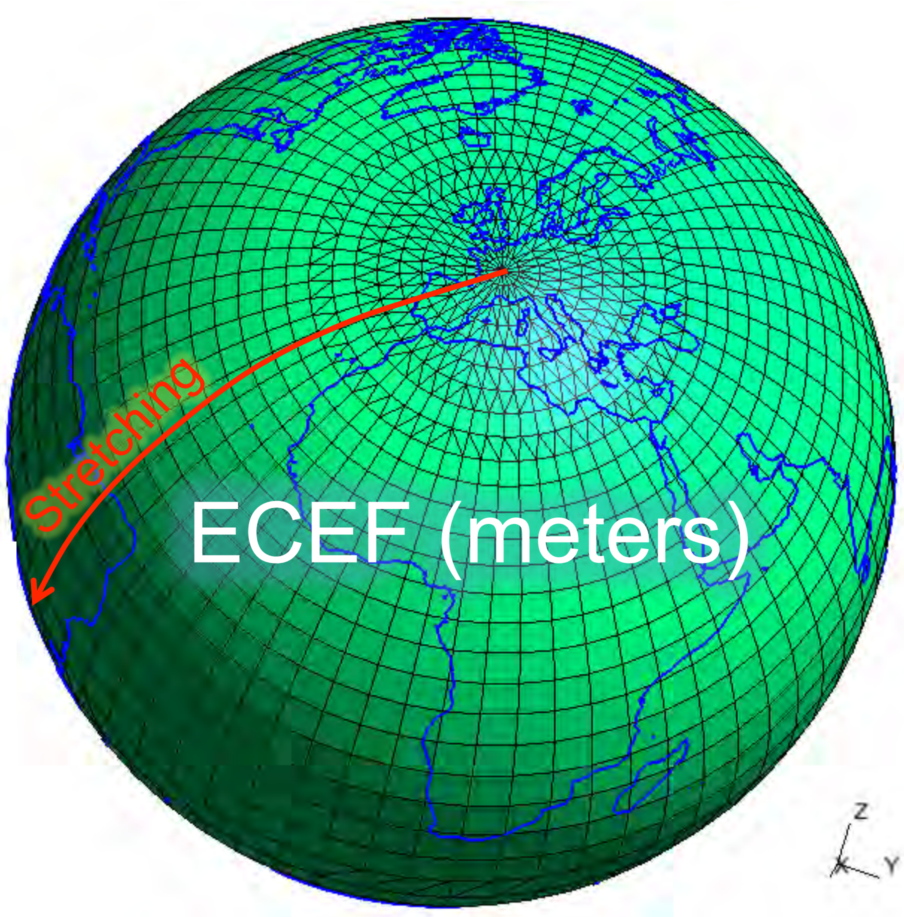
```
for( PointXY p : grid.xy() ) {
    double x = p.x();
    double y = p.y();
}
```

Geographic coordinates (lon,lat)

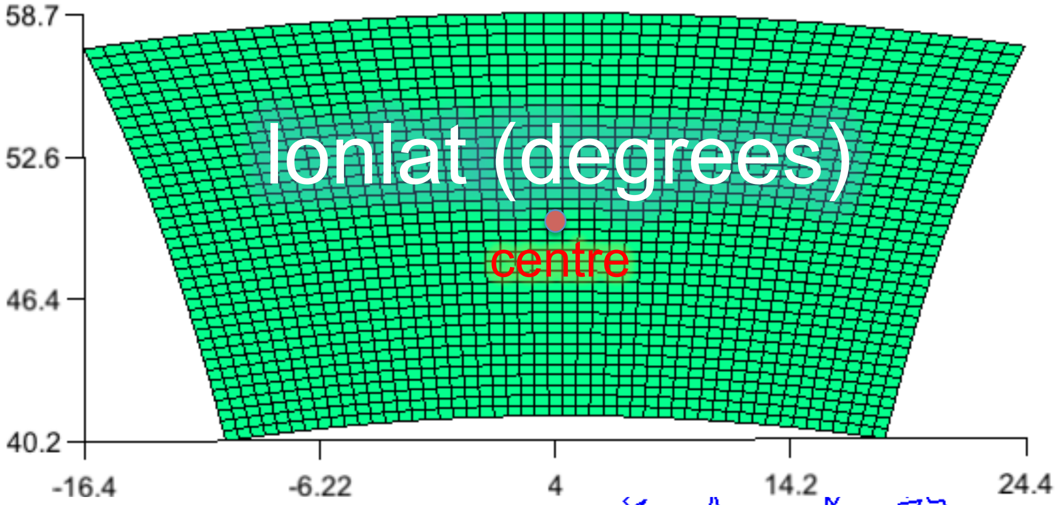
```
for( PointLonLat p : grid.lonlat() ) {
    double lon = p.lon();
    double lat = p.lat();
}
```

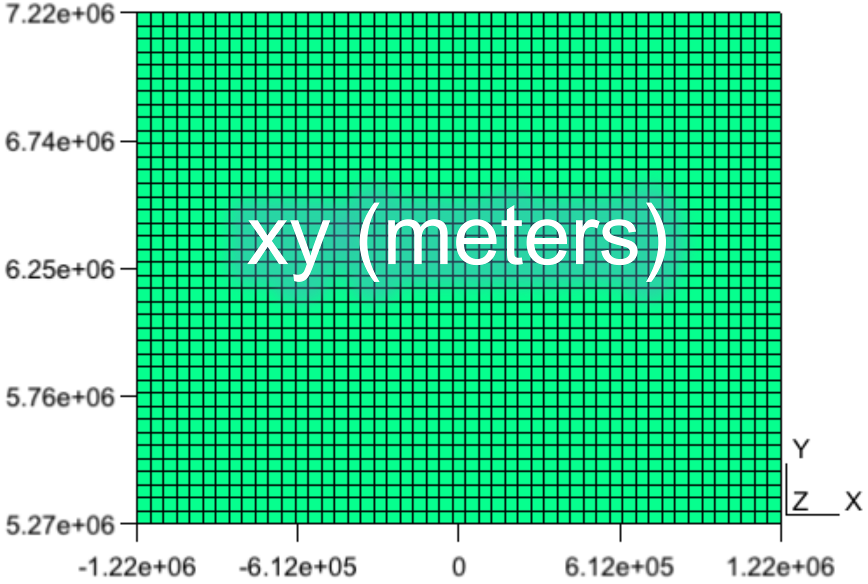
```
{
  "type" : "classic_gaussian",
  "N" : 16
  "projection" : {
     "type" : "rotated_schmidt",
     "north_pole"  : [3,47]
     "stretching_factor" : 2
  }
}
```

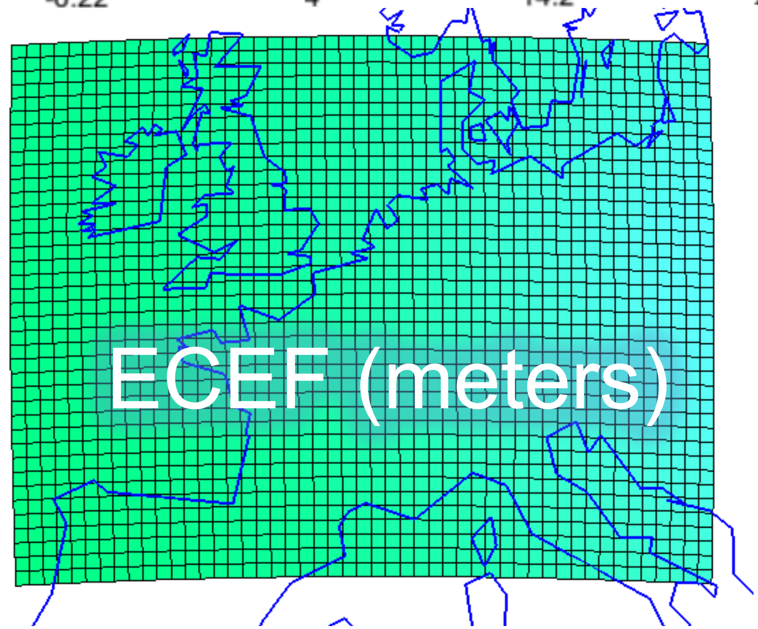




```
{
   "type" : "regional",
   "nx" : 50,   "dx" : 50000,
   "ny" : 40,   "dy" : 50000,
   "lonlat(centre)" : [4,50],
   "projection" : {
      "type" : "lambert",
      "latitude1"   : 50,
      "longitude0" : 4
   }
}
```

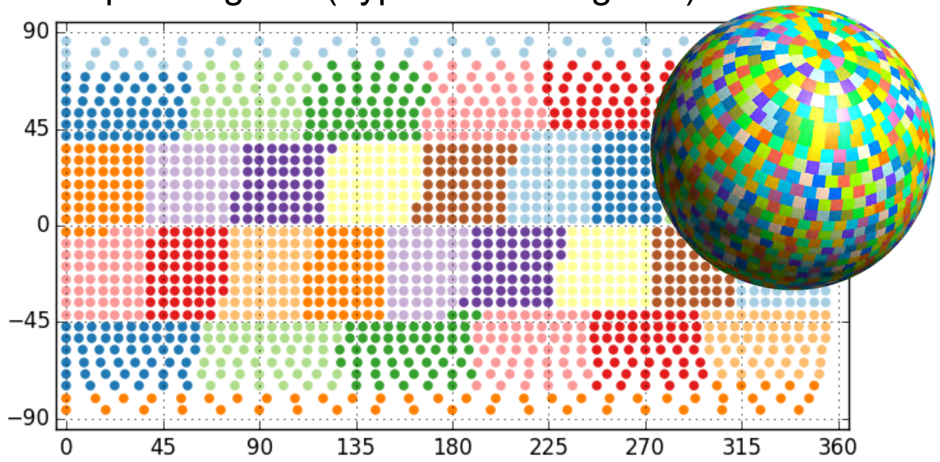




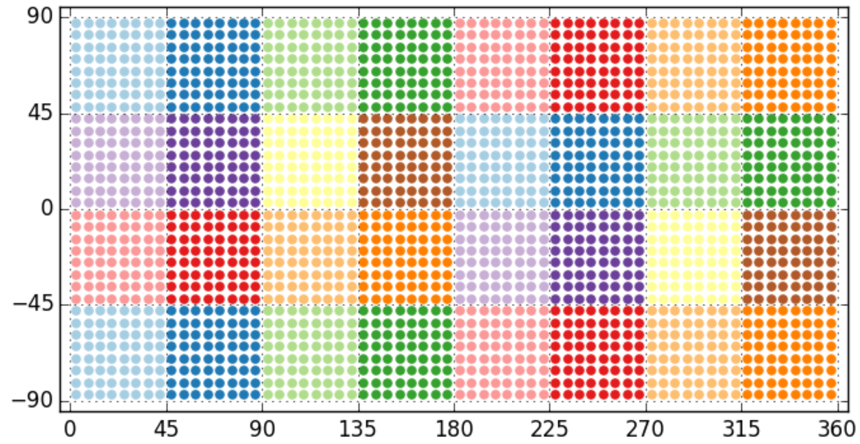


Multiple domain decomposition strategies

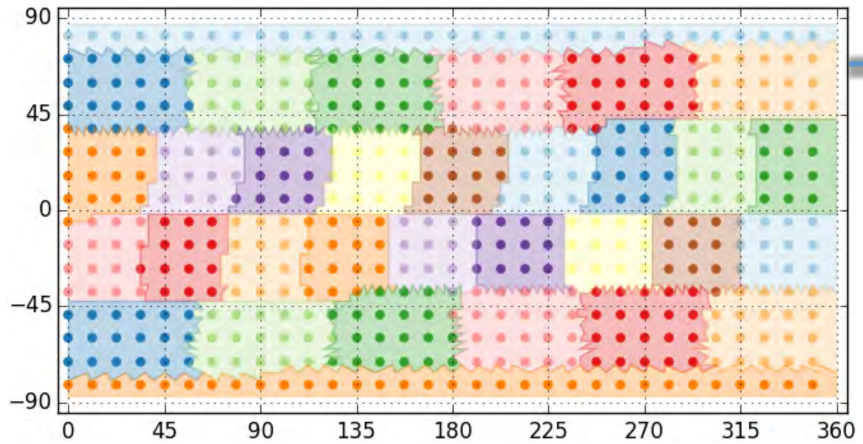
Equal Regions (typical for IFS grids)



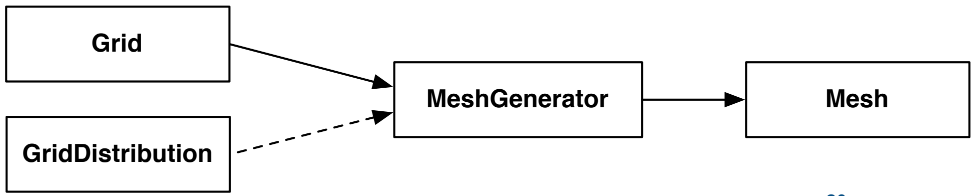
Checkerboard (typical for regional grids)



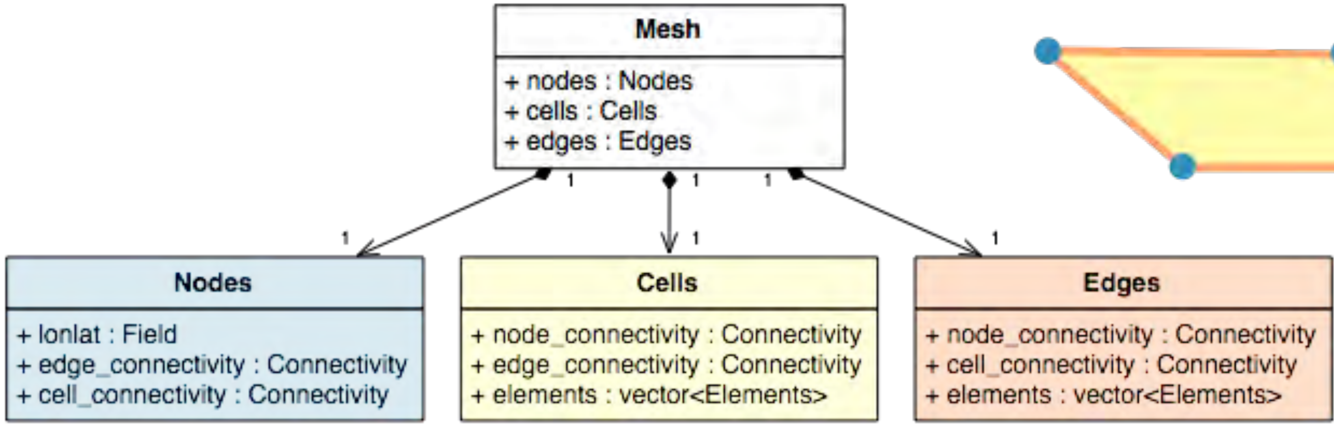
Matching Mesh

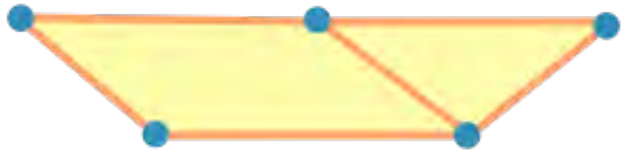


Any grid can follow the domain decomposition of an already distributed mesh

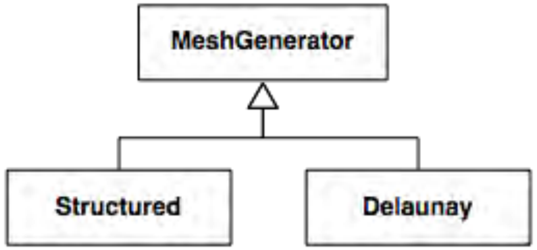


Mesh: connecting points (nodes) by edges and cells using connectivity tables





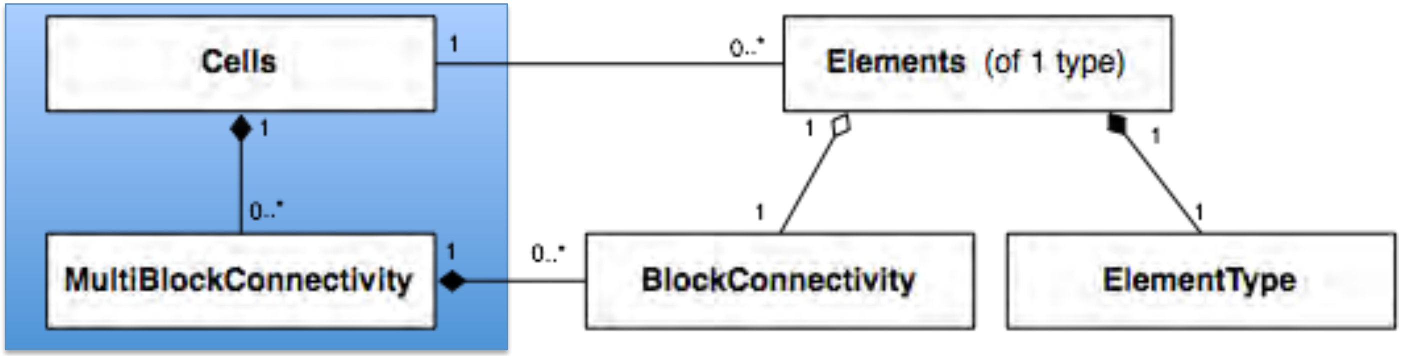
Mesh generation




```
MeshGenerator meshgen(“structured”);
Mesh mesh = meshgen.generate(grid);
```

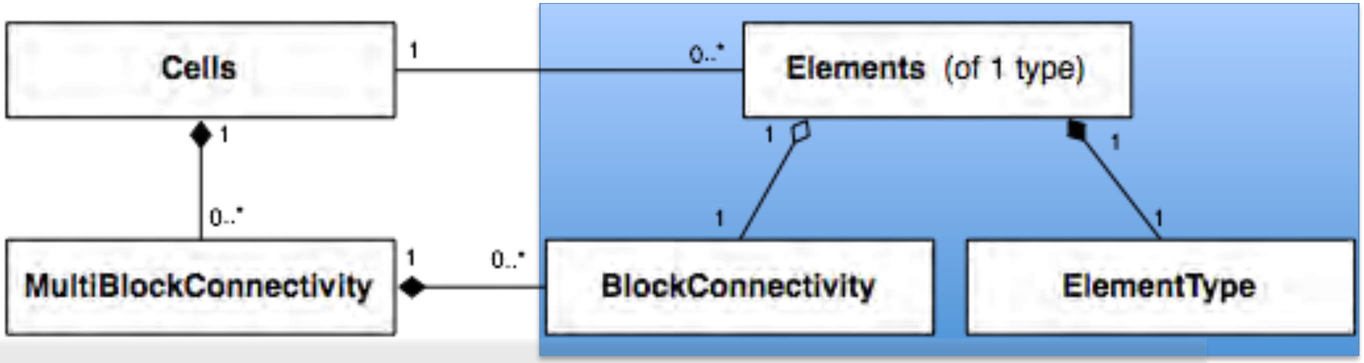
```
type(atlas_MeshGenerator) :: meshgen
type(atlas_Mesh)          :: mesh
meshgen = atlas_MeshGenerator(“structured”)
mesh = meshgen%generate(grid)
```

Example "for" over all elements



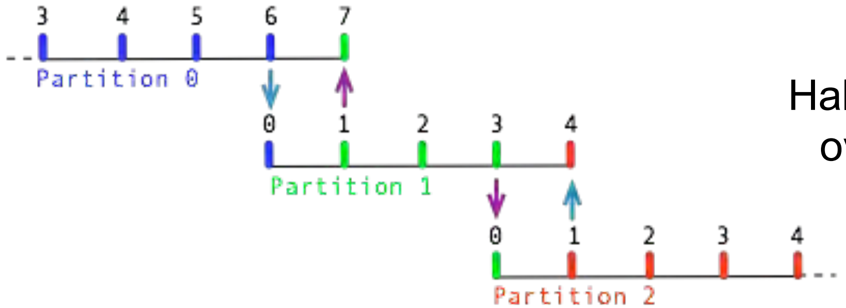

```
MultiBlockConnectivity& node_connectivity = mesh.cells().node_connectivity();

// Loop over ALL elements
for( size_t jelem=0; jelem<mesh.cells().size(); ++jelem ) {

    // Compute average over cell
    double cell_average = 0;
    for( size_t jnode=0; jnode<mesh.cells().nb_nodes(jelem);
        cell_average += field( node_connectivity(jelem,jnode) );
    cell_average /= double(mesh.cells().nb_nodes(jelem));
}
```

Example "for" per element type

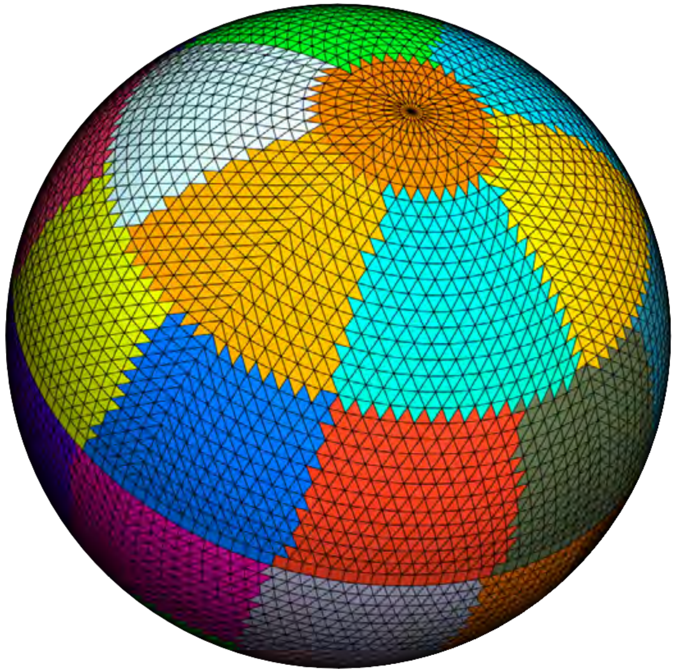


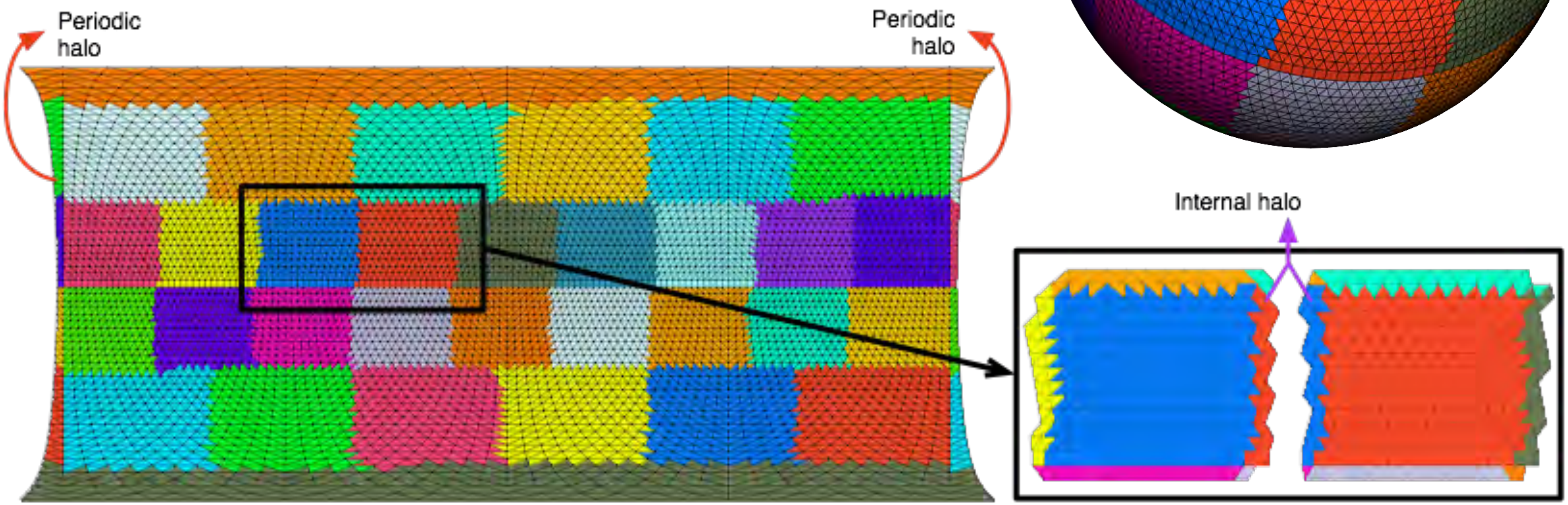

```
// Loop over element types
for( size_t jtype=0; jtype<mesh.cells().nb_types(); ++jtype ) {

   Elements& elements = mesh.cells().elements(jtype);
   BlockConnectivity& node_connectivity = elements.node_connectivity();

   // Loop over elements of one type
   for( size_t jelem=0; jelem<elements.size(); ++jelem ) {

      // Compute average over cell
      double cell_average = 0;
      for( size_t jnode=0; jnode<elements.nb_nodes();
         cell_average += field( node_connectivity(jelem,jnode) );
      cell_average /= double(elements.nb_nodes());
   }
}
```

Halo exchanges

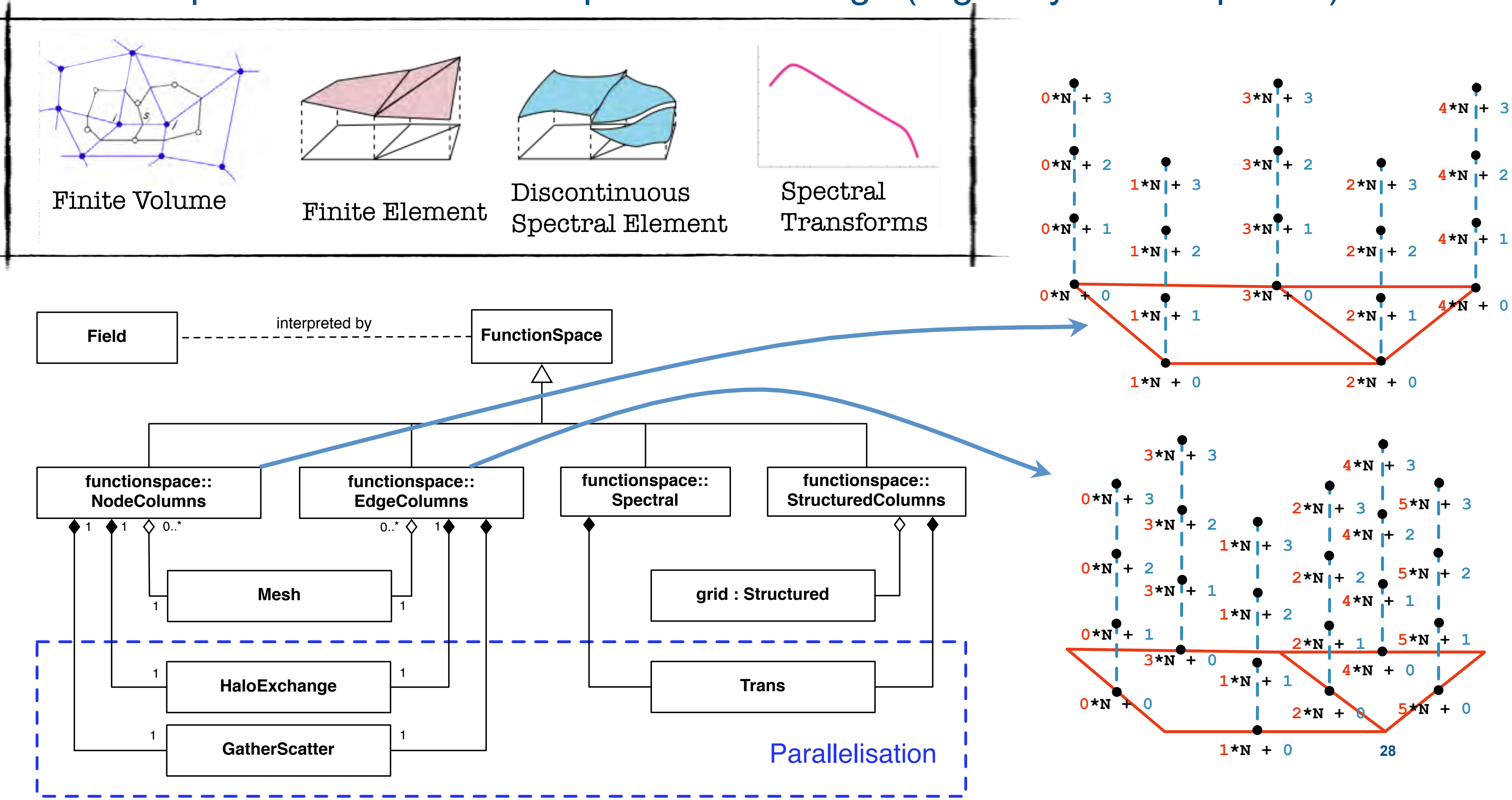


HaloExchange in overlap regions



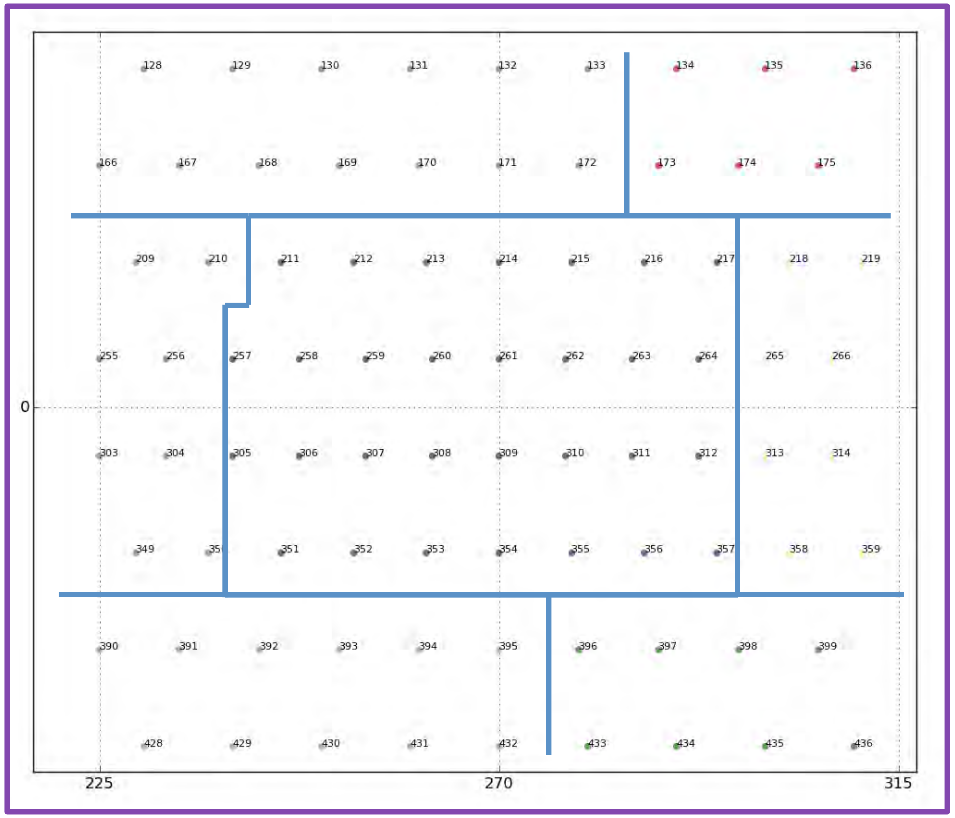


FunctionSpaces: Discretisation specific knowledge (arguably model specific)



StructuredColumns FunctionSpace

- What?
  - Discretisation of Fields without a Mesh (only StructuredGrid, cfr. IFS)
  - Distributed view of horizontal grid, plus structured vertical levels
- Halos
  - Fast algorithm to create halo
  - HaloExchange capabilities !!!
  - Halo's over pole !!!



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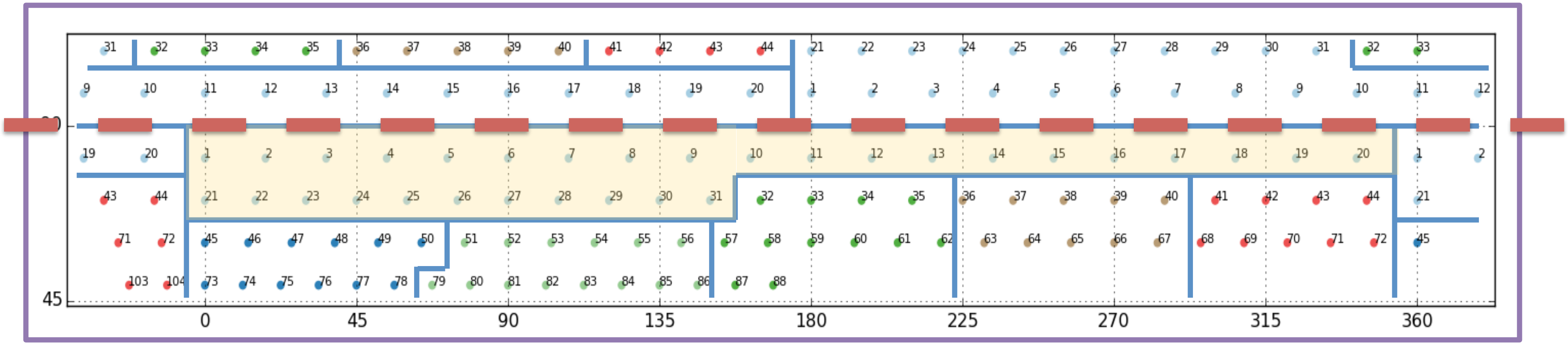
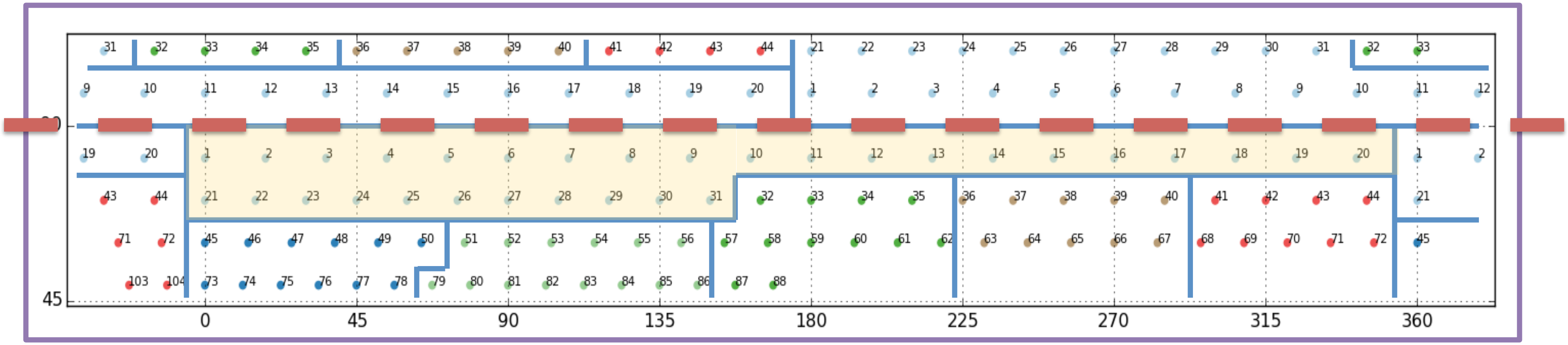
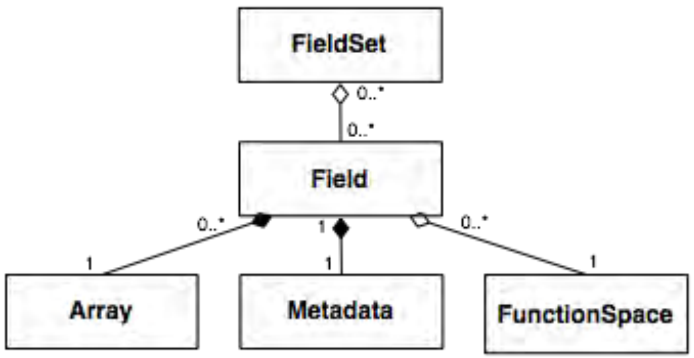


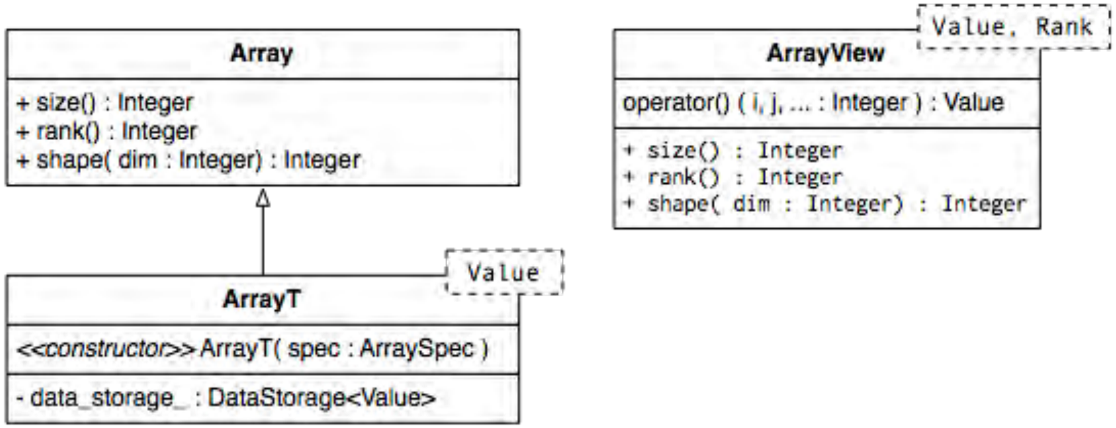
StructuredColumns FunctionSpace

- How?
  - Mapping (i , j) → local index
  - Indirect addressing but… increased flexibility
    - Room to optimise cache efficiency using space-filling curve
    - One-to-one mapping with mesh-based functionspace (excluding halo)
    - Halo points added at the end



Field: container for data with metadata

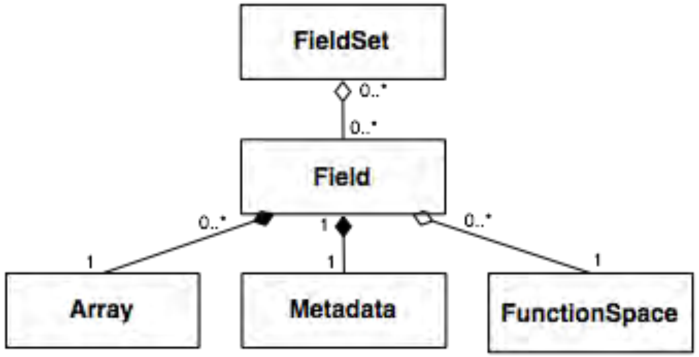


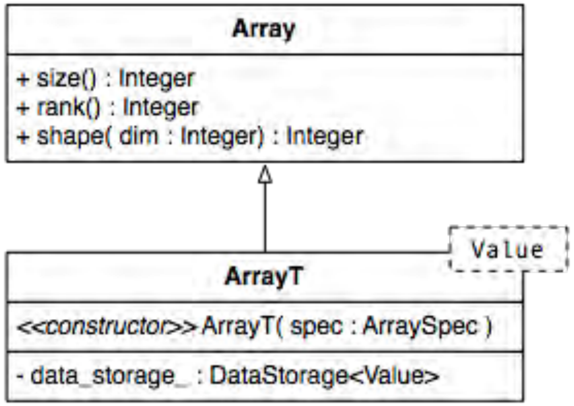


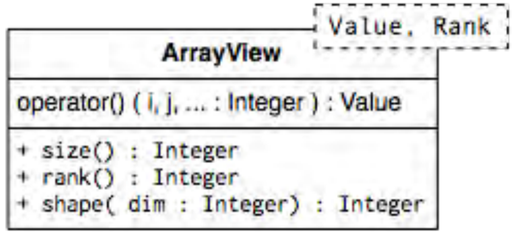

```
Field field = Field(
   /* name  */  "P",
   /* kind  */  make_datatype<double>(),
   /* shape */  make_shape(npts,nlev) );

field.metadata().set("units","hPa")
field.metadata().set("time",450)
```

```
type(atlas_Field)    :: field
type(atlas_Metadata) :: field_metadata

field = atlas_Field(                &
           name="P",                &
           kind=atlas_real(jprb),   &
           shape=[nlev,npts] )

field_metadata = field%metadata()
call field_metadata%set("units","hPa")
call field_metadata%set("units",450)
```

Acces to field data







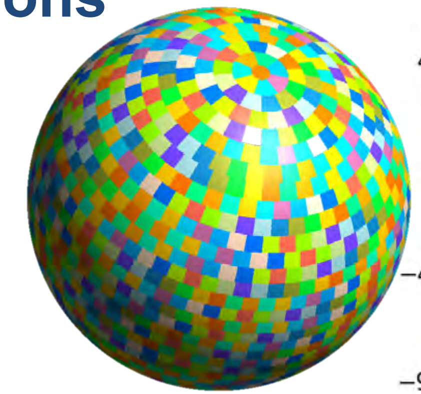

```
auto field_data =
        make_view<double,2>( field );

for( int jnode=0; jnode<npts; ++jnode ) {
    for( int jlev=0; jlev<nlev; ++jlev ) {
        field_data(jnode,jlev) = …
    }
}
```

```
real(8), pointer :: field_data(:,:)

call make_view( field, field_data )
do jnode=1,npts
    do jlev=1,nlev
        field_data(jlev,jnode) = …
    enddo
enddo
```

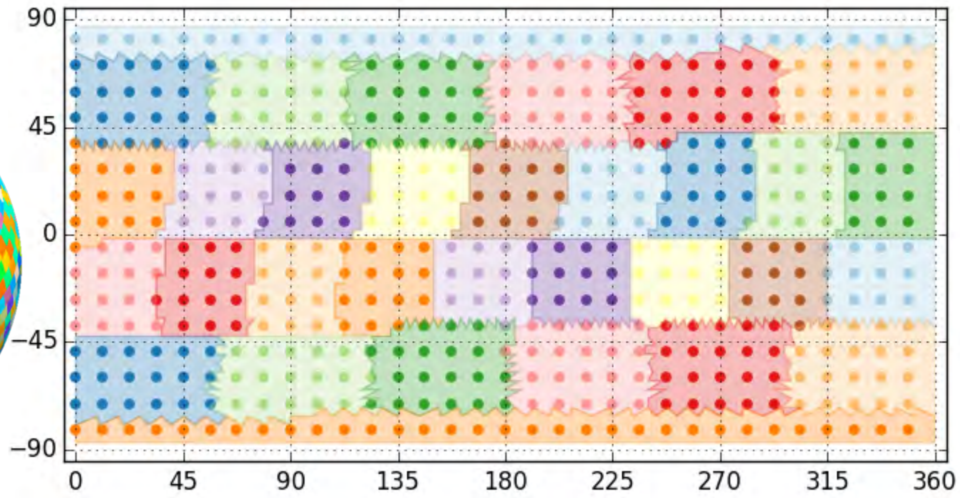
Remapping, using matching domain decompositions

- Domain decompositions match to avoid MPI communication

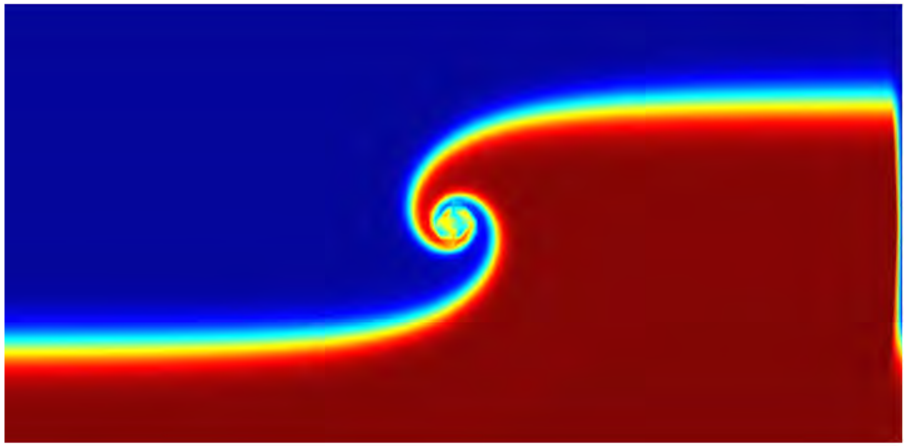
- Parallel interpolation:
  - nearest neighbour
  - k-nearest neighbour
  - linear element-based

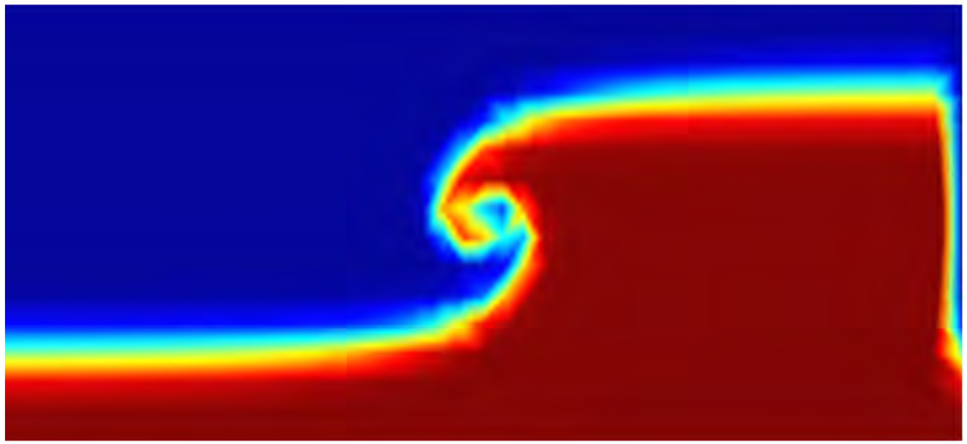


Thanks to Pedro Maciel (ECMWF)

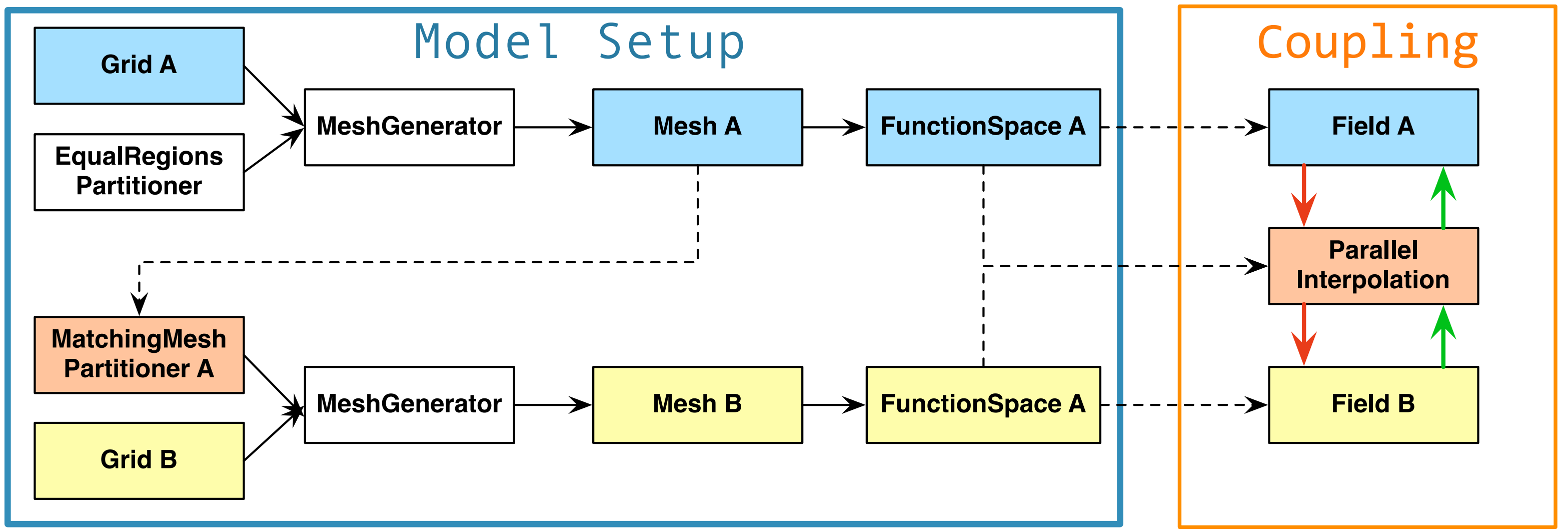


Example interpolation: O32 to F8





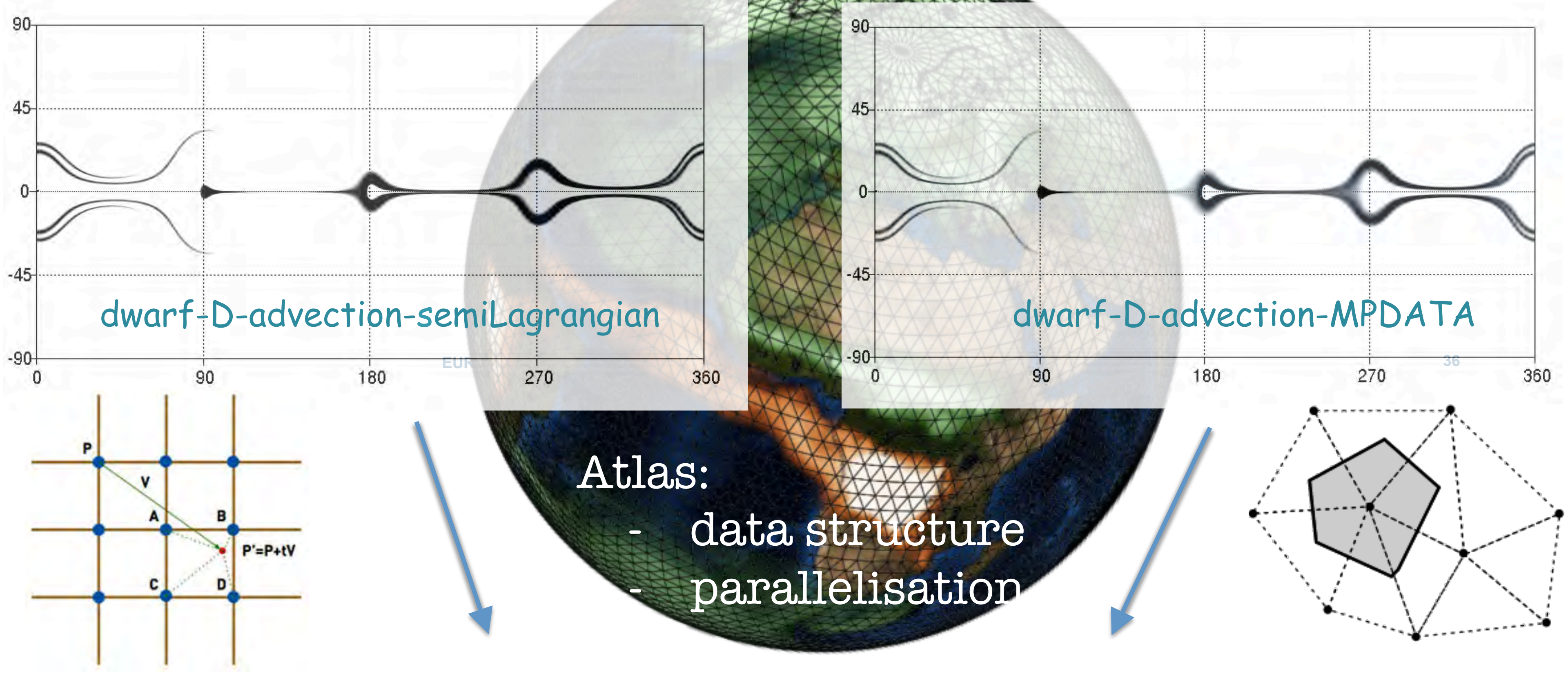
Remapping using matching domain decompositions




```
grid_A          = atlas_Grid("O1280")
partitioner_A   = atlas_EqualRegionsPartitioner()
mesh_A          = meshgenerator % generate(grid_A, partitioner_A)
fs_A            = atlas_functionspace_NodeColumns(mesh_A)

grid_B          = atlas_Grid("O640")
partitioner_B   = atlas_MatchingMeshPartitioner(mesh_A)
mesh_B          = meshgenerator % generate(grid_B, partitioner_B)
fs_B            = atlas_functionspace_NodeColumns(mesh_B)

interpolation_AB = atlas_Interpolation(type="finite-element",
                                       source=fs_A, target=fs_B)
```

```
call interpolation_AB %
              execute(field_A, field_B)
```

IFS and Advection dwarfs

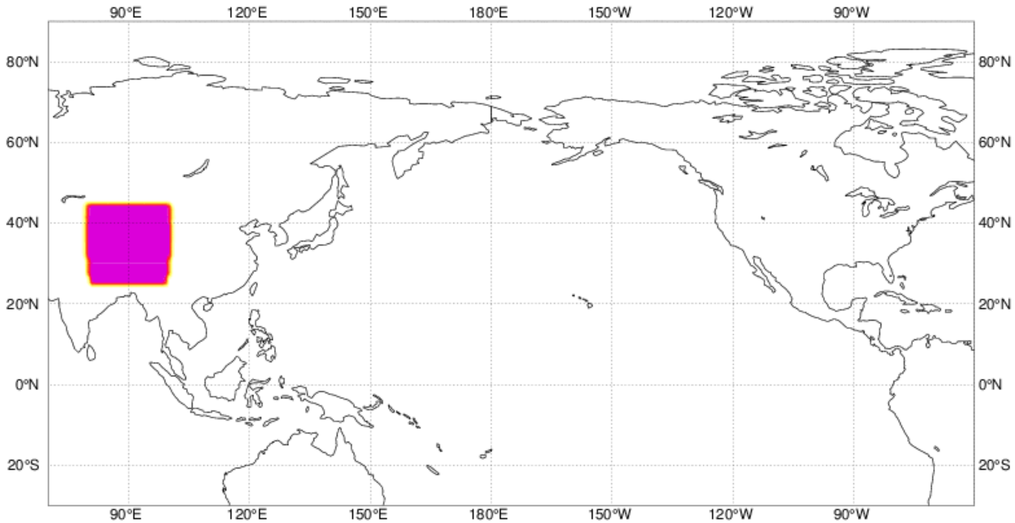


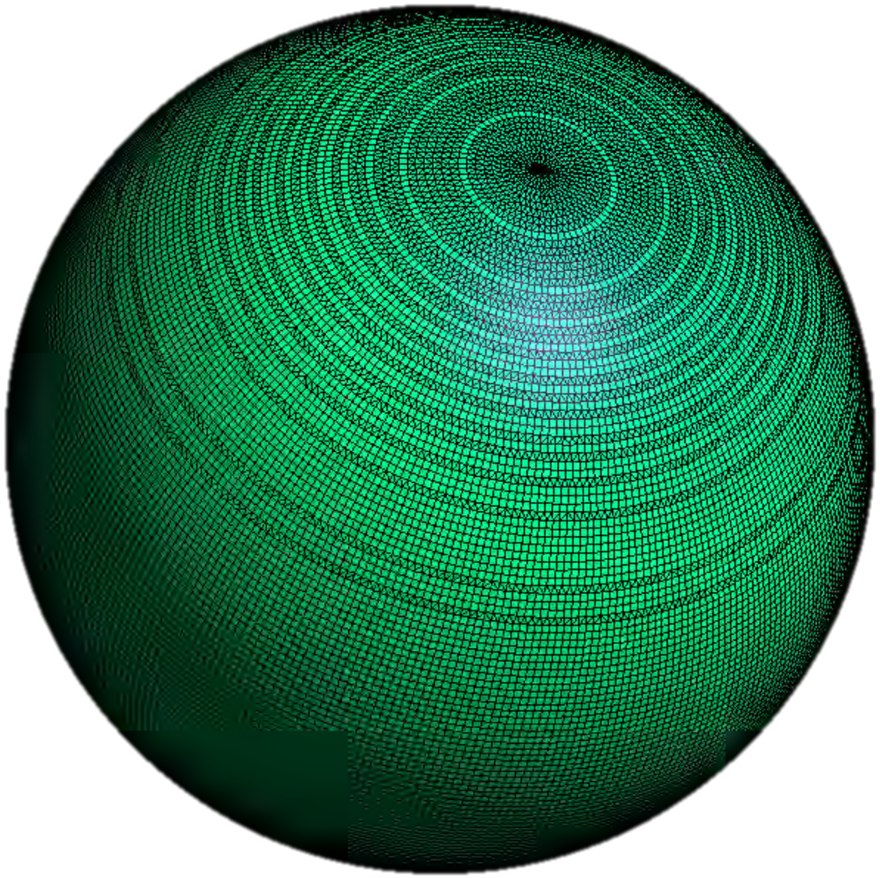
Advection abstraction in IFS based on Atlas

Thanks to Michail Diamantakis (ECMWF)

Passive tracer advection

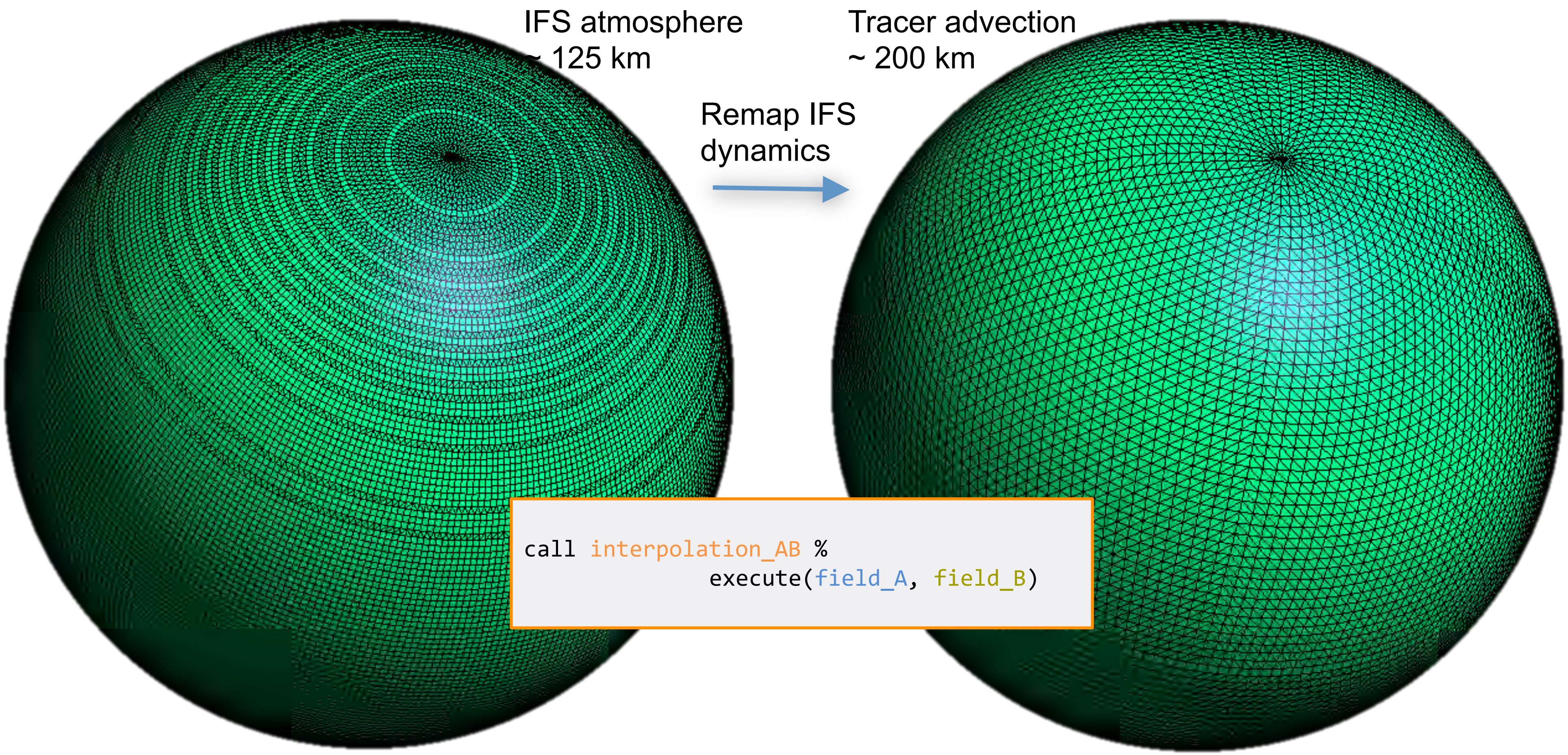
Tracer initialised over Asia – 125 km model resolution (N80)



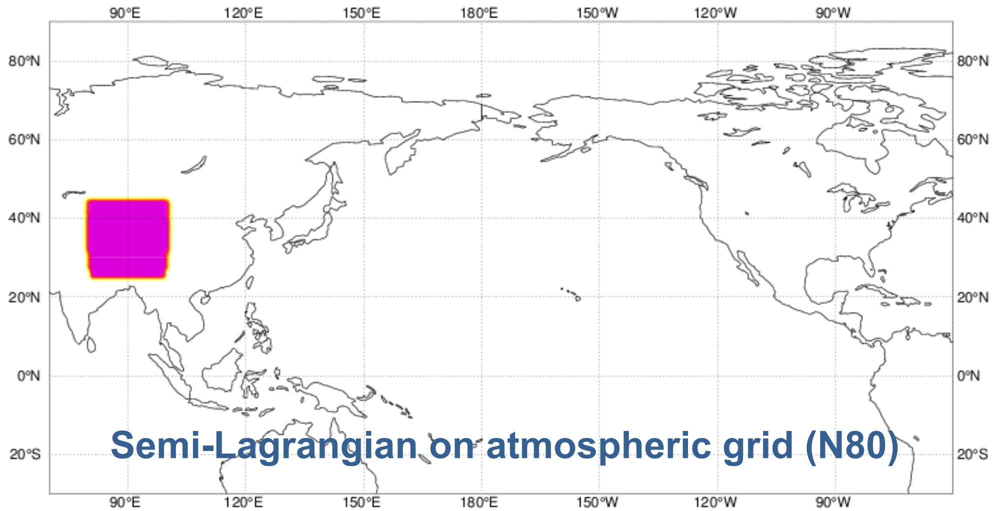


proof of concepts!
(read: poor Fortran code was abused in the process
to get quick results)

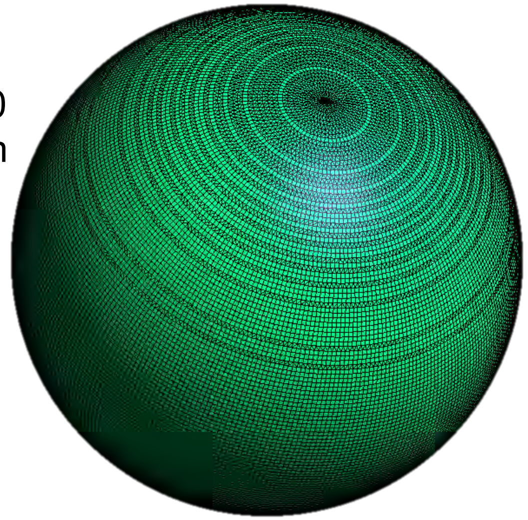
Can we use a coarser resolution for advection, but with wind from fine resolution?

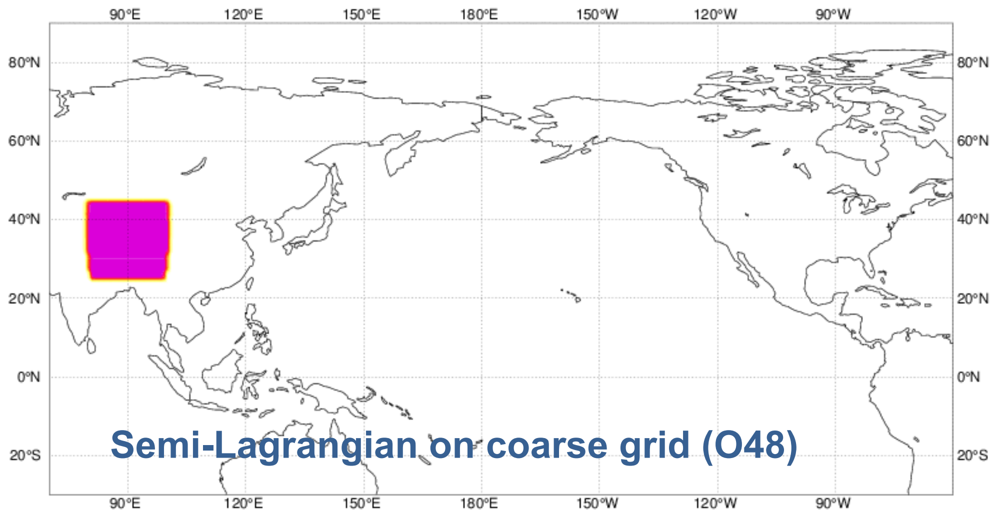



```
call interpolation_AB %
          execute(field_A, field_B)
```

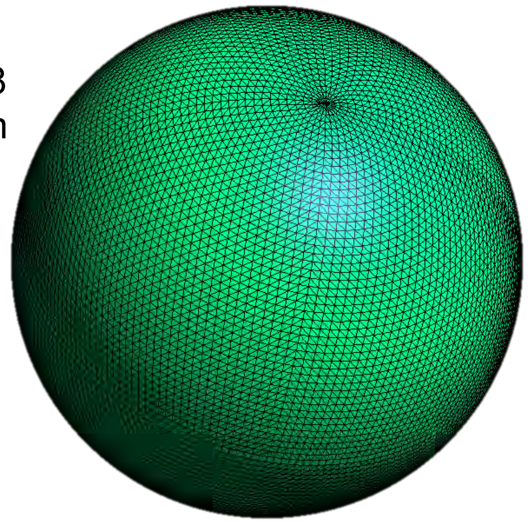


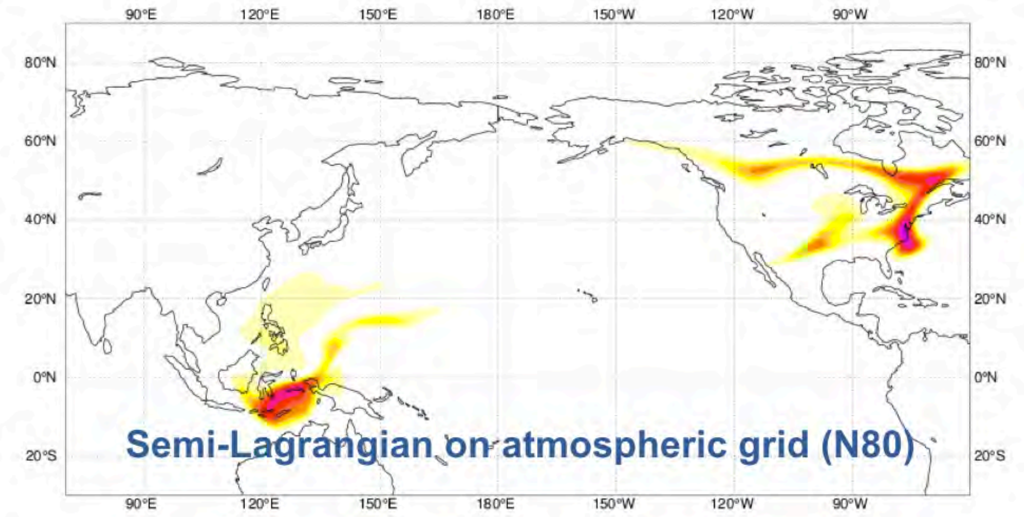
N80
~ 125 km



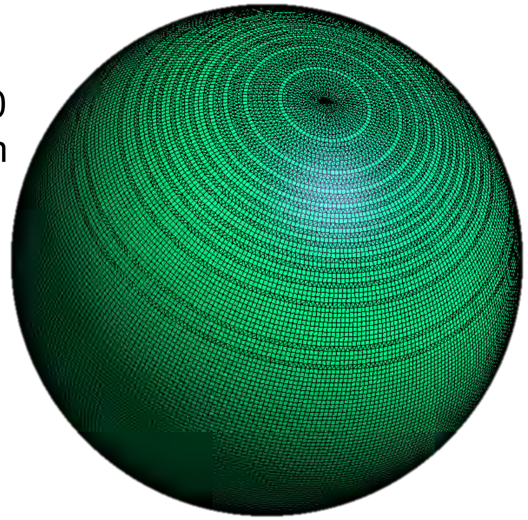


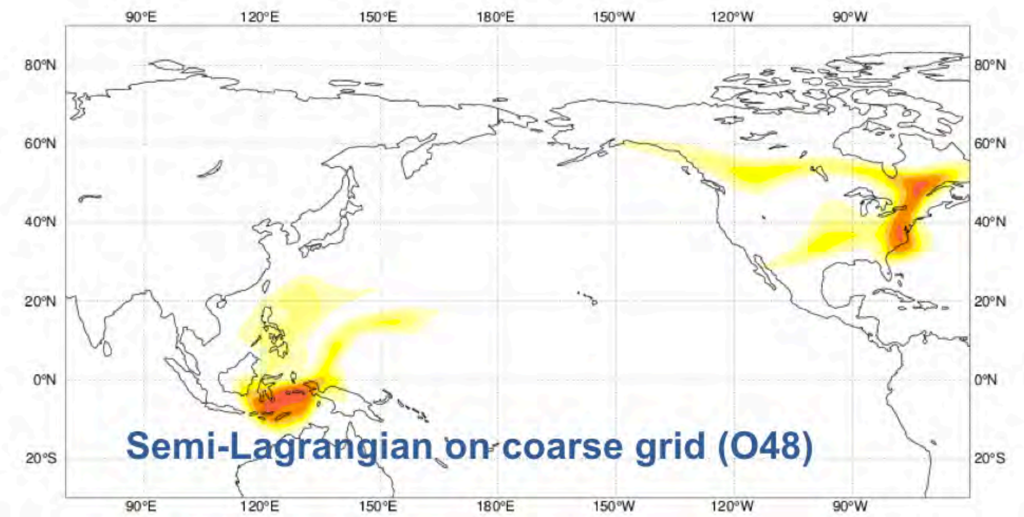
O48
~ 200 km



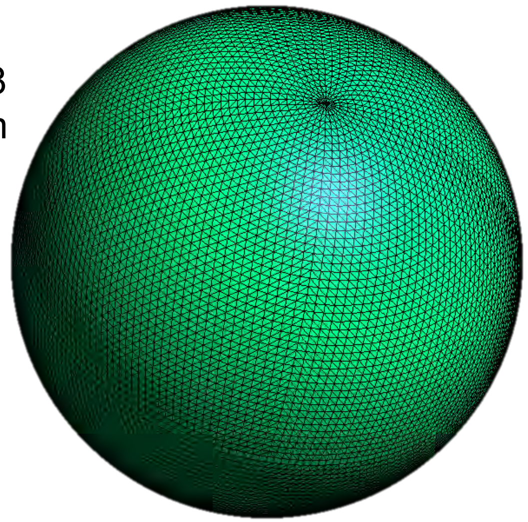


N80
~ 125 km





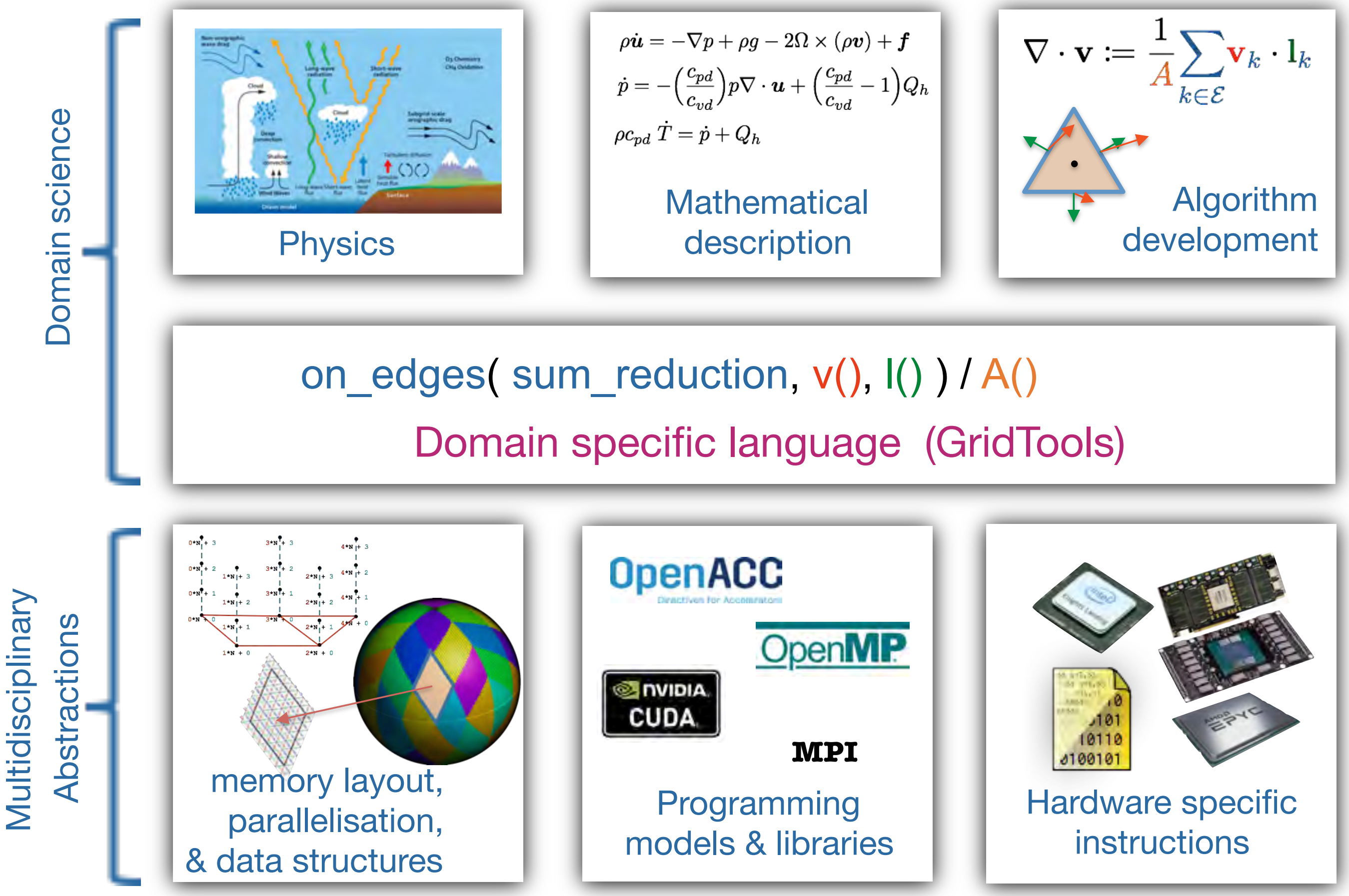
O48
~ 200 km



Atlas – GridTools integration

What is GridTools?

GridTools is a Domain-Specific-Language (DSL), developed by MeteoSwiss and CSCS, to express computational kernels that can be run on different hardware (CPU / GPU / MIC-KNL).



Atlas – GridTools integration

- Prior to ESCAPE, GridTools only worked on **specific regular grids** as used in COSMO
- In ESCAPE we extended this for **unstructured meshes based on Atlas**

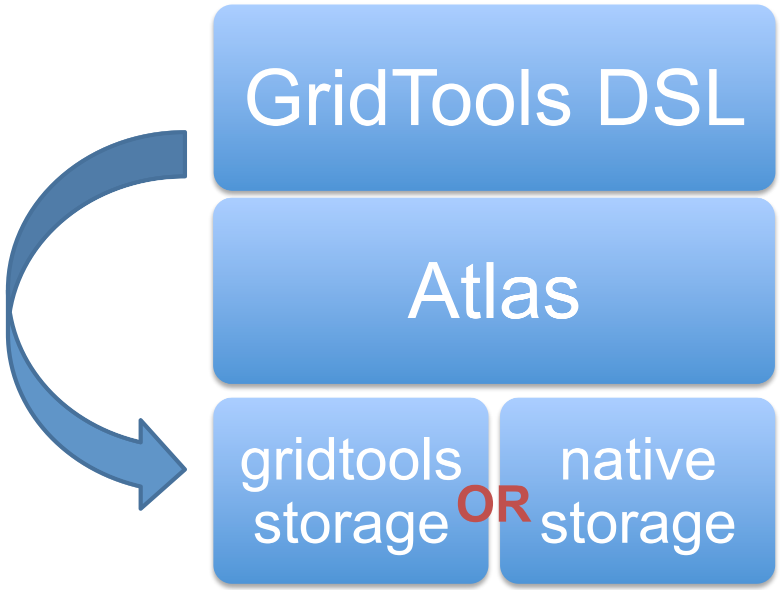
- GridTools has an internal data-storage framework that handles copying the data back-and-forth between the host (CPU) and device (e.g. GPU), and the DSL uses this extensively.

- **Challenge: How can we allow the GridTools DSL to recognise Atlas fields instead?**

Approach

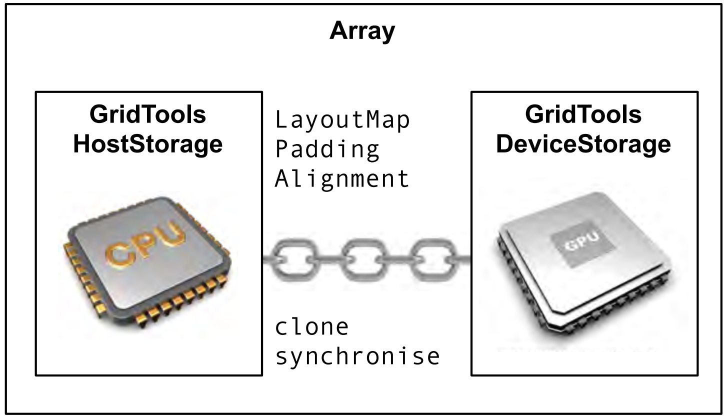
- Encapsulate the gridtools_storage features as a standalone module.

- Atlas Arrays and Fields can be compiled with gridtools_storage module for its internal storage.



Atlas on GPUs

- **Two linked memory spaces:**
  host (CPU) and device (GPU)
- **Built on GridTools storage layer**



Thanks to Carlos Osuna (MeteoSwiss)

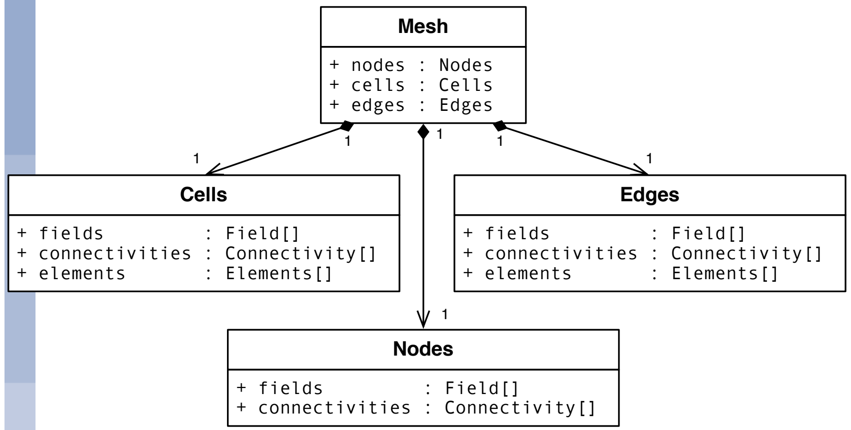
C++ example

```
// Create field (double precision, with 2 dimensions)
auto field = Field( datatype("real64"), shape(Ni,Nj) );

// Create a host view to interpret as 2D Array of doubles
auto host_view = make_host_view<double,2>(field);

// Modify data on host
for ( int i=0; i<Ni; ++i ) {
  for ( int j=0; j<Nj; ++j ) {
    host_view(i,j) = ...
}}

// Synchronise memory-spaces
field.syncHostDevice();

// Create a device view to interpret as 2D Array of doubles
auto device_view = make_device_view<double,2>(field);

// Use e.g. CUDA to process the device view...
some_cuda_kernel<<<1,1>>>(device_view);

// ... or GridTools or Kokkos
```

Atlas on GPUs with OpenACC for Fortran

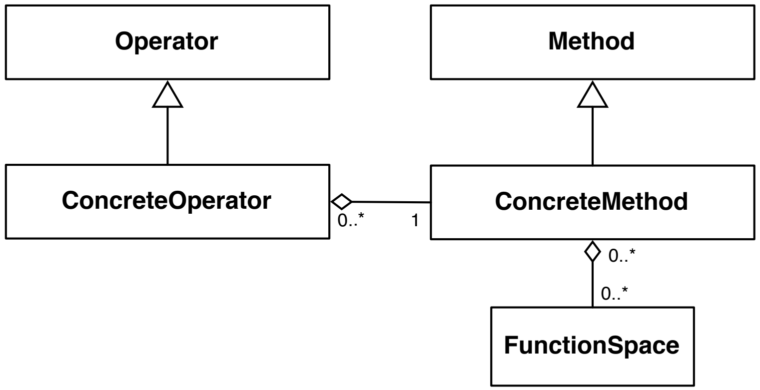
- **GPU enabled data structures**

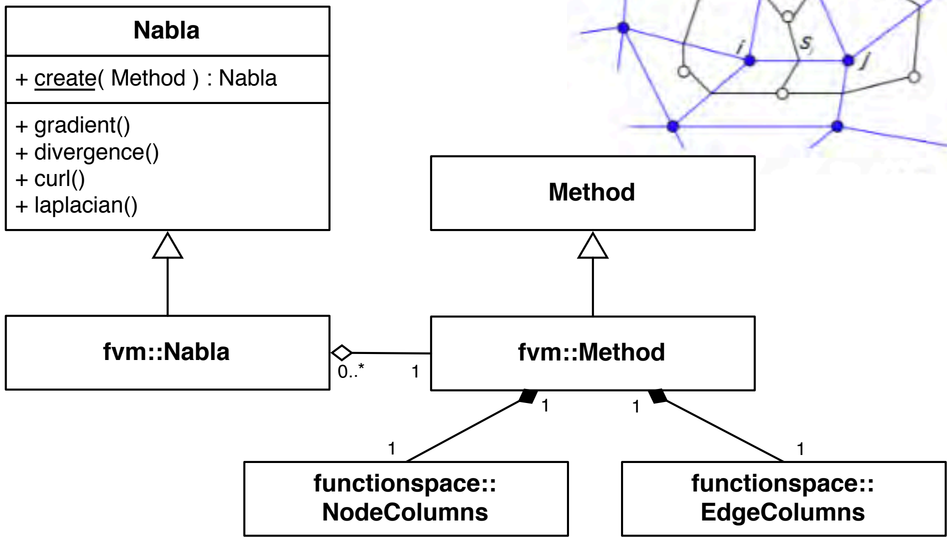
- Cloning mesh to device recursively clones all encapsulated components to device

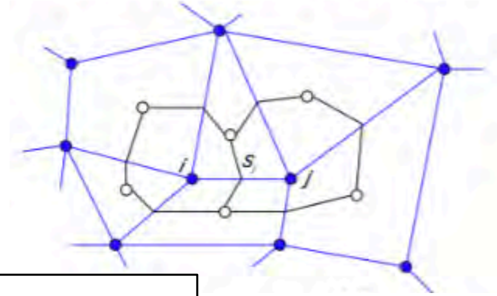



```fortran
type(atlas_Mesh) :: mesh             ! Assume created
type(atlas_mesh_Nodes) :: nodes ! Nodes in the Mesh
type(atlas_Field) :: field_xy    ! Coordinate field of nodes
real(8), pointer :: xy           ! Raw data pointer

!-----------------------------------------------------------
!

nodes    = mesh % nodes()            ! Access nodes
field_xy = nodes % xy()              ! Access coordinate field
call make_view( field_xy, xy )       ! Access raw data

call mesh % update_device()          ! Copy entire mesh to GPU

!$acc data present(xy)
!$acc kernels
do j=1,nodes % size()                ! Operate on GPU data
   xy(1,j) = ...                     ! e.g. modify X-coordinate
enddo
!$acc end kernels
!$acc end data

call field_xy % update_host()        ! Update changed field
```

Mathematical operations







Example Fortran code to create and apply the Nabla operator to compute gradient and laplacian

```
method = atlas_fvm_Method( mesh, levels=137 )
nabla  = atlas_Nabla( method )

call nabla%gradient ( scalarfield, gradfield )
call nabla%laplacian( scalarfield, laplfield )
```

Spectral Transforms in Atlas

C++ example

```
Grid grid("O1280");

StructuredColumns gp ( grid, levels(137) );
Spectral sp( 1279, levels(137) );

Field gpfield = gp.createField<double>();
Field spfield = sp.createField<double>();

Trans trans( gp, sp );   // TCo1279

trans.dirtrans( gpfield, spfield );
trans.invtrans( spfield, gpfield );
```

- Grid (Octahedral Gaussian O1280)
- FunctionSpaces gp and sp
- Creation of fields through FunctionSpace
- Internally sets up IFS-trans
- Transforms

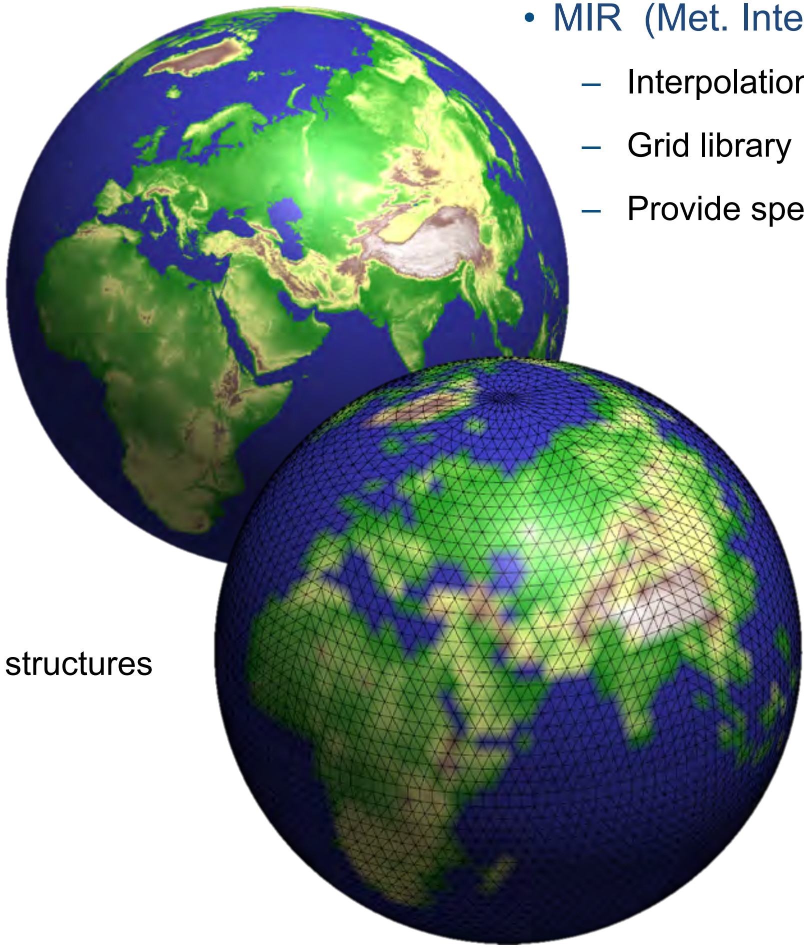
MIR

Similar in Fortran

FVM

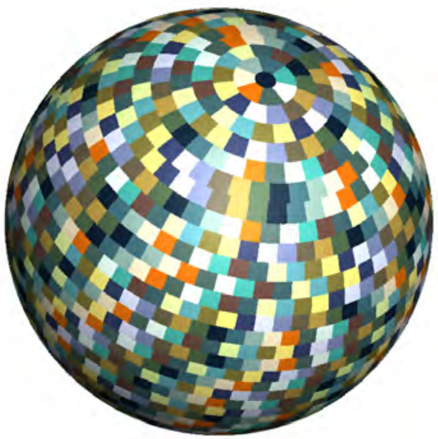
Atlas not the solution (i.e. not the library to develop in), but enabling new research

- ESCAPE dwarfs
  - Object Oriented data structures
  - LAM grids
  - GPU aware memory storage
    - IFS (not operational)
      - Grid-point derivatives
      - Parallel interpolations
      - Multiple grids / coupling



- MIR (Met. Interpol. & Regrid.)
  - Interpolation
  - Grid library
  - Provide spectral transforms

  - MARS
  - MetView
  - prodgen



- FVM
  - Object Oriented data structures
  - Parallelisation

Atlas, a library for NWP and climate modelling

5th ENES HPC Workshop
17-18 May 2018, Lecce

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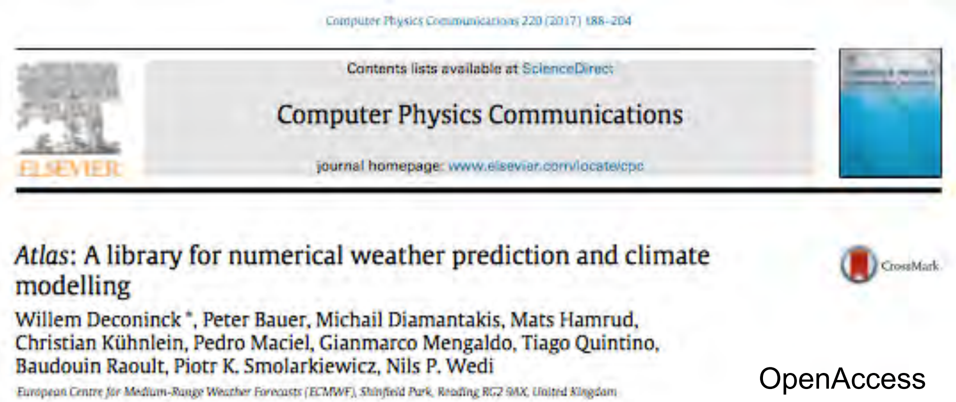
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