LFRic: Introduction and hands-on

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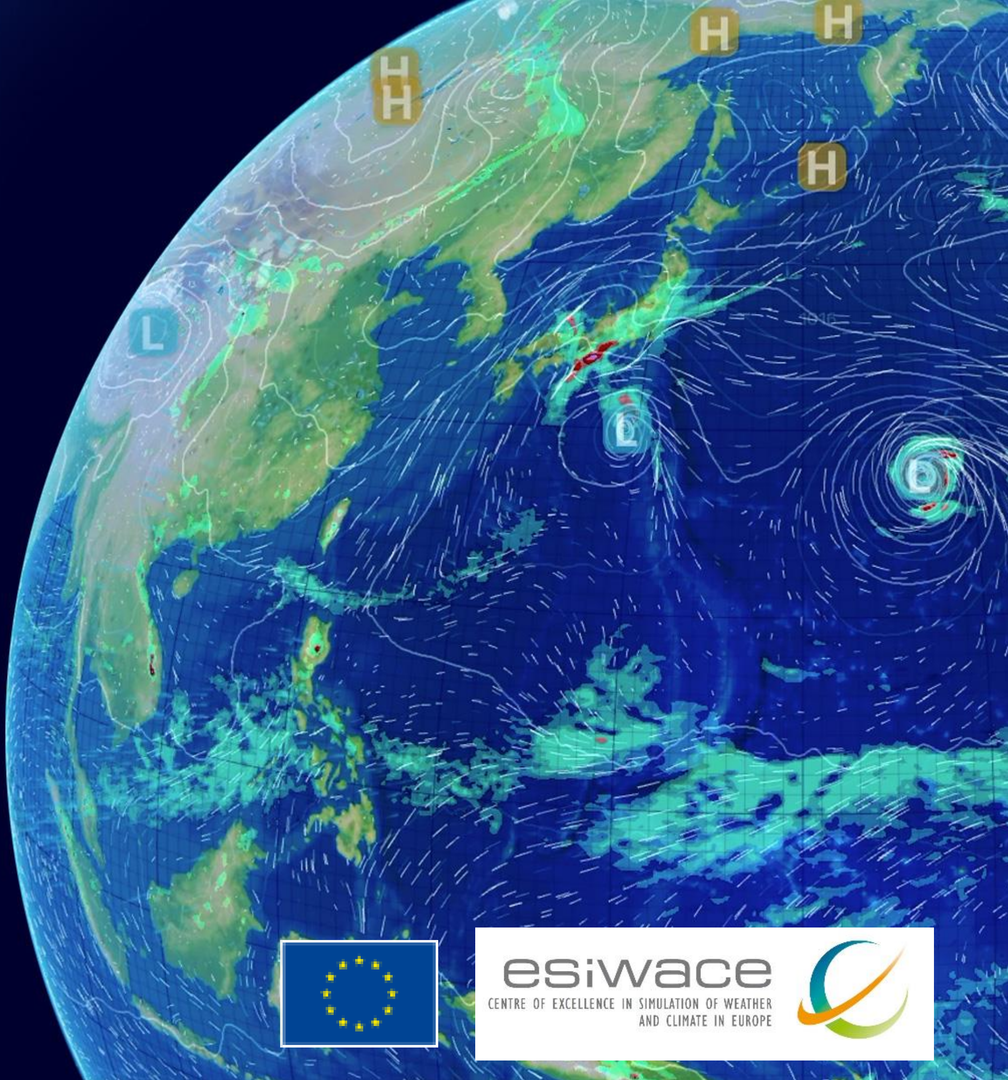
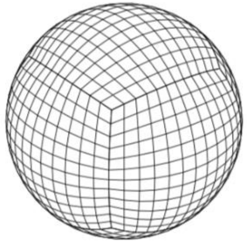
ESiWACE-2 DSL Training, 23 November 2020



LFRic (*after **L**ewis **F**ry **Ric**hardson*) is the new weather and climate modelling system being developed by the UK Met Office to replace the existing Unified Model in preparation for exascale computing in the 2020s

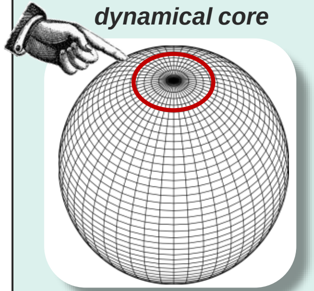
- Uses the **GungHo dynamical core**
- Runs on a **semi-structured cubed-sphere mesh**
- Uses **PSyclone** to generate **parallel code**



PSyclone

Increased resolution in NWP → Exascale computation

Unified Model & ENDGame dynamical core



Need a more scalable dynamical core

Need to make porting the codes from machine to machine easier: Flexible Implementation

New Dynamical Core – GungHo 工合

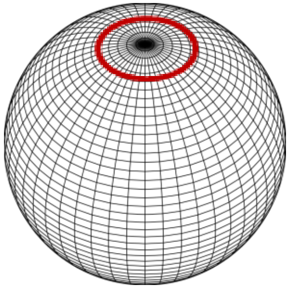
New Infrastructure – LFRic

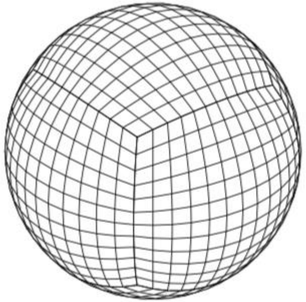
- **GungHo project:** Met Office, NERC (UK Universities) and STFC collaboration (2010 – 2015)
- **Future architectures?** – MPI, OpenMP Accelerators, GPUs, ARM, …?
- Complex parallel code + Complex parallel architectures + Complex compilers = **Complex optimisation space** → no single solution
- *Single source science code & performance portability(???) →* ***generated parallel code***

Conclusions from GungHo

- Keep the best of current MO ENDGame **dynamical core** and **improve** where possible (e.g. conservation)
  - Staniforth & Thuburn (2012) "Ten essential and desirable properties of a dynamical core"
  - Inspired by UM iterative-semi-implicit semi-Lagrangian scheme
- **Layered, "single-model" structure:** separate development teams for science (**GHASP**), infrastructure (**LFRic**) and parallelisation and optimisation (**PSyclone**)
- Optimisations provided by a code generator (***PSy + clone*** = *PSy layer generation*)
- Language: Object-orientated **Fortran 2003**
- Bring in **Physics parameterisations**: Reuse of UM code where possible; Couple these finite-different codes to the new finite-element core

Preparation for exascale: From UM/ENDGame to LFRic/GungHo





Unified Model (UM) & ENDGame dynamical core

- *Staggered Finite Differences (FDM)*
- Fully structured Lat-Lon mesh
- Hard-coded optimisations

LFRic system & GungHo dynamical core

- *Mixed Finite Elements (FEM)*
- Horizontally unstructured, vertically structured quasi-uniform mesh
- Generated optimisations

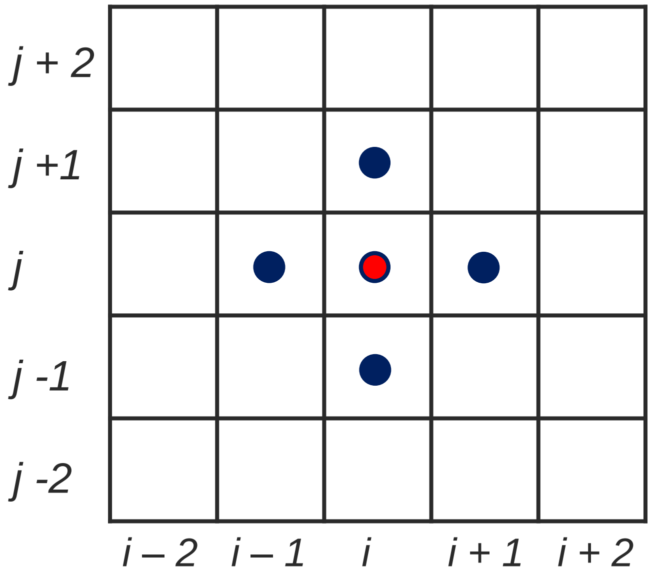
FDM on a structured mesh

- $f(x) \approx p_n(x), \frac{\mathrm{d}f(x)}{dx} \approx \frac{p'_n(x)}{\mathrm{dx}} + O(dx^{(n)})$
- Example: 2D Laplacian, equidistant mesh

$\nabla f(x_i, y_j) \approx [f(x_{i-1}, y_j) + f(x_i, y_{j-1})$ - $4f(x_i, y_j)$
$+ f(x_{i+1}, y_j) + f(x_i, y_{j+1})]/h^2$

→ Mesh layout explicit in the **stencil**: **location** and **connectivity**

→ Stencil representation relatively simple: *go_stencil(010,111,010)* in PSyclone GOcean 1.0 API
(depth and direction information for halo exchages)



$f(x_i, y_j)$

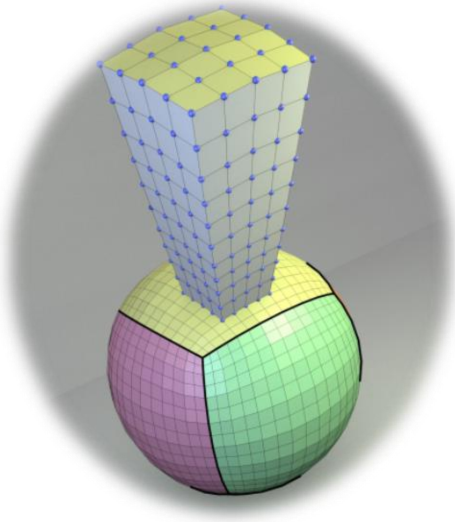
Mixed FEM on a **semi-structured mesh** (software engineers)

Global 2D Mesh
- Entities (vertices, edges, cells)
- Global IDs
- Connectivity (lookup arrays)

Partition
- Strategy (mesh type, ranks)
- Range of cells (owned and halos)
- Interface to distributed memory communication

Local 3D mesh
- Entities (vertices, edges, faces, cells)
- Local IDs
- Connectivity (lookup arrays)

2D cubed-sphere mesh extruded into 3D levels (*courtesy of Ricky Wong, animation on MO LFRic Wiki*)



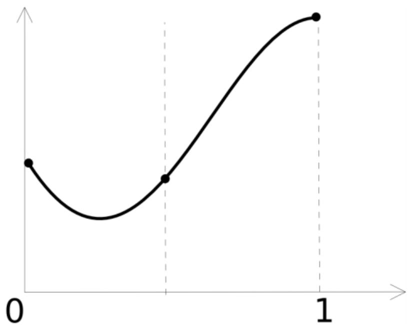
- Horizontal adjacency lost
- **Vertically** adjacent cells **contiguous** in memory → operate on **columns** of data

Mixed **FEM** on a semi-structured mesh

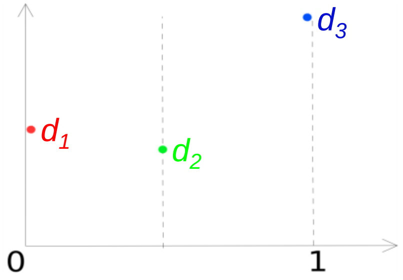
$$f(x) = \sum_{i=1}^{n} d_i \sigma_i(x)$$

Field

$$\sum_{i=1}^{3} =$$



$$\frac{df(x)}{dx} \sim \sum_{i=1}^{n} d_i \frac{d\sigma_i(x)}{dx}$$



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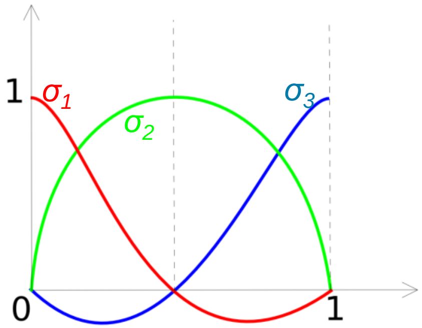


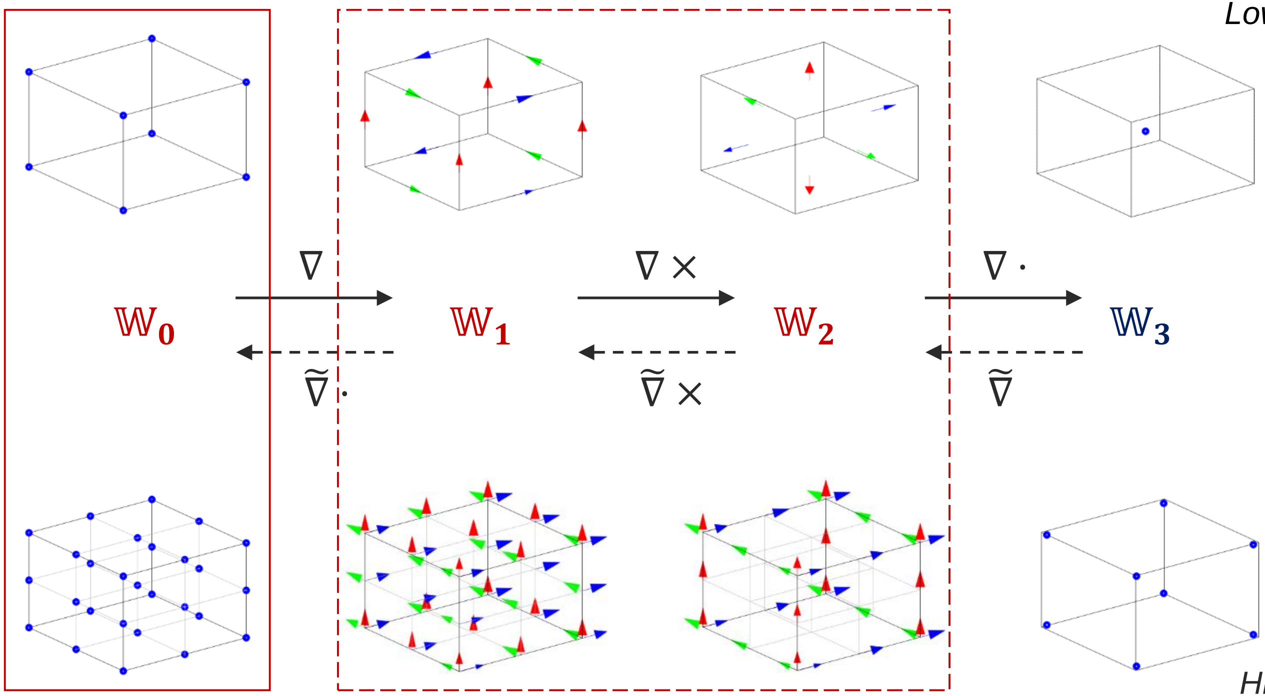
Degrees of Freedom ("dof"s)

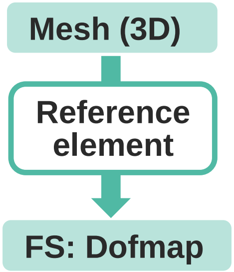
Function Space (FS)

Basis Functions

Mixed FEM (scientists): continuous + discontinuous

Lowest order (k = 0) reference element



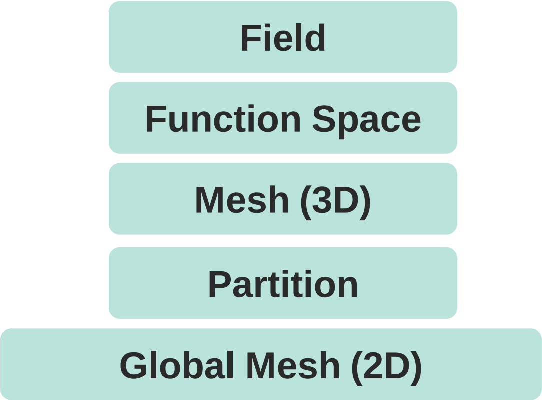


No shared dofs: W_3

Shared dofs: W_0 (fully), W_1 (tangential components) & W_2 (normal components)

Higher order (k = 1) reference element

LFRic hierarchy of classes (data + procedures)



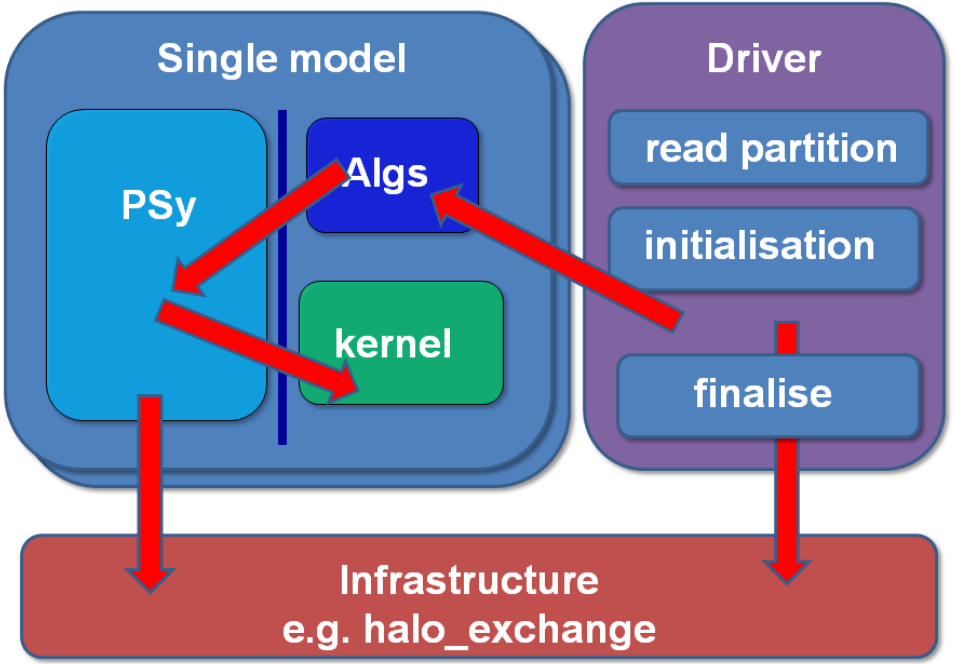
LFRic infrastructure: Hierarchy of classes

Role of infrastructure

- Provide **support** for **science** operations
- Construct and handle **data objects** (e.g. mesh, field, reference element, function space)
- **Support** for **distributed** and **shared memory** parallelism (e.g. dofmap, colouring for FS with shared dofs, halo exchange)
- **Interface** **external libraries** (e.g. YAXT for MPI communications, XIOS for parallel IO)

PSyKAl Separation of Concerns

between parallel code (*PSy*) and science code (*KAl*)



Algorithms (Natural Science: operations on ***whole field objects***)

⇩

Parallel-Systems (Computational Science: accesses field data and applies optimisations – ***generated code***)

⇩

Kernels (Natural Science: operations on ***data points***)

Use of “PSy” + clone in LFRic

- **Optimisations:** generates optimised PSy-layer code *(and soon transformed kernels – work in progress).*
- **Development**
  - Generates **kernel stubs** (argument declarations and ordering).
  - **fparser2** (F2003-2008): base for the **LFRic code style checker**.
- **Tools (profiling, DataAPI)**
  - Insert calls to profiling tools (interface in PSyclone) – tested (and used) in LFRic.
  - Extract data for running smaller code units as stand-alone applications (microbenchmarks) – work in progress.

Rules of engagement: LFRic ⟷ PSyclone Dynamo0.3 API

LFRic

- **Rules** (e.g. writing algorithms & kernels, data properties)
- Kernel **metadata**
- **Infrastructure support** (e.g. dofmap, colouring, MPI)

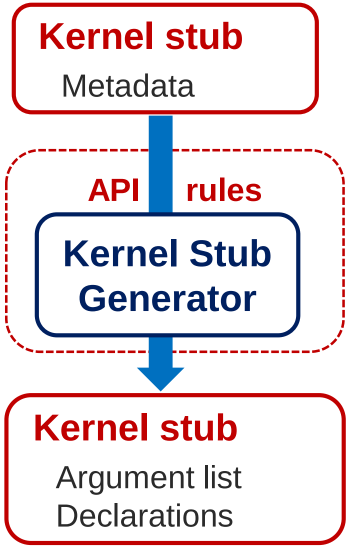
Dynamo0.3 API

- Flexible **optimisations**
- Support for data structures & properties following **API rules**
- Development mandated by requirements

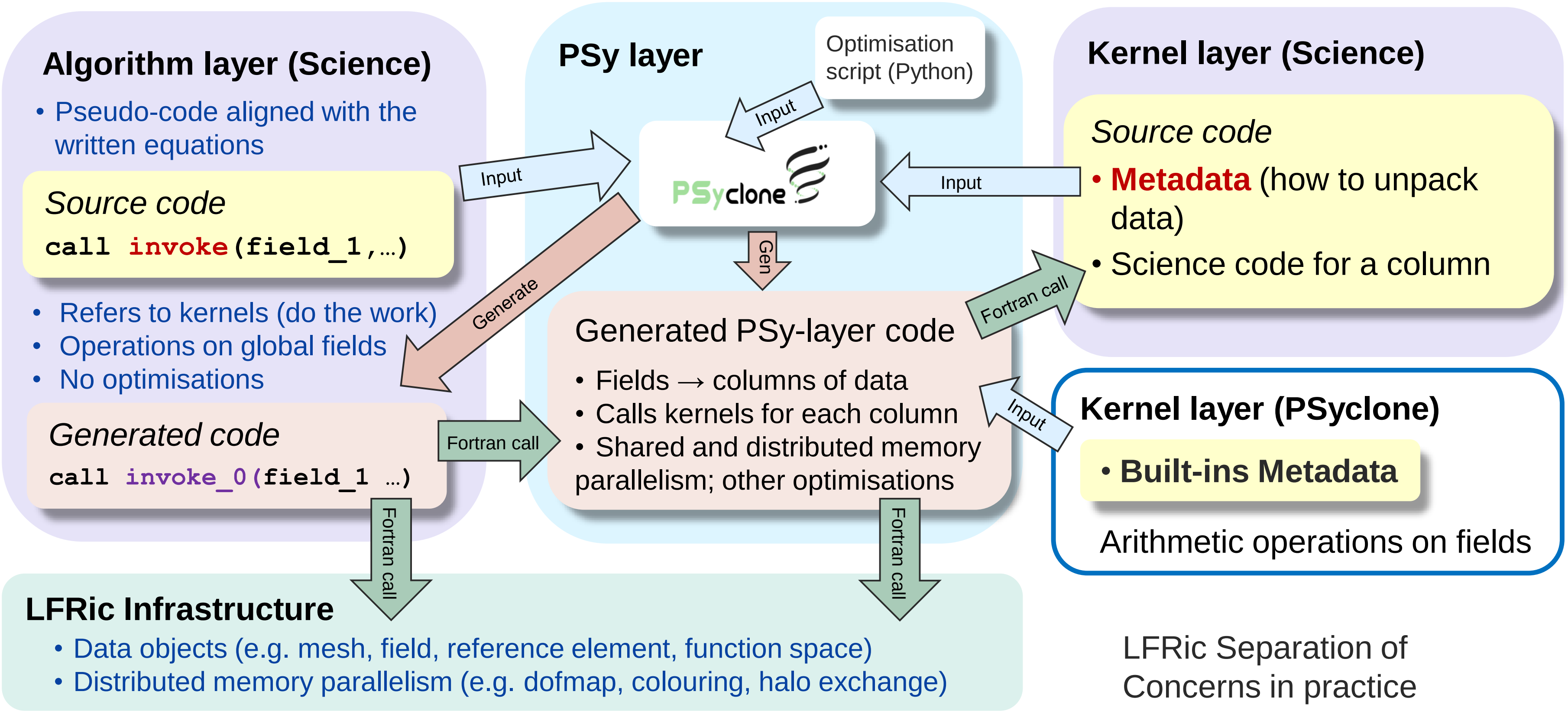
PSyKAl-lite

Required functionality (hand-written)

Kernel Stub Generator (R. Ford & A. Porter): *Metadata + Rules = Help in LFRic development*



DSL in action: LFRic – PSyclone communication



LFRic Separation of Concerns in practice

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LFRic: Algorithm code

Written by Scientists (DSL embedded in Fortran)

```
module lhs_alg_mod
…
 subroutine on_the_fly_lhs_alg(lhs, state, ref_state, … )
   use rtheta_kernel_mod,        only: rtheta_kernel_type
   use matrix_vector_kernel_mod, only: matrix_vector_kernel_type
   implicit none
   type(field_type), target, intent(in) :: state(bundle_size)
   type(field_type), target, intent(inout) :: lhs(bundle_size)
   …
   call invoke( name = "Compute lhs_theta",                         &
                rtheta_kernel_type( lhs_tmp(igh_t), theta_ref, u, qr ), &
                matrix_vector_kernel_type( lhs(igh_t), theta, mm_wtheta ), &
                inc_X_plus_bY( lhs(igh_t), tau_t_dt, lhs_tmp(igh_t) )
  …
  end subroutine on_the_fly_lhs_alg
end module lhs_alg_mod
```

Global fields:

data layout hidden

Kernel (LFRic)

- Loops over columns of cells

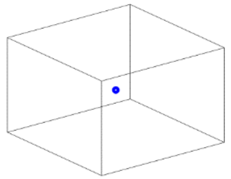
Built-in (PSyclone)

- Loops over all field dofs (arithmetic operations)

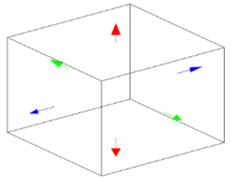
LFRic Kernel code *(Written by Scientists (Fortran))*

Metadata tells PSyclone how to unpack data

```
module rtheta_kernel_mod
…
  type, public, extends(kernel_type) :: rtheta_kernel_type
    private
    type(arg_type) :: meta_args(4) = (/                          &
         arg_type(GH_FIELD, GH_READWRITE, Wtheta),                &
         arg_type(GH_FIELD, GH_READ,      ANY_DISCONTINUOUS_SPACE_1), &
         arg_type(GH_FIELD, GH_INC,       W2),                    &
         arg_type(GH_FIELD, GH_READ,      ANY_SPACE_1),           &
         /)
    type(func_type) :: meta_funcs(2) = (/                        &
         func_type(Wtheta, GH_BASIS, GH_DIFF_BASIS),              &
         func_type(W2,     GH_BASIS, GH_DIFF_BASIS)               &
         /)
    integer :: iterates_over = CELLS
    integer :: gh_shape = GH_QUADRATURE_XYoZ
  contains
    procedure, nopass ::rtheta_code
  end type
…
```

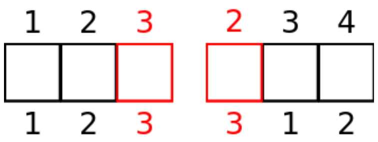


Discontinuous *function spaces: no shared DoFs*



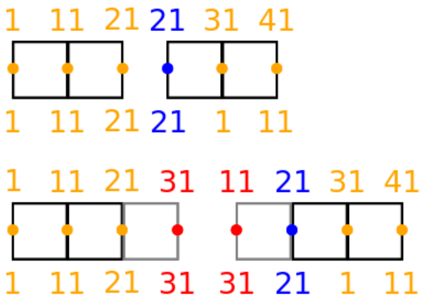
Continuous *function spaces: shared DoFs*

Updating fields in parallel in PSy layer: continuous vs discontinuous spaces



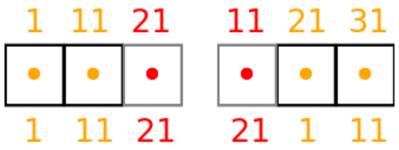
Continuous fields: *PSy-layer* ***cell loop****, kernel calls*

- Dofs on **owned** cells + redundant computation in the level-1 **halo**
- **GH_INC (R + W)** access in kernel code – requires colouring for OpenMP



Continuous fields:
PSy-layer ***DoF loop****, built-in calls*

- **Owned** dofs or redundant computation into **annexed** dofs (configuration option)



Discontinuous fields

- ***Cell loop****:* dofs on **owned** cells (redundant computation optional)
- ***Dof loop****:* **owned** dofs
- **GH_READWRITE (R + W)** or **GH_WRITE (W)** access – no colouring required for OpenMP

LFRic: Kernel code

Written by Scientists ("Fortran 90" style – **no objects allowed!**)

```
…
  subroutine rtheta_code( … r_theta, heat_flux, u, &
…sizes, maps, basis functions,
 quadrature points for all function spaces )
…
    real(kind=r_def), dimension(undf_wtheta), &
                      intent(inout) :: r_theta
    real(kind=r_def), dimension(undf_2d),     &
                      intent(in)    :: heat_flux
    real(kind=r_def), dimension(undf_w2),     &
                      intent(in)    :: u
…
    do k = 0, nlayers-1
      do df = 1, ndf_wtheta
        r_theta( map_wtheta(df) + k ) =  &
        r_theta( map_wtheta(df) + k ) - rtheta_e(df)
      end do
    end do
…
  end subroutine rtheta_code
end module rtheta_kernel_mod
```

Science code for a **column of *nlayers* levels**:

- **k-outer** over cells (layers)
- **dof-inner** over DoFs in a cell

Work in progress:

- *Kernel transformations & loop re-ordering (PSyclone)*
- *i-first fields for Physics parameterisation schemes (LFRic infrastructure and PSyclone)*

Hands-on sessions

https://github.com/stfc/PSyclone/blob/master/tutorial/practicals/LFRic/building_code/README.md

LFRic layers and what we are working on

1. Creating and calling kernels

2. Using built-ins

3. Time evolution of a field (time-permitting)

LFRic Driver layer overview – not for hands-on tutorial

Driver layer: set up and control of a model run

- Set up of the LFRic object stack: **global 2D mesh → partition → local 3D partitioned mesh → function space → field**
- Model initialisation (science configurations, initial data)
- Controls of a model run (e.g. time-step loop, checkpoint) includes wrappers to external libraries (e.g. YAXT, XIOS)

Simplified example in Tutorial 3

LFRic layers for hands-on tutorials

- **Algorithm layer**: Operations on whole field (and other) objects using ***invoke*** DSL syntax
- **Kernel layer**: Operations on field (and other) object data using ***metadata*** DSL syntax and ***loops*** to update data
- **PSy layer**: From algorithms to kernels
  - **Unpacks and access object data via accessor classes (*proxy*)**
  - **Calls kernels for each column**
  - Shared and distributed memory parallelism *(see sessions on distributed and shared memory support)*

Tutorial 1, Part 1: Create simple kernels to update fields on specific LFRic function spaces

https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/building_code/1_simple_kernels/part1

- Open the README.md document in a browser tab
- Open the LFRic kernel structure document in a browser tab
- Open a terminal, make sure that the hands-on environment is working and navigate to

  `tutorial/practicals/LFRic/building_code/1_simple_kernels/part1`
- We will follow steps in the README.md document

Tutorial 1, Part 2: Create simple kernels to update fields on generic LFRic function spaces

https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/building_code/1_simple_kernels/part2

- Open the README.md document in a browser tab
- Open the LFRic kernel structure document in a browser tab
- Open a terminal, make sure that the hands-on environment is working and navigate to

  `tutorial/practicals/LFRic/building_code/1_simple_kernels/part2`

- We will follow steps in the README.md document

Tutorial 2: Using built-ins

https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/building_code/2_built_ins

- Open the README.md document in a browser tab
- Open the PSyclone LFRic (Dynamo 0.3 API) built-ins documentation in a browser tab
- Open a terminal, make sure that the hands-on environment is working and navigate to

  `tutorial/practicals/LFRic/building_code/2_built_ins`
- We will follow steps in the README.md document

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Tutorial 3: Time evolution of a field on a planar mesh

https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/LFRic/building_code/3_time_evolution

- Open the README.md document in a browser tab
- Open a terminal, make sure that the hands-on environment is working and navigate to

  `tutorial/practicals/LFRic/building_code/3_time_evolution`

- We will follow steps in the README.md document

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Questions?

Acknowledgements

LFRic team, GungHo Atmospheric Science team and other LFRic developers

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Links and references

- LFRic: https://code.metoffice.gov.uk/trac/lfric/wiki
- LFRic container recipes (to be hosted on https://github.com/MetOffice):
  - https://github.com/eth-cscs/ContainerHackathon/tree/master/LFRIC
  - https://github.com/tinyendian/lfric_reader
- PSyclone and fparser
  - https://github.com/stfc/PSyclone
  - https://psyclone.readthedocs.io
  - https://github.com/stfc/fparser
  - https://fparser.readthedocs.io
- PSyclone in LFRic: https://code.metoffice.gov.uk/trac/lfric/wiki/PSycloneTool
- GHASP (GungHo Atmospheric Science): https://code.metoffice.gov.uk/trac/lfric/wiki/GungHoScience
- stylist: https://github.com/MetOffice/stylist
- Adams et al. (2019), *LFRic: Meeting the challenges of scalability and performance portability in Weather and Climate models*, Journal of Parallel and Distributed Computing,132, 383-396