LFRic approach to performance portability

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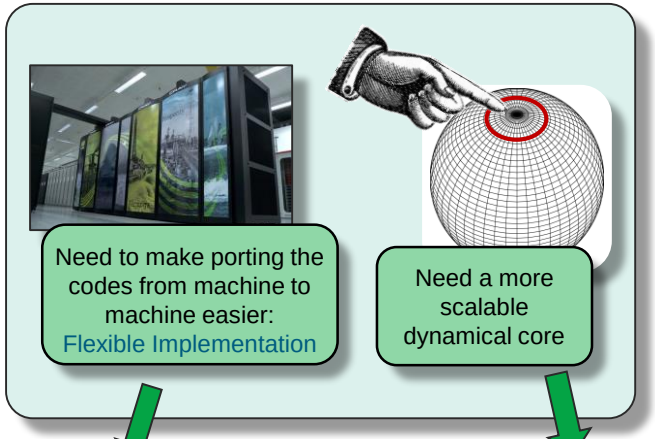
Overview

What is LFRic and how it talks to PSyclone

Utilising API information for performance

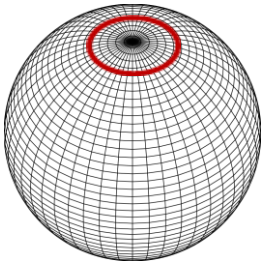
Summary

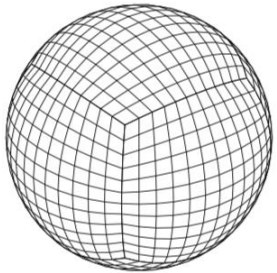
In the beginning: GungHo project



- Met Office, NERC (UK Universities) and STFC collaboration (2010 – 2015)
- Future architectures - MPI? OpenMP? Accelerators? GPUs? ARM? …?
- Increased resolution → exascale computation
- Scientific code can be ~ 10^6 lines (of Fortran)
- Complex parallel code + Complex parallel architectures + Complex compilers = Complex optimisation space => no single solution
- Single source science code & Performance portability

LFRic/GungHo: Preparation for exascale





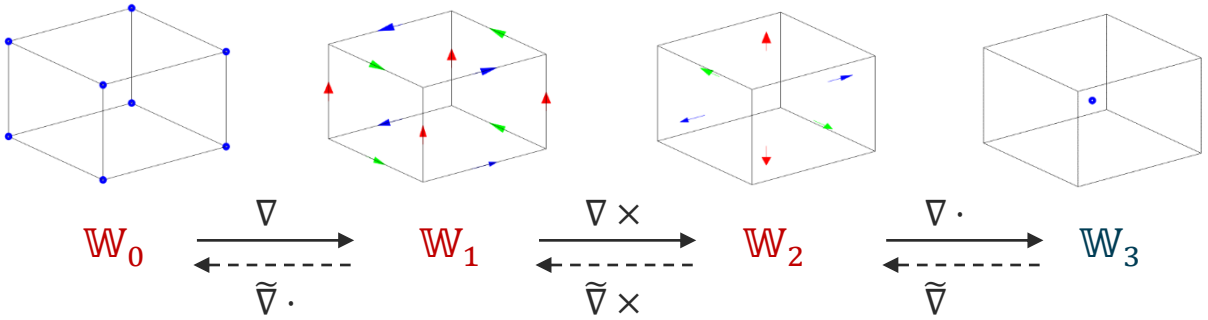
Unified Model (UM) & ENDGame dynamical core

- Staggered Finite Differences
- Fully structured Lat-Lon mesh
- Hard-coded optimisations

LFRic system & GungHo dynamical core

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

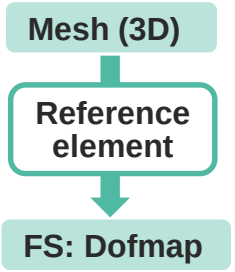
Mixed FEM (continuous + discontinuous)



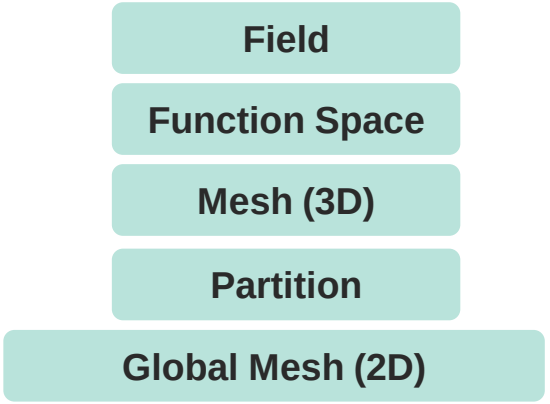
Lowest order (k = 0) reference element

Shared dofs (degrees of freedom):
W_0 (all), W_1 (tangential components) & W_2 (normal components)

No shared dofs: W_3



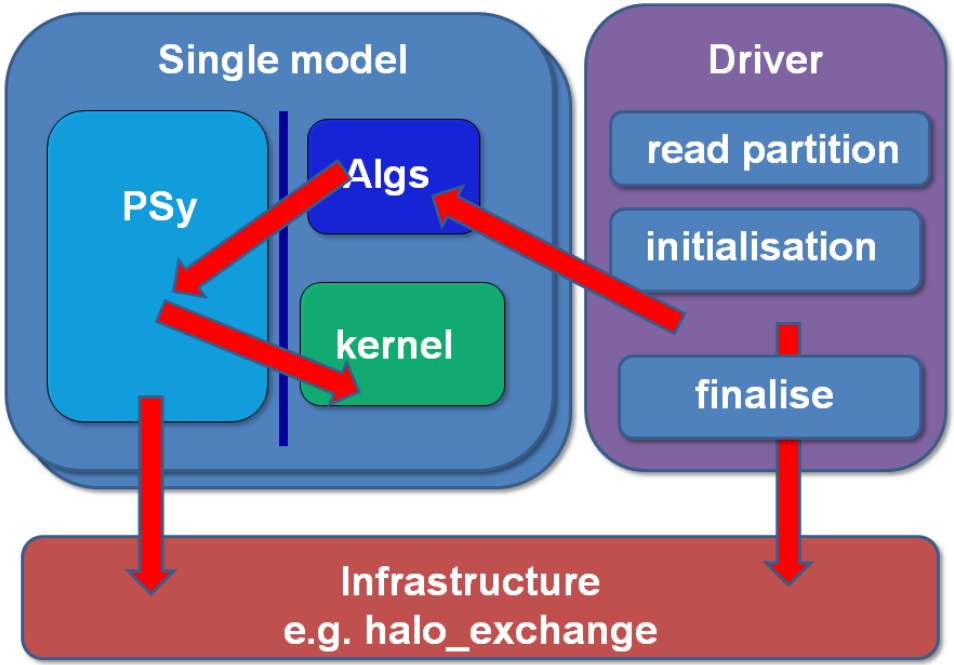
LFRic infrastructure: Hierarchy of objects



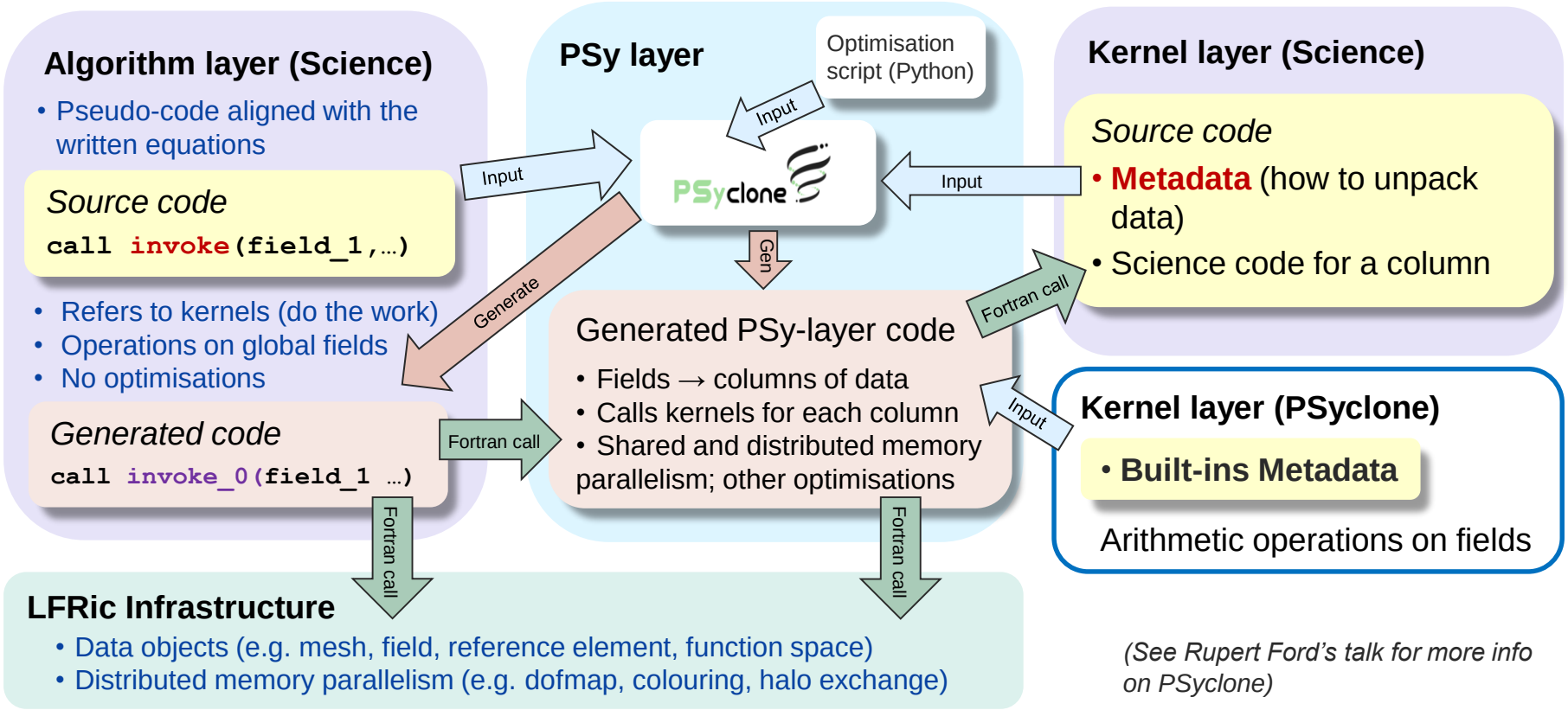
Separation of Concerns

PSyKAl

- **Parallel-Systems:** Computational Science, applies optimisations – ***generated code***
- **Kernels:** Natural Science, operations on (columns of) data points
- **Algorithms:** Natural Science, operations on whole fields



PSyKAl Infrastructure in LFRic: Parallel-Systems, Kernels, Algorithms

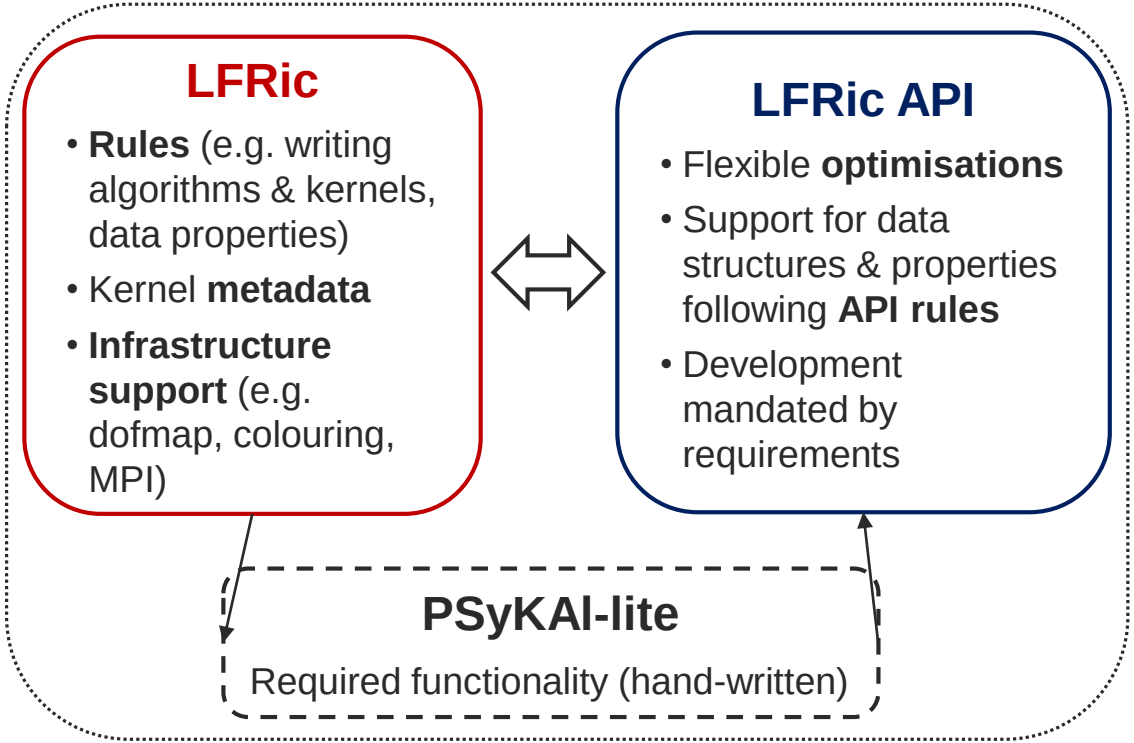


(See Rupert Ford's talk for more info on PSyclone)

Use of “PSy + clone” in LFRic

- **Optimisations:** generates optimised PSy-layer code *(and soon transformed kernels – work in progress).*
  - Optimisations encoded as a ‘recipe’ rather than baked into the scientific source code.
  - Different recipes for different architectures.
- **Development**
  - Generates **kernel stubs** (argument declarations and ordering).
  - **fparser2** (F2003-2008) parses LFRic code (also tested on the Unified Model) and 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 (micorbenchmarks) – work in progress.

Rules of engagement: LFRic ⟷ PSyclone LFRic API



Distributed + shared memory parallelism

PSyclone transformations

- Dynamo0p3ColourTrans
- Dynamo0p3OMPLoopTrans
- OMPParallelTrans

⇩

LFRic support

- Halo exchange
- Colouring (cell & halo) for fields on continuous FS

…

LFRic: Kernel code

Written by Scientists (Fortran)

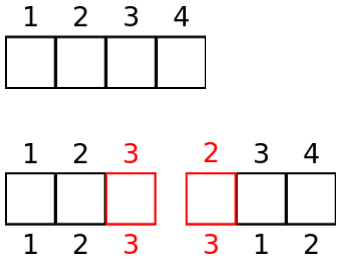
Metadata tells PSyclone how to unpack data

```
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
…
```

Science code for a column of *nlayers* levels

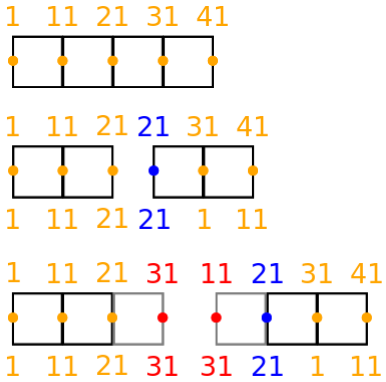
```
…
   subroutine rtheta_code( … r_theta, heat_flux, u, &
…sizes, maps, basis functions,
 quadrature points for all function spaces )
…
    real(kind=r_def), dimension(undf_wtheta), &
                      intent(inout) :: r_theta
    real(kind=r_def), dimension(undf_2d),     &
                      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
```

Updating fields on continuous vs discontinuous spaces



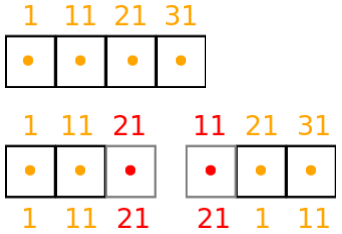
Continuous fields (cell loop)

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



Continuous fields (dof loop)

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



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
- *Kernel code*

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Example of optimisation based on API knowledge

- LFRic utilises existing parameterisation schemes for UM *(until they need to be refactored).*
- **Interfacing** ("Physics" kernels) **UM Physics**, **SOCRATES** ("Suite Of Community RAdiative Transfer codes") and **JULES** (land surface) models.
- Consequences: "stuck" with data layout and hard-coded OpenMP implementation for UM, **limited scope for optimisation** (e.g. for now not safe to call UM Physics with more than 1 thread).
- **PSyclone: ANY_DISCONTINUOUS_SPACE** metadata in LFRic "Physics" kernels and **redundant computation** switch to **reduce communication costs** (number of halo exchanges).

Halo exchanges	**C48: 6*48*48 columns, ≈ 200 km in horizontal**			**C96: 6*96*96 columns, ≈ 100 km in horizontal**		
Application	**AC**	**AD**	**AD+RC**	**AC**	**AD**	**AD+RC**
lfric_atm	324002	285919 (88.24 %)	150649 (46.49 %)	354851	312403 (88.03 %)	164024 (46.22 %)
slow_physics	5997	576 (9.6 %)	0	5997	576 (9.6 %)	0
fast_physics	15961	14046 (88 %)	10430 (65.35 %)	16009	14094 (88.03 %)	10454 (65.3 %)

Aquaplanet runs:
38 vertical levels,
dt = 300 s,
multigrid solver (4 levels)

ANY_**S**PACE (general function space, assumes continuity); **A**NY_**D**ISCONTINUOUS_SPACE ("knows" that most Physics schemes are cell-volume based, no shared dofs); **AD** and **R**edundant **C**omputation into annexed dofs.

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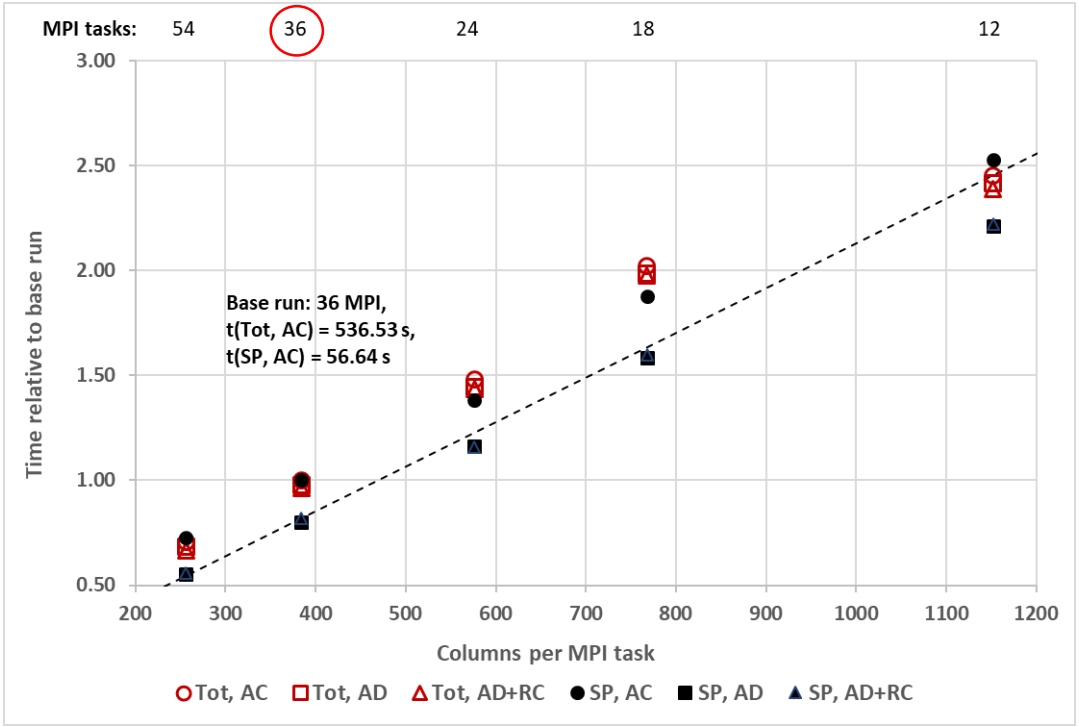
Aquaplanet run, C48 MG (6*48^2 columns ≈ 200 km hor; L38; dt = 300 s)

(Cray XC40/XCS, Aries interconnect, dual socket 18-core Broadwell Intel Xeon node, i.e. 36 CPU cores per node)



Speed-up (%) compared to runtime of AC Physics metadata runs (**Tot**al, **S**low **P**hysics and **F**ast **P**hysics runtimes)

Col per task	Tot, AD	SP, AD	FP, AD
256	2.83	23.84	2.56
384	2.46	20.09	3.35
576	2.44	16.03	1.16
768	1.82	15.58	1.89
1152	1.53	12.61	1.79

Col per task	Tot, AD+RC	SP, AD+RC	FP, AD+RC
256	5.63	23.40	6.48
384	3.62	18.22	4.46
576	3.28	16.09	2.42
768	2.38	14.97	3.19
1152	2.72	12.11	2.26

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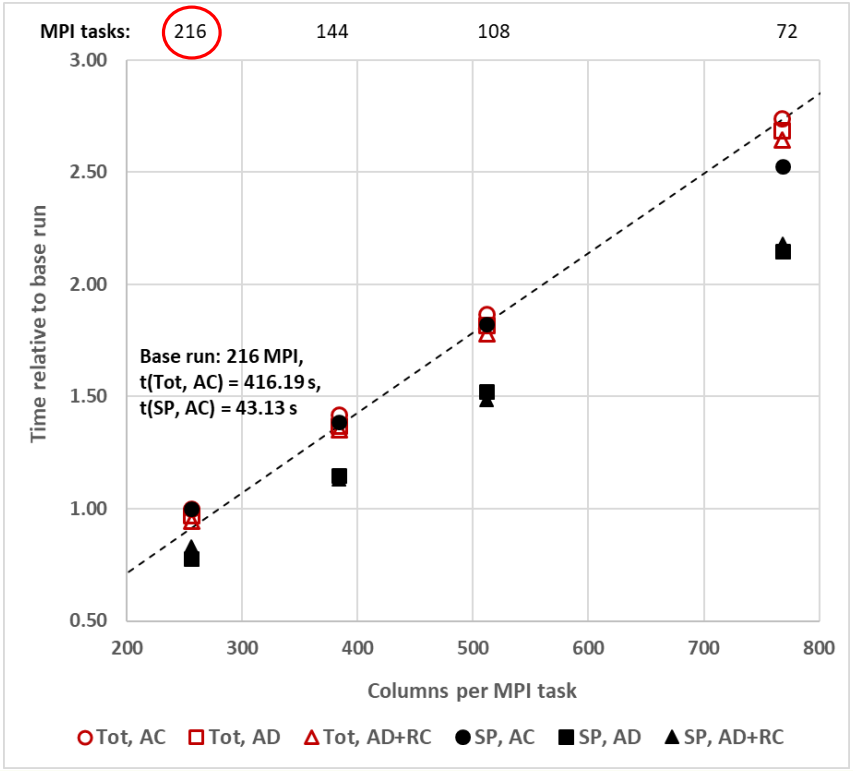
Aquaplanet run, C96 MG (6*96^2 columns ≈ 100 km hor; L38; dt = 300 s)

(Cray XC40/XCS, Aries interconnect, dual socket 18-core Broadwell Intel Xeon node, i.e. 36 CPU cores per node)



Speed-up (%) compared to runtime of AC Physics metadata runs (**Tot**al, **S**low **P**hysics and **F**ast **P**hysics runtimes)

Col per task	Tot, AD	SP, AD	FP, AD
256	3.25	22.14	4.37
384	3.42	17.15	3.80
512	2.60	16.62	3.04
768	1.98	15.00	2.75

Col per task	Tot, AD+RC	SP, AD+RC	FP, AD+RC
256	5.41	16.81	4.94
384	4.70	18.44	3.73
512	4.53	18.59	4.40
768	3.40	13.80	4.06

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Summary and (some) work in progress

- Separation of concerns → flexible optimisations
- Flexible optimisations + API knowledge → performance improvements

Work in progress (and future)

- Implement kernel transformation and optimisation
- Kernel extraction (creating microbenchmarks)
- Portability
  - Run LFRic with GPU (start with OpenACC from PSyclone NEMO API)
  - LFRic container tests on PizDaint (Broadwell - baseline) and Hawk (AMD)

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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