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PSyclone, a source-to-source transformation and optimisation tool for Fortran

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ExCALIBUR Workshop, 17th-18th October, 2024

Overview

1. Motivation
2. PSyclone in ExCALIBUR
    1. Marine-systems models
    2. OpenMP Tasking
    3. [xDSL]
3. Conclusions

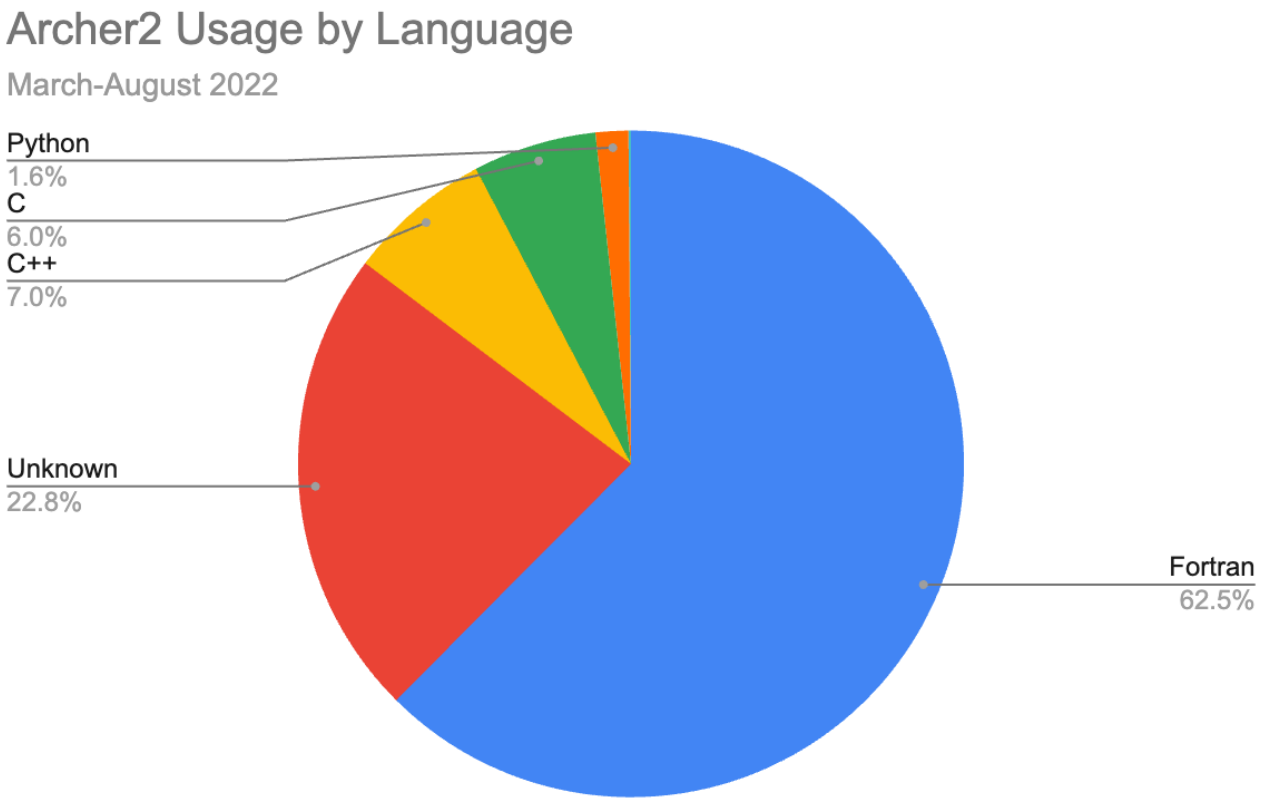
1. Motivation

HPC is heterogeneous (and diverse)

Top 500 June ‘24 list

#	Name	Processor	Linpack PFlop/s
1	Frontier	AMD EPYC Milan 64c AMD Instinct MI250X	1,207
2	Aurora	Intel Xeon Max 9470 52c Intel Data Center GPU Max	1,012
3	Eagle	Intel Xeon Platinum 8480C 48c Nvidia H100	846
4	Fugaku	Fujitsu A64FX 48c	442
5	Lumi	AMD EPYC Milan 64c AMD Instinct MI250X	379
6	Alps	Nvidia Grace 72c Nvidia GH200	270
7	Leonardo	Intel Xeon Platinum 8358 32c Nvidia A100 SMX4	241

Many HPC applications still use Fortran



Code	Language	Percentage use
VASP	Fortran	27.29%
Unidentified	Unknown	22.35%
CP2K	Fortran	6.28%
GROMACS	C	4.53%
CASTEP	Fortran	4.03%
Met Office UM	Fortran	3.10%
SENGA	Fortran	2.92%
Nektar++	C++	2.81%
NEMO	Fortran	2.46%
LAMMPS	C++	2.40%
PDNS3D	Fortran	1.89%
iIMB	Fortran	1.71%

Source: https://cpufun.substack.com/p/is-fortran-a-dead-language - Jim Cownie
https://www.archer2.ac.uk/support-access/status.html#:~:text=0.0-,Historical%20usage%20data,-Period

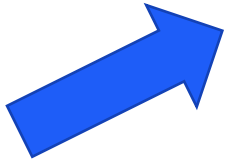
Collaborative development

- Some applications have many contributors from multiple institutions:
  - Run on different systems in each institution. Hard to maintain multiple implementations. It must be portable.
  - Contributors from different areas of expertise. Productivity, readability, maintainability are essential for the sustainability of the project.
  - Millions LOCs of FORTRAN (validated long-standing code).
  - Rewriting existing applications in a GPU-centric programming model is a challenging proposition.

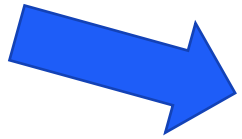
Fortran

```
A = B + maxval(C(:,3:8))
```

- High-level array notation
- Array intrinsics
- Slices
- Pure, Elemental
- Where, Masks
- Non-aliasing semantics



Expressive syntax



Good for optimising compilers

Fortran vs heterogeneous Fortran

```
A = B + maxval(C(:,3:8))
```

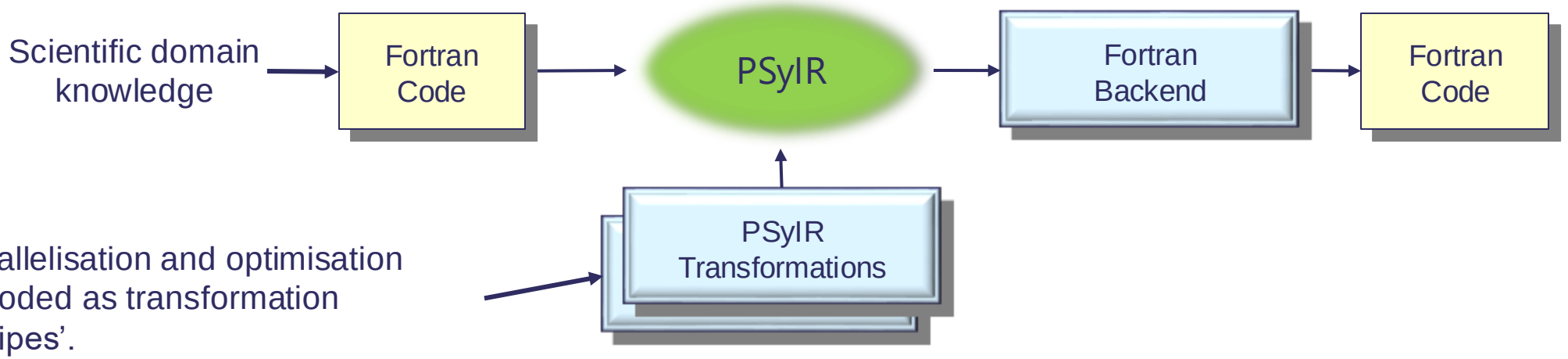
```
!$omp map data(from: B, C)
tmp = -huge(C)
!$omp target
!$omp loop collapse(2) reduction(tmp:max)
do i=1, N
    do j=3, 8
        tmp = max(tmp, C(i, j))
    end do
end do
!$omp end loop
!$omp loop collapse(2)
do i=1, N
    do j=1, M
        A(i,j) = B(i,j) + tmp
     end do
end do
!$omp end loop
!$omp end target
!$omp map data (to: A)
```

- Loses terse notation
- Harder to maintain, changing a line easily breaks directives

Is metaprogramming a solution?

- Start from a single-source science description in Fortran
- At build time generate the required specialised syntax to target a particular platform / programming model / set of parameters.

PSyclone (BSD 3-clause)
https://github.com/stfc/PSyclone



Separation of concerns

Perf portability: diff. recipes for each architectures

Visible "*readable*" output Standard debugging/profiling

Standard output composable w. other tools and vendor compilers

2. PSyclone for Marine Systems Models

Excalibur Marine Systems (‘nemo’) Design

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Hartree Centre
Met Office
National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL
NVIDIA
National Oceanography Centre

NEMO Ocean Model

- **N**ucleus for **E**uropean **M**odelling of the **O**cean (https://www.nemo-ocean.eu/)
- Written in Fortran (120 kLOCs) with MPI
- NEMO is intended to be a flexible tool for studying the ocean and its interactions with the other components of the earth climate system (atmosphere, sea-ice, biogeochemical tracers) over a wide range of space and time scales.
- The NEMO Consortium comprises five European institutes:

Fortran with PSyclone: NEMO loop example

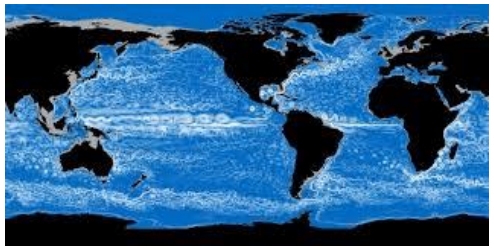
```
do jk = 1, jpkm1, 1
  zun(:,:,jk) = e2u(:,:) * e3u_n(:,:,jk) &
              & * (un(:,:,jk) + usd(:,:,jk))
enddo
```

```
for subroutine in psyir:

    for assign in subroutine.walk(Assignment):
        ArrayRange2LoopTrans.apply(assign)

    for loop in subroutine.walk(Loop):
        try:
            OMPLoopTrans().apply(loop)
            directive = loop.ancestor(Directive)
            OMPTargetTrans().apply(directive)
        except TransformationEror as err:
            print("Loop not accelerated:", err)
```

```
!$omp target
!$omp loop collapse(3)
do jk = 1, jpkm1, 1
  do idx_6 = LBOUND(zun, dim=2), UBOUND(zun, dim=2), 1
    do idx_7 = UBOUND(zun, dim=1),LBOUND(zun, dim=1), 1
      zun(idx_7,idx_6,jk) = e2u(idx_7,idx_6) * e3u_n(idx_7,idx_6,jk) &
                          & * (un(idx_7,idx_6,jk) + usd(idx_7,idx_6,jk))
    enddo
  enddo
enddo
!$omp end loop
!$omp end target
```

Can also contain domain specific logic and whole program optimisation!

NEMO 4 PSyclone-accelerated for GPUs

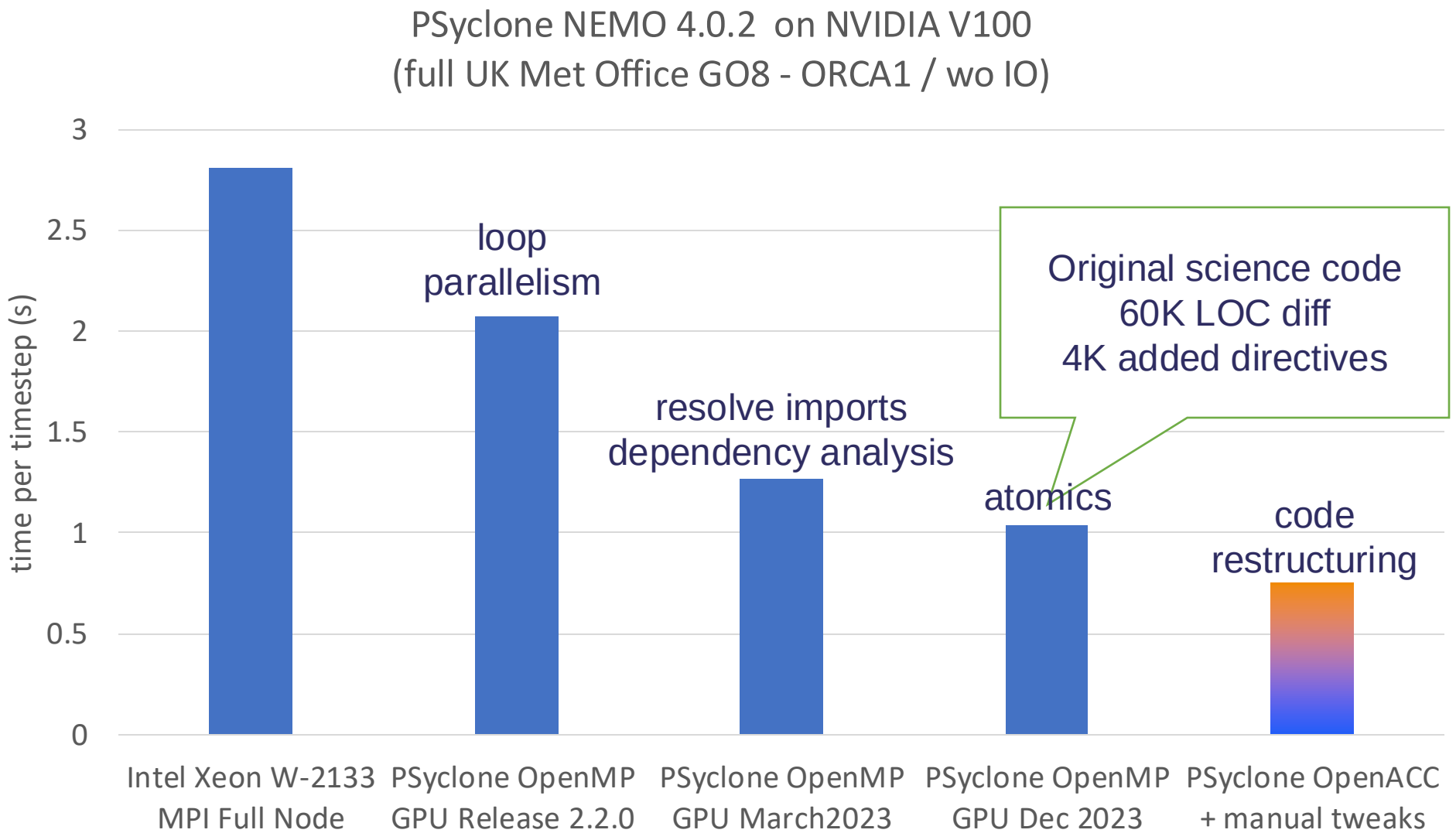


CPU:
Intel Xeon W-2133

GPU:
NVIDIA V100

Blue: original source
Orange: manual opt

Transformation:
~200 LOCs



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PSyclone for code transformation

- Provide performance portability to existing science code, incremental development.
- Successful at porting data-parallel, loop-centric code that already has MPI to GPUs.
- Performance portability can be fragile to code changes
  (DSL improves on this but not the subject of ExCALIBUR)

2. OpenMP Tasking in PSyclone

Excalibur Cross-Cutting Theme on Tasking

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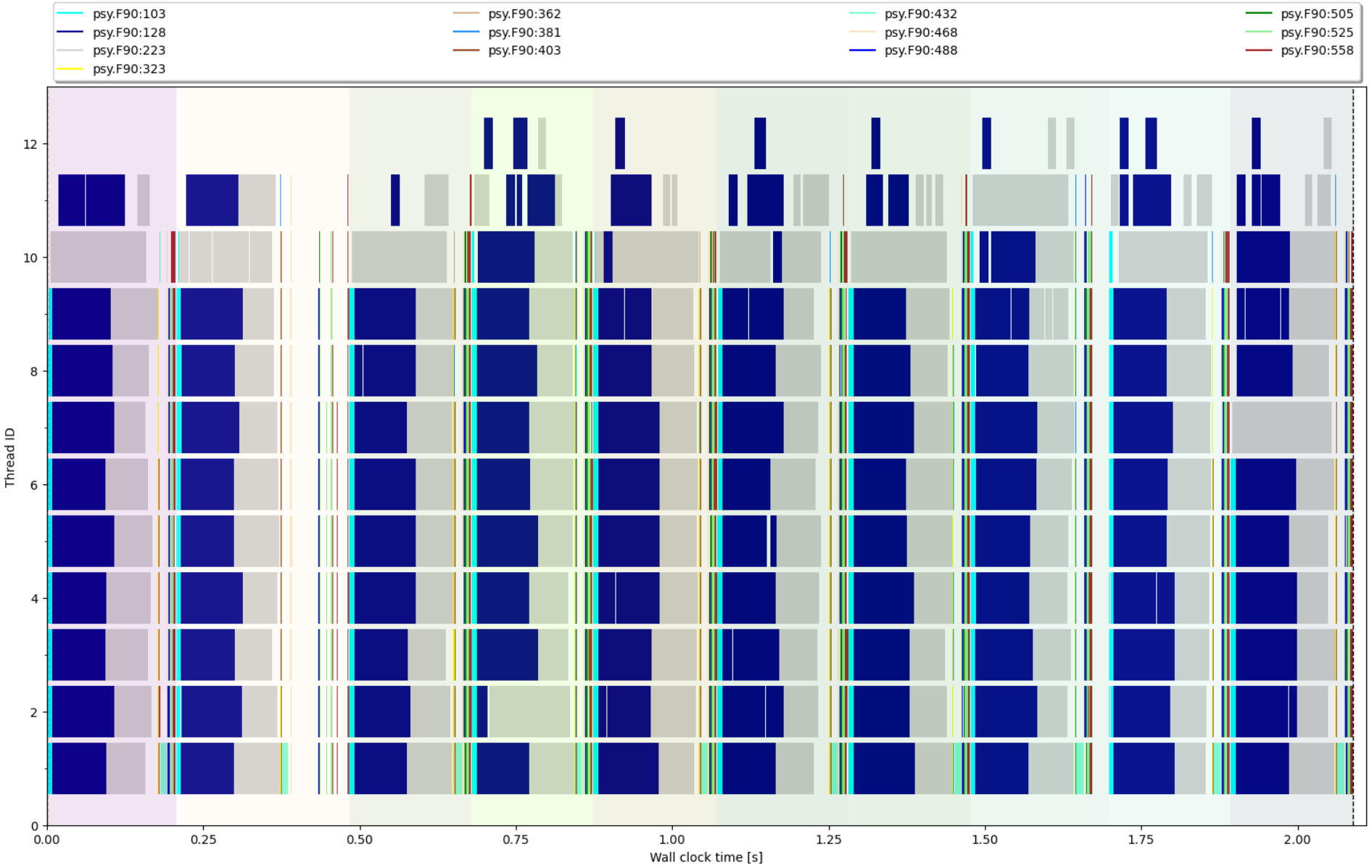
OpenMP tasking in PSyclone

- Goal: Can PSyclone add tasking into the generated code.
  - Primarily focused on the code transformation frontend in this project
- Strategy: Split loops into chunks, parallelise inner loop with tasks and dependencies.

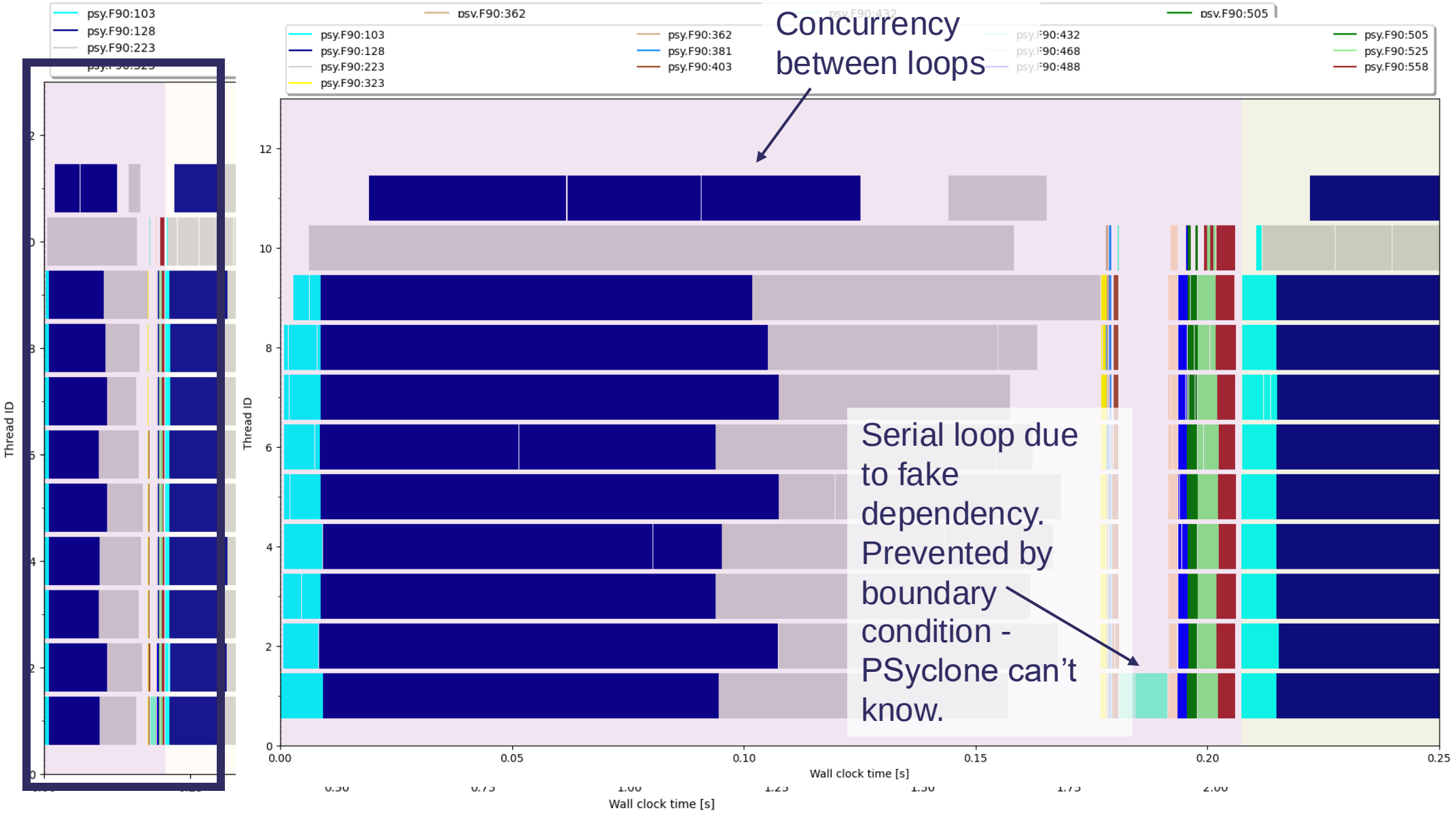
```
Do i = 1, N, 32
    !$omp task depend(.......)
      do j = i, i + 32, 1
```

- Challenges:
  - Dependency analysis to generate the depend clause(s).
  - Analysis of generated clauses to ensure correctness (`a(1:32)` and `a(2:31)` are *not* dependent in OpenMP 5.1 spec).

NemoLite2D Benchmark breakdown



NemoLite2D Benchmark Results - zoom



OpenMP Tasking Conclusions

- PSyclone is now capable of adding OpenMP tasking with dependencies into some code paths.
  - Full support for LFRic was too complex for this project's timeline.
- Performance can be competitive with traditional OpenMP looping code.
  - To be worthwhile, need a case with dependent loops with load imbalance, e.g. a lot of boundary condition sections.
- Some of the developments and improvements will benefit all future PSyclone development:
  - PSyclone may use a similar but simpler dependency analysis approach to launch `target` regions with `nowait` and add appropriate `taskwait` barriers into the code to increase GPU utilisation.

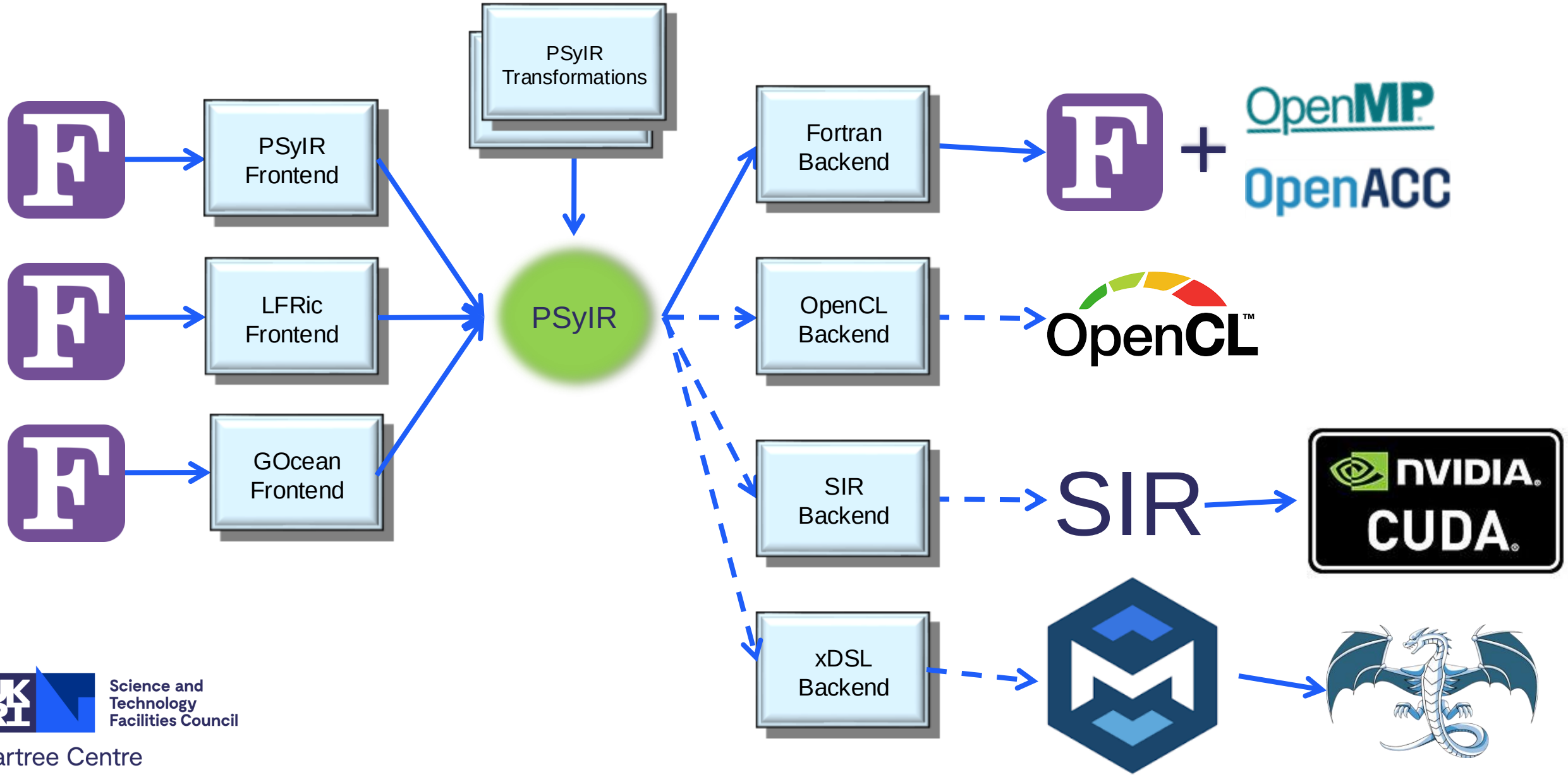
3. [PSyclone and xDSL]

Excalibur Cross-Cutting Theme on DSLs

Multi-Level Intermediate Representation

- Open-source compiler infrastructure, originally developed by Google
- “multi-level”: able to define multiple dialects and progressively convert towards machine code. This allows MLIR to retain information at a higher level of abstraction, which enables more accurate analyses and transformations.

PSyclone & xDSL



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Takeaways

- PSyclone is a Fortran source-to-source compiler that can be used with existing science code and to write DSLs.
- Provides separation of concerns and a tool for HPC experts.
- Support for
  - OpenMP threading, tasking and offload
  - OpenACC offload
  - Generic code transformations (inlining, hoisting, intrinsic replacement)
- Used with production/full configurations:
  - LFRic (multi-node parallelism for UK Met Office's atmospheric model)
  - NEMO (integrated in the build system and GPU demonstrator)
- Ongoing work on generalising the code-transformation approach and improving GPU offloading capabilities, especially within NG-Arch.

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Thank you

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