An Introduction to PSyclone

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ESIWACE2 training course on Domain-specific Languages in Weather and Climate, 23rd-27th November 2020

Overview

- Motivation
- PSyclone
  - What it is and what it does
  - Modes of Operation
  - Levels of Abstraction
- The LFRic Domain
- The GOcean Domain
- The NEMO Domain
- Other Features

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Motivation

See previous talk on DSLs but essentially:

- 3P's : Performance, Portability and Productivity
  - Maintainable high performance software
  - Single-source science code
  - Performance portability
- Complex parallel code + Complex parallel architectures + Complex compilers = Complex optimisation space => unlikely to be a single solution
- Single-source optimised code is unlikely to be possible
- So … separate science specification/code from code optimisation

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PSyclone 1.9.0
BSD 3-clause
https://github.com/stfc/PSyclone
https://psyclone.readthedocs.io

```
> pip install psyclone
```

- A domain-specific compiler for embedded DSL(s)
  - Configurable: FD/FV NEMO, GOcean, FE LFRic
  - Currently Fortran -> Fortran/OpenCL
  - Supports distributed- and shared-memory parallelism
  - Supports code generation and code transformation
- A tool for use by HPC experts
  - Hard to beat a human (debatable)
  - Work round limitations/bugs
  - Optimisations encoded as a 'recipe' rather than baked into the scientific source code
  - Different recipes for different computer architectures
  - Enables scriptable, whole-code optimisation

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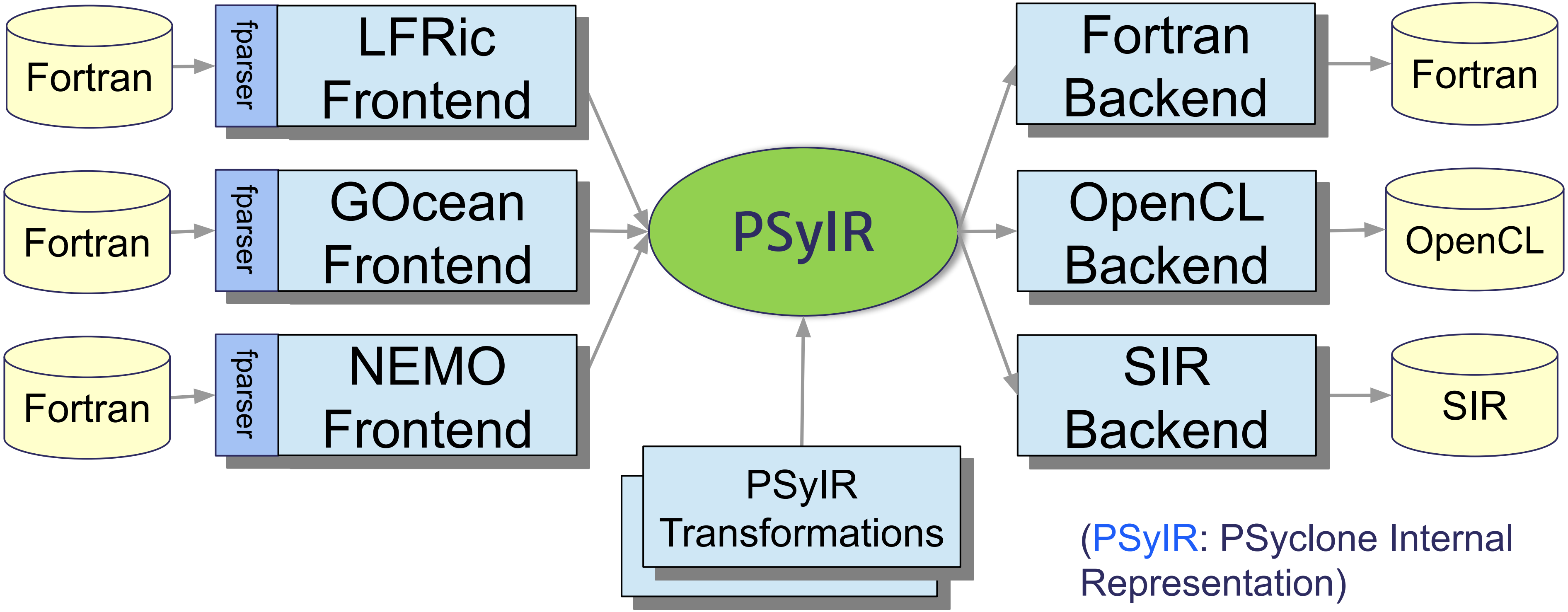
Basic Structure



(PSyIR: PSyclone Internal Representation)

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Fparser

Pure Python Fortran parser:

- Supports Fortran 2003 + some 2008
- Open source BSD3 licence
- Developed on GitHub
- Can fully parse UM, LFRic and NEMO source
- Work-in-progress to parse IFS source
- Used by PSyclone, Stylist, Loki

https://github.com/stfc/fparser
https://fparser.readthedocs.io/

```
> pip install fparser
```

```fortran
PROGRAM copy_stencil
  IMPLICIT NONE
  INTEGER, PARAMETER :: n = 10, np1 = 11
  INTEGER :: i, j, k
  REAL, DIMENSION(np1, n, n) :: out, in
  DO k = 1, n
    DO j = 1, n
      DO i = 1, n
        out(i, j, k) = in(i + 1, j, k)
```

```
child type =  <class 'fparser.two.Fortran2003.Execution_Part'>
  child type =  <class 'fparser.two.Fortran2003.Block_Nonlabel_Do_Construct'>
    child type =  <class 'fparser.two.Fortran2003.Nonlabel_Do_Stmt'>
      child type =  <class 'str'> 'DO'
      child type =  <class 'fparser.two.Fortran2003.Loop_Control'>
        child type =  <class 'NoneType'>
        child type =  <class 'tuple'>
        child type =  <class 'NoneType'>
    child type =  <class 'fparser.two.Fortran2003.Block_Nonlabel_Do_Construct'>
      child type =  <class 'fparser.two.Fortran2003.Nonlabel_Do_Stmt'>
        child type =  <class 'str'> 'DO'
        child type =  <class 'fparser.two.Fortran2003.Loop_Control'>
          child type =  <class 'NoneType'>
          child type =  <class 'tuple'>
          child type =  <class 'NoneType'>
      child type =  <class 'fparser.two.Fortran2003.Block_Nonlabel_Do_Construct'>
        child type =  <class 'fparser.two.Fortran2003.Nonlabel_Do_Stmt'>
          child type =  <class 'str'> 'DO'
```

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PSyclone: Two Modes of Operation

Revolution

Process code written in a DSL

Currently two Domains supported:

- LFRic - Mixed finite elements, mesh unstructured in horizontal, structured in vertical, embedded in Fortran
- GOcean - DSL for 2D, finite difference, stretched, structured grid, embedded in Fortran

Evolution

Process existing code that follows strict coding conventions

Recognise certain code structures and construct higher-level Internal Representation

Transformations applied to this IR

In development for NEMO (plus associated models, e.g. SI^3, MEDUSA). Also applied to ROMS.

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Levels of Abstraction

Domain-specific: LFRic IR, NEMO IR, GOcean IR

Language-independent: PSyIR

Language-specific: Fortran, C, … OpenMP, OpenACC, MPI, …

DSLs

Not DSLs!

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The LFRic Domain

(Revolution)

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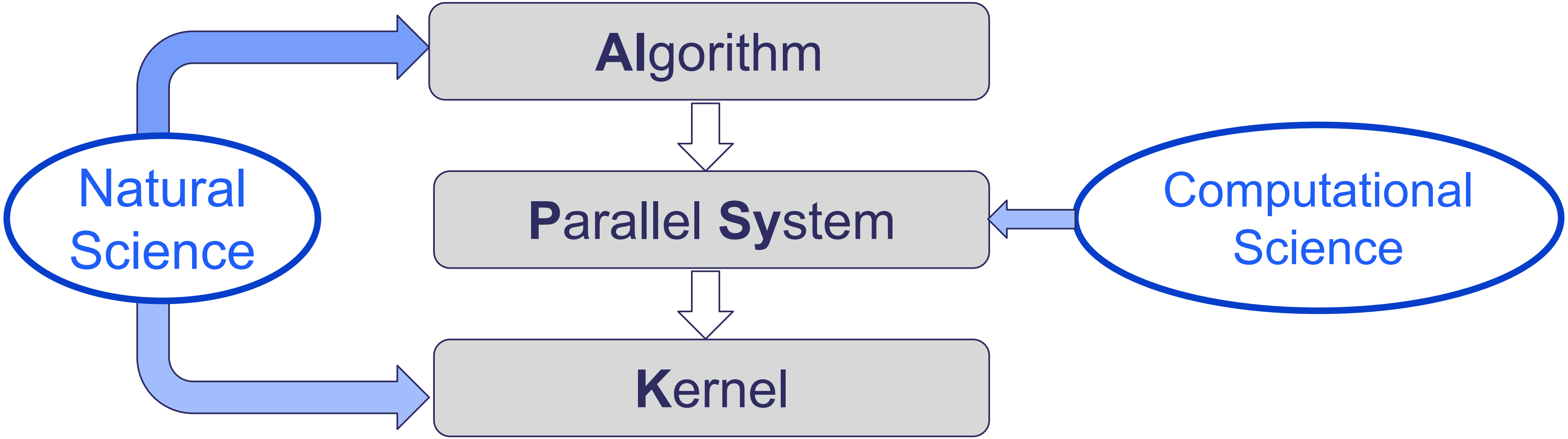
LFRic: Separation of Concerns



PSyKAl : Separate the Natural Science from the Computational Science (performance)

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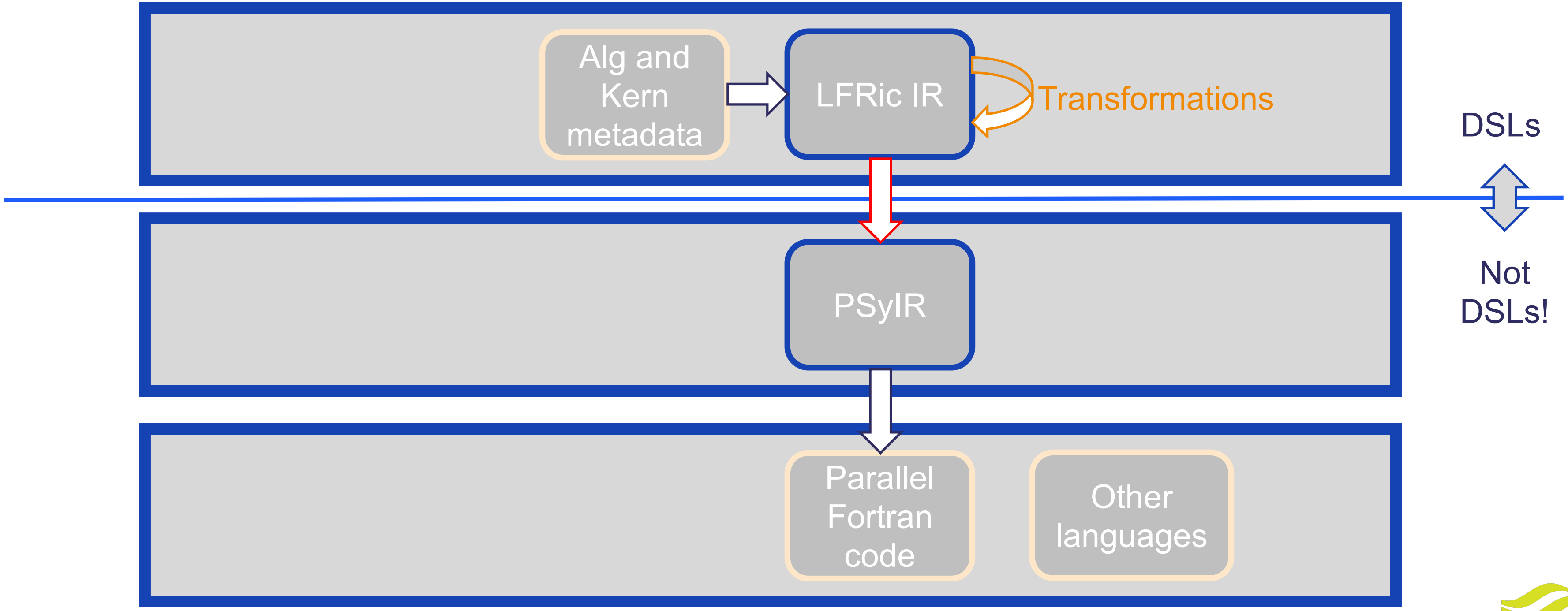
LFRic DSL PSy Layer



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LFRic DSL: Algorithm Layer Example

```
type(field_type) :: hb_inv
type(field_type), private :: grad_p
```

Logically-global field objects

```
call invoke( setval_c(grad_p, 0.0_r_def),                          &
             scaled_matrix_vector_kernel_type(grad_p, p, div_star,  &
                                             hb_inv),
             enforce_bc_kernel_type( grad_p ),
             apply_variable_hx_kernel_type(
                  Hp, grad_p, mt_lumped_inv, p,
                  compound_div, p3theta, ptheta2, m3_exner_star,
                  tau_t, timestep_term) )
```

Specify kernels to execute using an invoke()

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LFRic DSL: Kernel Metadata Example

```
type, public, extends(kernel_type) :: apply_variable_hx_kernel_type
  private
  type(arg_type) :: meta_args(10) = (/                                      &
       arg_type(GH_FIELD,    GH_WRITE, W3),                                 &
       arg_type(GH_FIELD,    GH_READ,  W2),                                 &
       arg_type(GH_FIELD,    GH_READ,  ANY_SPACE_1),                        &
       arg_type(GH_FIELD,    GH_READ,  W3),                                 &
       arg_type(GH_OPERATOR, GH_READ,  W3, W2),                             &
       arg_type(GH_OPERATOR, GH_READ,  W3, ANY_SPACE_1),                    &
       arg_type(GH_OPERATOR, GH_READ,  ANY_SPACE_1, W2),                    &
       arg_type(GH_OPERATOR, GH_READ,  W3, W3),                             &
       arg_type(GH_REAL,     GH_READ),                                      &
       arg_type(GH_REAL,     GH_READ)                                       &
       /)
  integer :: iterates_over = CELLS
contains
  procedure, nopass :: apply_variable_hx_code
end type
```

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LFRic DSL: Vanilla PSy-layer Code

```
      DO df=1,undf_aspc1_grad_p
        grad_p_proxy%data(df) = 0.0_r_def
      END DO
      DO cell=1,grad_p_proxy%vspace%get_ncell()
        !
        CALL scaled_matrix_vector_code(nlayers, grad_p_proxy%data, p_proxy%data, div_star_proxy%data, hb_inv_proxy%data, ndf_aspc1_grad_p, undf_aspc1_grad_p, map_aspc1_grad_p(:,cell), ndf_aspc2_p, undf_aspc2_p, map_aspc2_p(:,cell), ndf_w3, undf_w3, map_w3(:,cell))
      END DO
      DO cell=1,grad_p_proxy%vspace%get_ncell()
        !
        CALL enforce_bc_code(nlayers, grad_p_proxy%data, ndf_aspc1_grad_p, undf_aspc1_grad_p, map_aspc1_grad_p(:,cell), boundary_dofs_grad_p)
      END DO
```

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LFRic Transformation Example
(PSyclone/examples/lfric/eg3)

Consider a simpler example where an invoke() contains a single, user-supplied kernel. Algorithm code:

```
type(field_type), intent(inout)    :: lhs
type(field_type), intent(in)       :: rhs
type(mesh_type),  intent(in)       :: mesh
type(field_type), intent(in)       :: chi(3)

integer(i_def),                 intent(in) :: solver_type
type(quadrature_type), optional, intent(in) :: qr
```

```
call invoke( w3_solver_kernel_type(lhs, rhs, chi, ascalar, qr) )
```

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LFRic Transformation Example

Corresponding PSyIR representation:

```
InvokeSchedule[invoke='invoke_0_w3_solver_kernel_type', dm=False]
    0: Loop[type='', field_space='w3', it_space='cells', upper_bound='ncells']
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Schedule[]
            0: CodedKern solver_w3_code(lhs,rhs,chi,ascalar) [module_inline=False]
```

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Transformation script:

```
def trans(psy):
    ''' PSyclone transformation script for the dynamo0p3 api to apply
    colouring and OpenMP generically.'''
    ctrans = Dynamo0p3ColourTrans()
    otrans = DynamoOMPParallelLoopTrans()

    # Loop over all of the Invokes in the PSy object
    for invoke in psy.invokes.invoke_list:

        schedule = invoke.schedule

        # Colour all of the loops over cells unless they are on
        # discontinuous spaces
        cschedule = schedule
        for child in schedule.children:
            if isinstance(child, Loop) \
               and child.field_space.orig_name \
               not in FunctionSpace.VALID_DISCONTINUOUS_NAMES \
               and child.iteration_space == "cells":
                cschedule, _ = ctrans.apply(child)
        # Then apply OpenMP to each of the colour loops
        schedule = cschedule
        for child in schedule.children:
            if isinstance(child, Loop):
                if child.loop_type == "colours":
                    schedule, _ = otrans.apply(child.loop_body[0])
                else:
                    schedule, _ = otrans.apply(child)
```

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LFRic Transformation Example

Transformed PSyIR representation:

```
InvokeSchedule[invoke='invoke_0_w3_solver_kernel_type', dm=False]
    0: Directive[OMP parallel do]
        Schedule[]
            0: Loop[type='', field_space='w3', it_space='cells', upper_bound='ncells']
                Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
                Literal[value:'NOT_INITIALISED', Scalar<INTEGER, UNDEFINED>]
                Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                Schedule[]
                    0: CodedKern solver_w3_code(lhs,rhs,chi,ascalar) [module_inline=False]
```

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LFRic Transformation Example

Generated Fortran (PSy layer):

```fortran
      !
      !$omp parallel do default(shared), private(cell), schedule(static)
      DO cell=1,lhs_proxy%vspace%get_ncell()
        !
        CALL solver_w3_code(nlayers, lhs_proxy%data, rhs_proxy%data, chi_proxy(1)%data, chi_proxy(2)%data, chi_proxy(3)%data, ascalar, ndf_w3, undf_w3, map_w3(:,cell), basis_w3_qr, ndf_wchi, undf_wchi, map_wchi(:,cell), diff_basis_wchi_qr, np_xy_qr, np_z_qr, weights_xy_qr, weights_z_qr)
      END DO
      !$omp end parallel do
      !
```

Transformed Algorithm code:

```fortran
CALL invoke_0_w3_solver_kernel_type(lhs, rhs, chi, ascalar, qr)
```

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The GOcean Domain

(Revolution)

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A PSyKAl-based API for Finite Difference

Directly-addressed on 2D, stretched, regular grid

Much simpler than LFRic

Used in 2 shallow-water benchmarks & a Tsunami code

Simplicity lends itself to prototyping work, e.g.:

- OpenCL and Kokkos backends
- kernel extraction with PSyData

See PSyData tutorial (Tues) & Sergi's presentation (Weds)

```
type, extends(kernel_type) :: compute_cu
   type(go_arg), dimension(3) :: meta_args =     &
        (/ go_arg(GO_WRITE, GO_CU, GO_POINTWISE),                  &
           go_arg(GO_READ,  GO_CT, GO_STENCIL(000,110,000)), &
           go_arg(GO_READ,  GO_CU, GO_POINTWISE)                   &
         /)
   !> This kernel writes only to internal points of the
   !! simulation domain.
   integer :: ITERATES_OVER = GO_INTERNAL_PTS

   !> The U,V and F points that share the same index as a given
   !! are those immediately to the South and West of it.
   integer :: index_offset = GO_OFFSET_SW

contains
  procedure, nopass :: code => compute_cu
end type compute_cu
```

Point-wise kernels

```
!> Compute the mass flux in the x direction at point (i,j)
subroutine compute_cu_code(i, j, cu, p, u)
  implicit none
  integer,  intent(in) :: I, J
  real(go_wp), intent(out), dimension(:,:) :: cu
  real(go_wp), intent(in),  dimension(:,:) :: p, u

  CU(I,J) = 0.5d0*(P(i,J)+P(I-1,J))*U(I,J)
```

The NEMO Domain

(Evolution)

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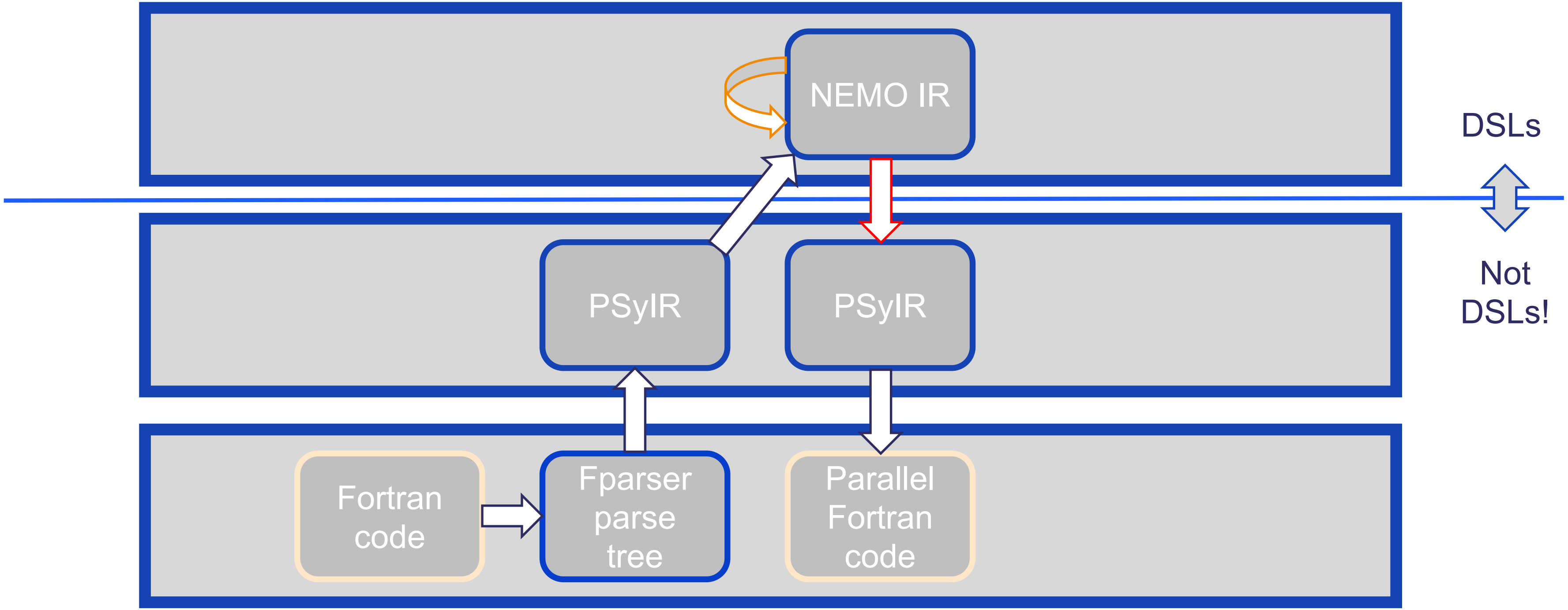
NEMO DSL

Construct high-level representation of existing source code:



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NEMO Transformation Example

(PSyclone/examples/nemo/eg2)

Original code (`tral_ldf_iso` routine):

```
!                                                         ! ===========
DO jn = 1, kjpt                                           ! tracer loop
   !                                                      ! ===========
   !
   !!----------------------------------------------------------------------
   !!   I - masked horizontal derivative
   !!----------------------------------------------------------------------
 bug.... why (x,:,:)?   (1,jpj,:) and (jpi,1,:) should be sufficient....
   zdit (1,:,:) = 0._wp     ;     zdit (jpi,:,:) = 0._wp
   zdjt (1,:,:) = 0._wp     ;     zdjt (jpi,:,:) = 0._wp
   !!end

   ! Horizontal tracer gradient
   DO jk = 1, jpkm1
      DO jj = 1, jpjm1
         DO ji = 1, jpim1   ! vector opt.
            zdit(ji,jj,jk) = ( ptb(ji+1,jj  ,jk,jn) - ptb(ji,jj,jk,jn) ) * umask(ji,jj,jk)
            zdjt(ji,jj,jk) = ( ptb(ji  ,jj+1,jk,jn) - ptb(ji,jj,jk,jn) ) * vmask(ji,jj,jk)
         END DO
      END DO
   END DO
   IF( ln_zps ) THEN      ! botton and surface ocean correction of the horizontal gradient
      DO jj = 1, jpjm1                ! bottom correction (partial bottom cell)
```

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PSyIR constructed by PSyclone:

```
4: Loop[type='levels', field_space='None', it_space='None']
    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Reference[name:'jpkm1']
    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Schedule[]
        0: Loop[type='lat', field_space='None', it_space='None']
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Reference[name:'jpjm1']
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Schedule[]
                0: Loop[type='lon', field_space='None', it_space='None']
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Reference[name:'fs_jpim1']
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Schedule[]
                        0: InlinedKern[]
                            Schedule[]
                                0: Assignment[]
                                    ArrayReference[name:'zdit']
                                        Reference[name:'ji']
                                        Reference[name:'jj']
                                        Reference[name:'jk']
                                    BinaryOperation[operator:'MUL']
```

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NEMO Transformation Script

```
def trans(psy):
    ''' Transform a specific Schedule by making all loops
    over levels OpenMP parallel.

    :param psy: the object holding all information on the PSy layer \
                to be modified.
    :type psy: :py:class:`psyclone.psyGen.PSy`

    :returns: the transformed PSy object
    :rtype:  :py:class:`psyclone.psyGen.PSy`

    '''
    from psyclone.psyGen import TransInfo
    from psyclone.nemo import NemoKern
    # Get the Schedule of the target routine
    sched = psy.invokes.get('tra_ldf_iso').schedule
    # Get the transformation we will apply
    ompt = TransInfo().get_trans_name('OMPParallelLoopTrans'
    # Apply it to each loop over levels containing a ker
    for loop in sched.loops():
        kernels = loop.walk(NemoKern)
        if kernels and loop.loop_type == "levels":
            sched, _ = ompt.apply(loop)
    # Return the modified psy object
    return psy
```

Parallelises all loops over vertical levels using OpenMP

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Transformed PSyIR:

```
    Literal[value:'0.', Scalar<REAL, wp: <Scalar<INTEGER, UNDEFINED>, unresolved>>]
4: Directive[OMP parallel do]
    Schedule[]
        0: Loop[type='levels', field_space='None', it_space='None']
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Reference[name:'jpkm1']
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Schedule[]
                0: Loop[type='lat', field_space='None', it_space='None']
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Reference[name:'jpjm1']
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Schedule[]
                        0: Loop[type='lon', field_space='None', it_space='None']
                            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                            Reference[name:'fs_jpim1']
                            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                            Schedule[]
                                0: InlinedKern[]
                                    Schedule[]
                                        0: Assignment[]
```

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Generated Fortran with OpenMP directives added

```
DO jn = 1, kjpt
  zdit(1, :, :) = 0._wp
  zdit(jpi, :, :) = 0._wp
  zdjt(1, :, :) = 0._wp
  zdjt(jpi, :, :) = 0._wp
  !$OMP parallel do default(shared), private(ji,jj,jk), schedule(static)
  DO jk = 1, jpkm1
    DO jj = 1, jpjm1
      DO ji = 1, fs_jpim1
         zdit(ji, jj, jk) = (ptb(ji + 1, jj, jk, jn) - ptb(ji, jj, jk, jn)) &
                  * umask(ji, jj, jk)
         zdjt(ji, jj, jk) = (ptb(ji, jj + 1, jk, jn) - ptb(ji, jj, jk, jn)) &
                  * vmask(ji, jj, jk)
      END DO
    END DO
  END DO
  !$OMP end parallel do
```

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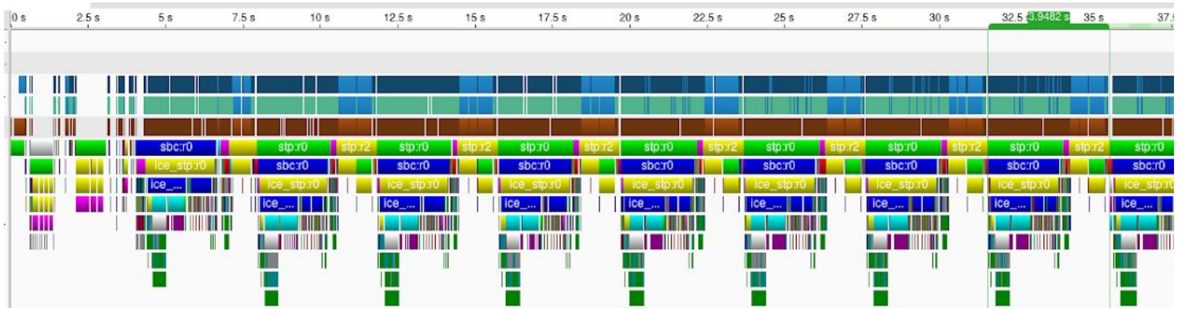
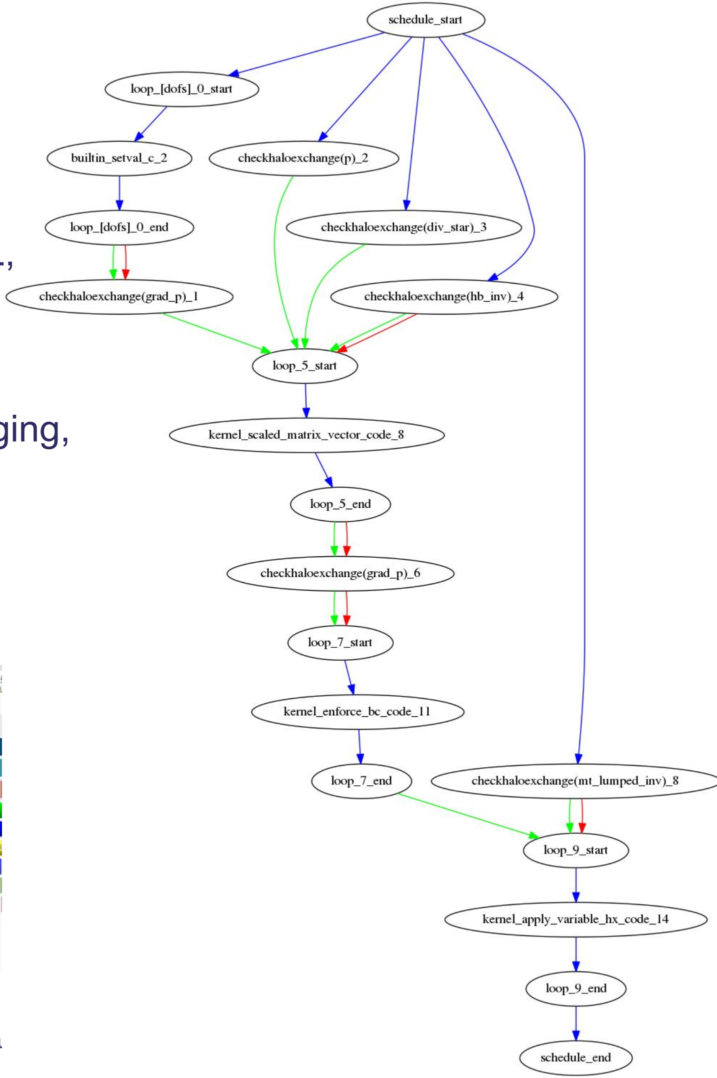
Other Features

Available transformations (loop fusion, OpenMP, OpenACC, OpenCL, asynchronous halo exchanges, redundant computation)
- Tuesday Sessions 2 & 3 and Wednesday Session 1

PSyData API - allows calipers to be inserted for e.g. profiling, debugging, validation, kernel (benchmark) extraction, on-line visualisation etc.
- Tuesday Sessions 1 & 4

DAG view of PSy-layer Schedules





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Summary

- PSyclone is a Domain-Specific Compiler for use with both DSLs and existing code
- Intended as a tool for use by an HPC expert
- Configurable:
    - LFRic & GOcean Domains (revolution)
    - NEMO Domain (evolution)
- Constructs a PSyclone Internal Representation of supplied code
- User transforms this representation using Python scripts
- Provides error checking and analysis functionality
- Generates Fortran (or OpenCL) for the transformed PSyIR

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Science and Technology Facilities Council

Thank you!

User, Developer and Reference Guides are available:

psyclone[-dev,-ref].readthedocs.io

For more information please contact:

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