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PSyclone – Separation of Concerns for HPC Codes

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PSyclone

- PSyclone developed by The Hartree Centre STFC Daresbury Laboratory, UK (since 2014)
  - Main developers:
    - Rupert Ford and Andy Porter
- In close cooperation with UK Met Office's Exascale Project
  - Used for the next generation Unified Model development (LFRic)
    - Expected to become operational in 2023
  - Based on 3d mixed finite elements
- International cooperation with UM Collaboration Partners
  - Including BOM
- Open source python program (BSD 3 clause) https://github.com/stfc/PSyclone

HPC Codes

```
call HaloExchange(da, …)
$OMP PARALLEL DO default(none) private(j) …
do j=2,nx-1
   dw(1:ny)=da(j,1:ny)
   call swlat(uw,qw,vw,dw,ny)
enddo
!$OMP END PARALLEL
...
   call swlon(...)


...


subroutine swlat(…)
  do i=2, ny-1
     d2=GA*t*((dw(ip)-dw(i))/h(i)-(dw(i)-dw(im))/h(im))
     u1(i)=uw(i)+rl-t1*((3.*uw(im)+qw(im)+3.*uw(ip)
```

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View of a Natural Scientist

```
    call swlat(uw,qw,vw,dw,ny)

...
    call swlon(...)

...

subroutine swlat(…)

      d2=GA*t*((dw(ip)-dw(i))/h(i)-(dw(i)-dw(im))/h(im))
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```

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Computational Science: Optimisation and Parallelisation

```
call HaloExchange(da, …)
$OMP PARALLEL DO default(none) private(j) …
do j=2,nx-1
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   call swlat(uw,qw,vw,dw,ny)
enddo
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...
   call swlon(...)


...

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```

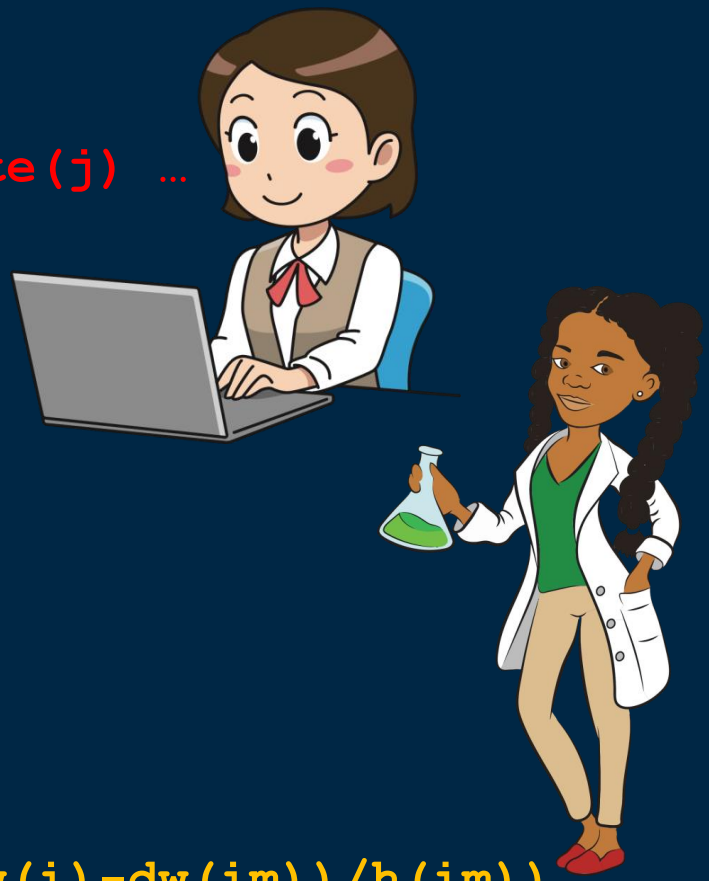

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HPC Code Analysis

- Typical HPC code combines skills from natural and computational science
  - Each one has its own special knowledge and experience
  - Highly interdisciplinary
- Optimised code looks different for different hardware:
  - OpenMP parallel, MPI, hybrid, GPU, Xeon Phi
  - What will future architectures look like?
- How can we manage and future-proof source code under these circumstances?

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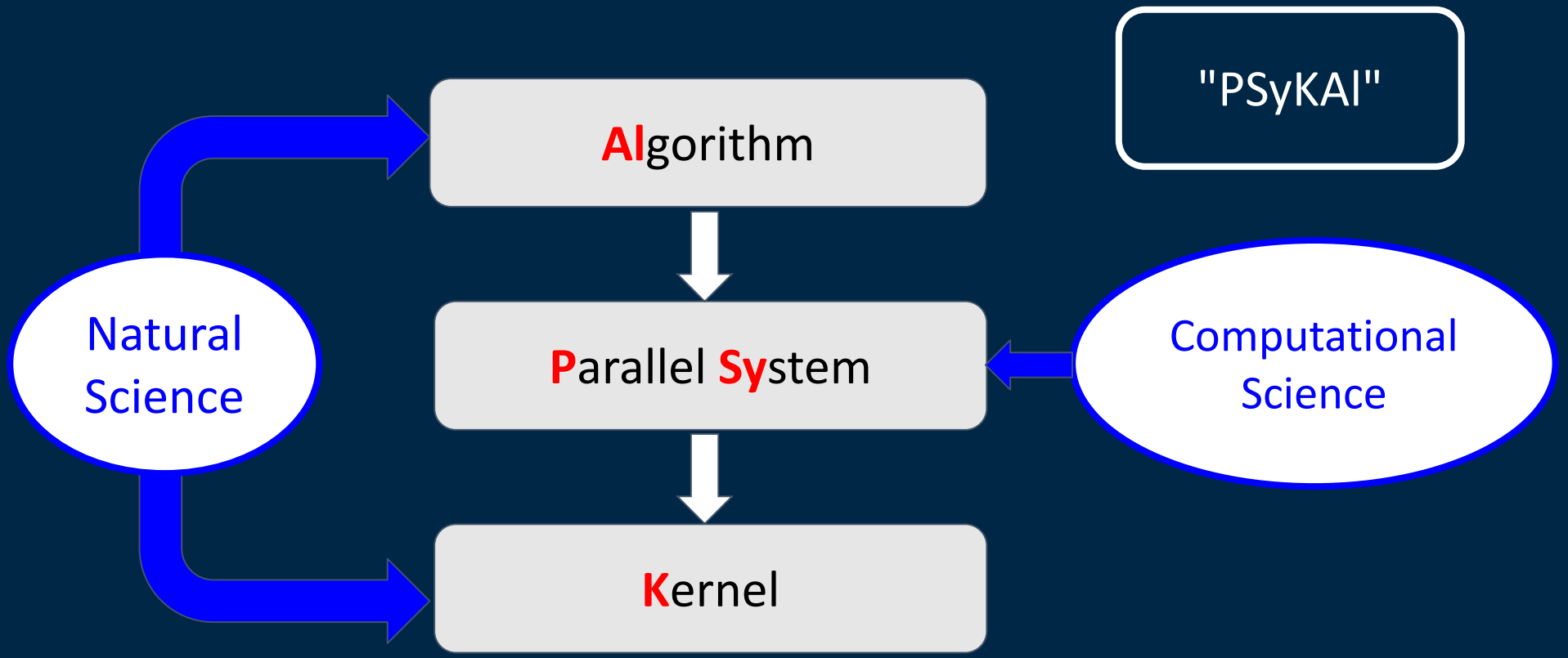
Separation of Concerns



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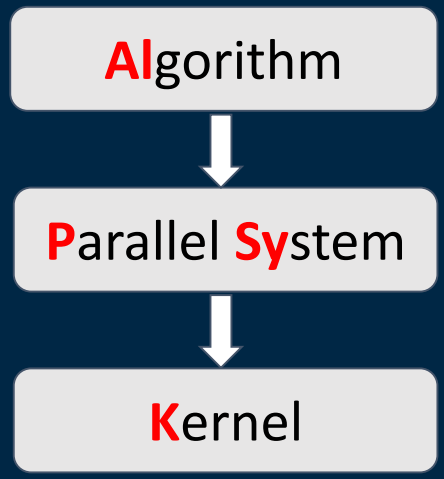
What is PSyclone?



- "Domain Specific Language" or a code generator
  - Reads high level algorithm and kernel
  - Creates the parallel system layer
    - I.e. the (potential parallel) loop structure
  - But it is plain Fortran
- Restricts the way you can program somewhat
  - You need to think of 'kernels'

- Helps with the separation of concerns:
  - Natural scientists can write code using/thinking of whole arrays and single elements
  - Computational scientists can work on optimisation and parallelisation **independently**

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Example: Algorithm Layer (High Level)

```
use compute_cu_mod, only: compute_cu
type(r2d_field) :: cu_fld, p_fld, u_fld, …

call invoke( copy(u_fld, uold_fld) )

call invoke( name="update_fields",
             compute_cu(CU_fld, p_fld, u_fld), &
             compute_cv(CV_fld, p_fld, v_fld) )

call invoke( time_smooth(u_fld, UNEW_fld, UOLD_fld), &
             time_smooth(v_fld, VNEW_fld, VOLD_fld), &
             time_smooth(p_fld, PNEW_fld, POLD_fld) )
```

PSyclone Rewrites Algorithm Layer

```
use compute_cu_mod, only: compute_cu
type(r2d_field) :: cu_fld, p_fld, u_fld


! call invoke( copy(u_fld, uold_fld) )
call invoke_0(u_fld, uold_fld)


!call invoke( name="update_fields",
!             compute_cu(CU_fld, p_fld, u_fld), &
!             compute_cv(CV_fld, p_fld, v_fld) )

call invoke_update_fields(CU_fld, p_fld, u_fld, &
                          CV_fld, v_fld)
```

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Pointwise Kernel Layer

```
subroutine copy_code(i, j, source, dest)
    implicit none
    integer,  intent(in) :: i, j
    real(wp), intent(out), dimension(:,:) :: dest
    real(wp), intent(in),  dimension(:,:) :: source

    dest(i, j) = source(i,j)

end subroutine copy_code
```

```
subroutine compute_cu_code(i, j, cu, p, u)
    ...
    cu(i,j) = 0.5d0*(p(i,j)+p(i-1,j))*u(i,j)…
end subroutine compute_cu_code
```

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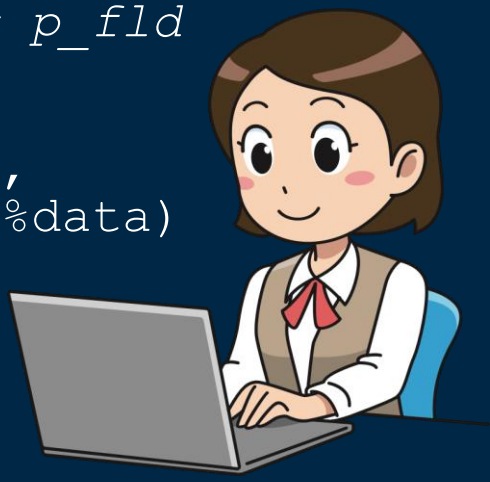
Automatically Created PSy Layer

```
Subroutine invoke_update_fields(cu_fld, p_fld, u_fld, &
                                cv_fld, v_fld)

USE compute_cu_mod, ONLY: compute_cu_code
istop = cu_fld%grid%simulation_domain%xstop
jstop = cu_fld%grid%simulation_domain%ystop

! In case of MPI: possible halo exchange for p_fld
DO j=2, jstop
   DO i=2,istop
      CALL compute_cu_code(i, j, cu_fld%data,
                           p_fld%data, u_fld%data)
   END DO
END DO

DO j=2, jstop
   DO i=2,istop
      CALL compute_cv_code(i, j, cv_fld%data,
                           p_fld%data, v_fld%data)
   END DO
END DO
```



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Kernels Need to Define Kernel Type

- Defines the iteration space and stencil operations:

```
type, extends(kernel_type) :: compute_cu
    type(arg), dimension(3) :: meta_args =      &
          (/ arg(WRITE, FIELD, POINTWISE),      & ! Cu
             arg(READ,  FIELD, STENCIL(010,     & ! P
                                       111,     &
                                       010)),   &
             arg(READ,  FIELD, POINTWISE)       & ! U
          /)
    integer :: ITERATES_OVER = INTERNAL_PTS
contains
    procedure, nopass :: code => compute_cu_code
end type compute_cu
```

- The type is defined only for PSyclone, not used anywhere else

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PSyclone Schedule

- Internal tree representation of loops and kernel invocations

```
GOSchedule[invoke='invoke_1',Constant loop bounds=True]
  Loop[type='outer',field_space='cu',it_space='internal_pts']
    Loop[type='inner',field_space='cu',it_space='internal_…']
      KernCall compute_cu_code(cu_fld,p_fld,u_fld)
  Loop[type='outer',field_space='cu',it_space='internal_pts']
    Loop[type='inner',field_space='cu',it_space='intern..']
      KernCall compute_cv_code(cv_fld,p_fld,v_fld)
```

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Transformations Act on Schedule

- Python scripts can act as transformations
- Transformations can be developed by computational scientist independent of Fortran code
- They can modify the schedule, e.g. adding halo exchanges, OMP directive nodes, fuse loops etc.

```
from psyclone.transformations import LoopFuse

def trans(psy):
    schedule =
        psy.invokes.get('invoke_compute_fields')
           .schedule
    schedule.view()
    fuse = LoopFuse() # Create fuse transform

    s1 = fuse.apply(schedule.children[0],
                    schedule.children[1])
```

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Result of Loop Fuse Transformation

```
GOSchedule[invoke='invoke_1',Constant loop bounds=True]
  Loop[type='outer',field_space='cu',it_space=…]
    Loop[type='inner',field_space='cu',it_space=…]
      KernCall compute_cu_code(cu_fld,p_fld,u_fld)
    Loop[type='inner',field_space='cu',it_space=…]
      KernCall compute_cv_code(cv_fld,p_fld,v_fld)
```

```
DO j=2,jstop
   DO i=2,istop
      CALL compute_cu_code(i, j, cu_fld%data, …)
   END DO
   i=2,istop
      CALL compute_cv_code(i, j, cv_fld%data, …)
   END DO
END DO
```

Transformations

- Transformations together with PSyclone can:
  - Optimise code (e.g. loop fuse, loop blocking/tiling, …)
  - Parallelise code using OpenMP or MPI
  - Generate code for different hardware architectures (OpenMP, OpenACC, …)
  - Generate different code for different compilers
- They are mostly independent of the actual code
  - To a certain degree ☺

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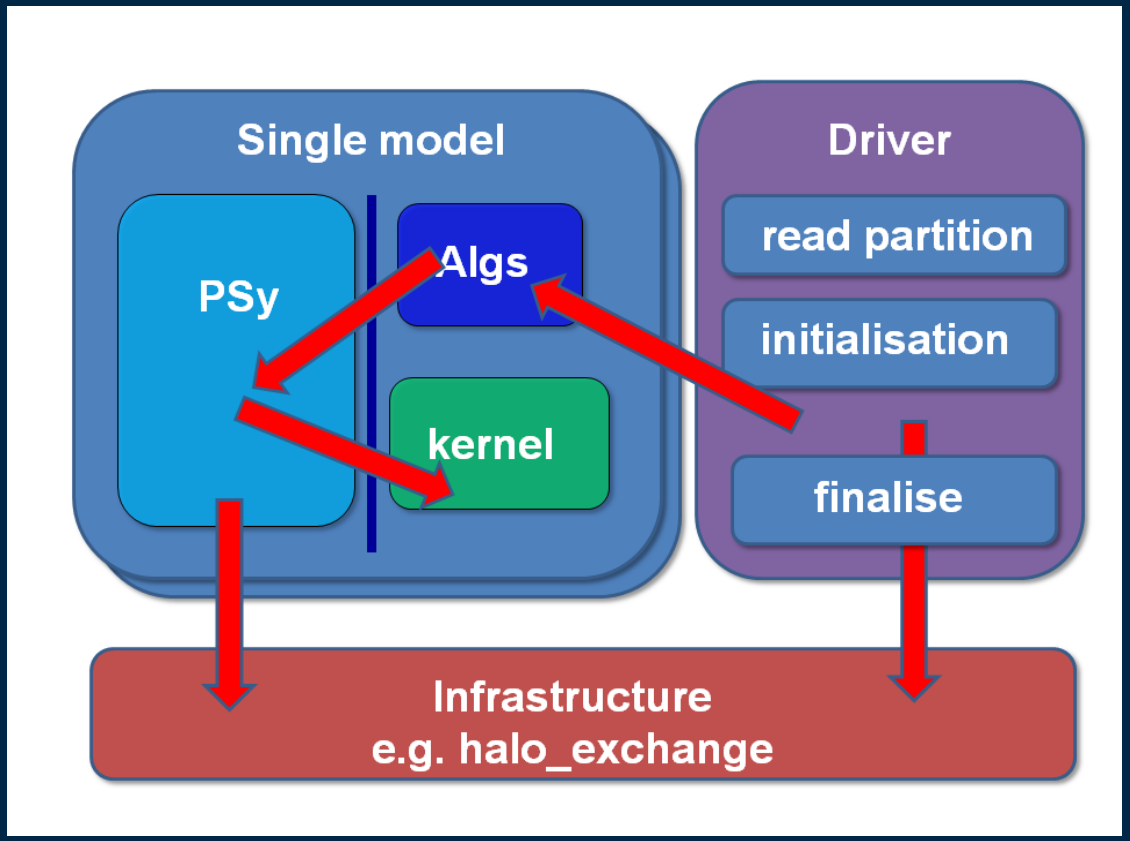
PSyclone Infrastructure Library

- Driver/runtime library needed for setting up parallel environment
  - LFRic: Earth System Modelling Framework, now:
  - YAXT: Yet Another eXchange Tool
  - GOcean: GOcean Library (GOLib v.1.0)
- Supplies field types etc.
- Support for 2d finite differences, and 3d finite elements



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Results: MOST

- Method of Splitting Tsunamis
  - Developed by the NOAA Pacific Marine Environmental Laboratory (PMEL)
- Optimised by stand-alone script to fuse loops and apply OpenMP statements
  - For GNU Fortran: additional module inlining support
- Compared with a manual developed and optimised C version

	Intel 17	Cray 8.4.5	GNU Fortran 5.1.0
Original code	111.0	115.6	102.4
PSyclone	48.5	31.4	88.7 → 70.4
Optimised C version	*49.0*	*47.0*	-

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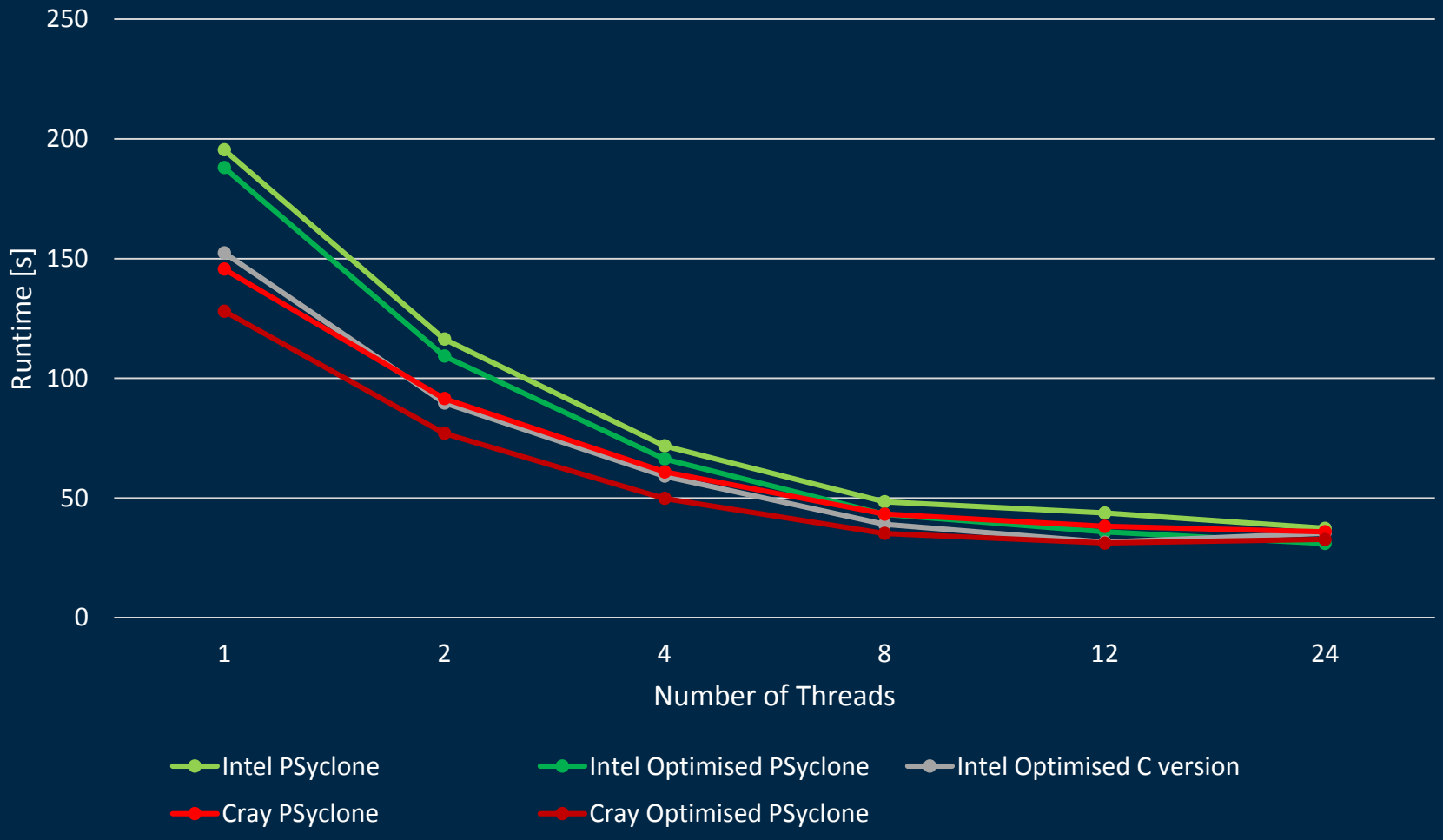
OpenMP Scaling – Added OpenMP Optimisations



Summary

- PSyclone helps with the separation of concern
  - Separate natural science code from computational science code
  - Natural science can be developed and maintained independent of optimisations (to a certain degree)
- Originally developed for 3d FEM, it can be used with other methods
- Domain-specific language 'in Fortran'
- Can automatically parallelise code, e.g. MPI, OpenMP
  - But of course restricts code development to 'kernels'
- Can create hardware-specific code
  - E.g. CPU, GPU, Xeon Phi
- Tools under development:
  - Profiler support, automatic test-case creation, perhaps automatic performance optimisation?

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Thank you

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Thanks to GDJ and oksmith from openclipart.org for the images of scientists

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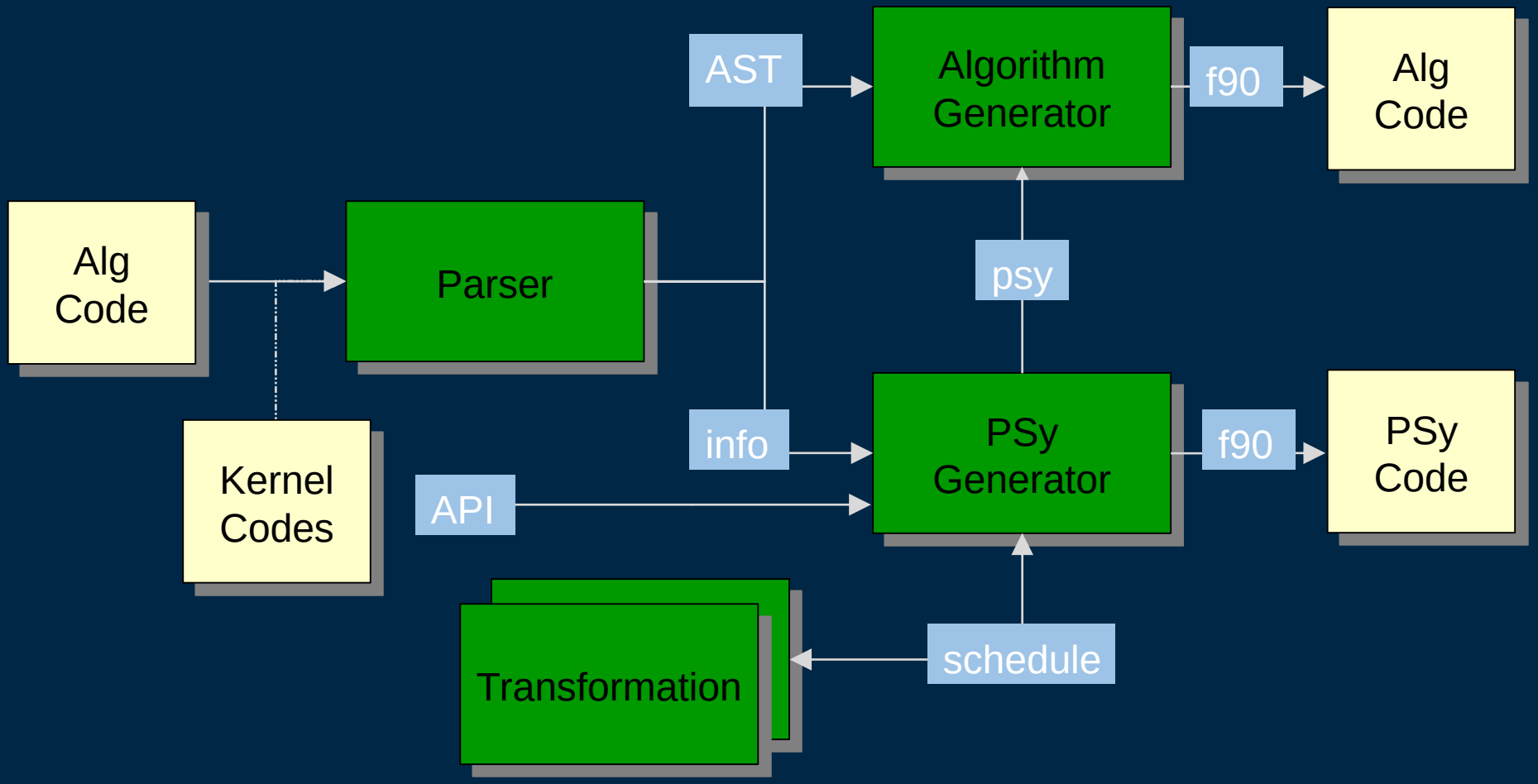
PSyclone Architecture



# Threads	Intel PSyclone Fortran		Cray PSyclone Fortran		Intel C, hand-tuned
1	195.45	188.0	145.65	128.0	152.4
2	116.38	109.3	91.49	77.0	89.7
4	71.78	66.3	60.93	49.8	59.1
8	48.42	43.2	43.24	35.2	39.0
12	43.70	35.9	38.12	31.2	31.5
24	37.33	31.0	35.88	32.7	35.3