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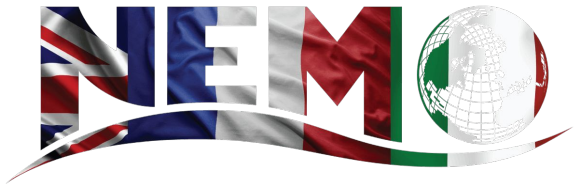
Overview of Using PSyclone with

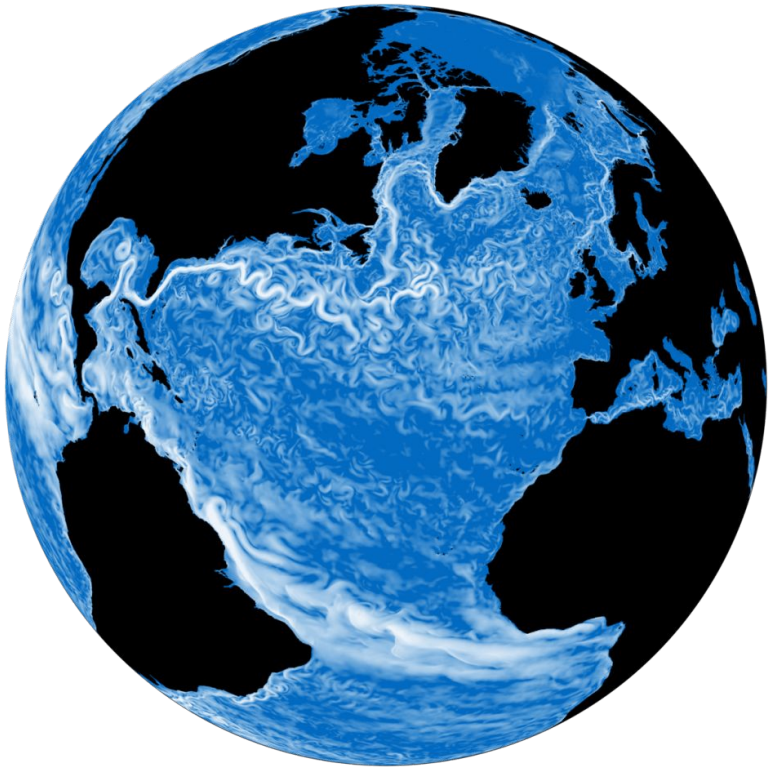


Andy Porter, STFC Hartree Centre

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

Outline

- The NEMO Ocean Model
- Performance characteristics
- Coding standards
- Using PSyclone with NEMO
- Existing code => PSyIR, navigating the PSyIR
- The tracer-advection mini-app



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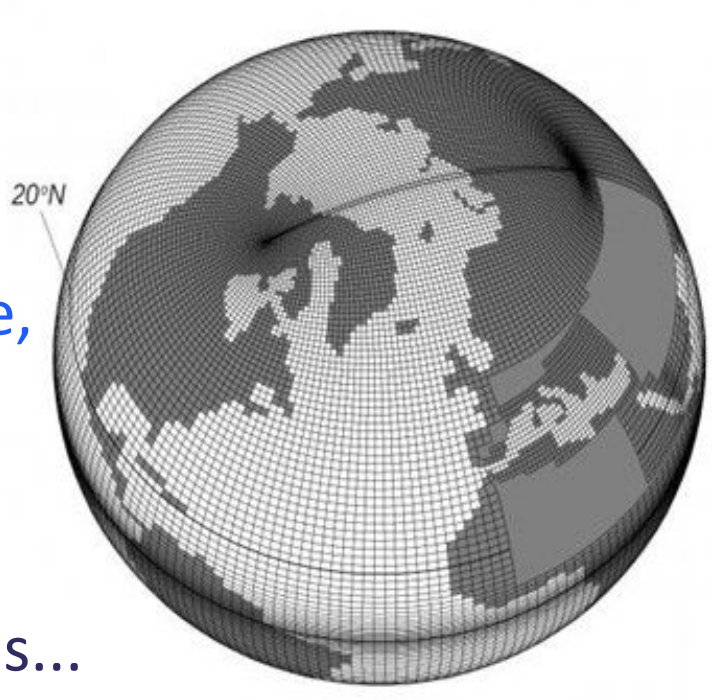
The NEMO Ocean Model



- Finite difference model using a tripolar, stretched latitude, longitude mesh ('ORCA')
- Three core components:
  - NEMO-OPA: ocean dynamics, thermodynamics
  - NEMO-SI^3: sea-ice (thermo)dynamics, brine inclusions...
  - NEMO-TOP/PISCES: tracer transport and biogeochemistry
- Mesh rotated so that poles are over land
  - Can go to high resolution without the 'pole problem'
  - No need to fundamentally change the code
- Relatively large (core of ~100K lines of Fortran)

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NEMO continued...

- Large user base (Met Office, ECMWF, CERFACS...)
  - Trusted part of CMIP experiments
- Constantly under scientific development
- Developers are typically oceanographers, not computer scientists
- ~20 years old (and counting...)
- Focus on:
  - Scientific correctness
  - Maintainability (aka Productivity)
  - Portability
- Run either in serial or MPI parallel
  - => CPU only

```
121 ./ICE/icetab.F90
317 ./ICE/icesbc.F90
264 ./ICE/icerst.F90
1649 ./ICE/icedyn_adv_umx.F90
166 ./ICE/icethd_sal.F90
573 ./ICE/icethd.F90
483 ./ICE/ice.F90
251 ./ICE/icethd_pnd.F90
755 ./ICE/iceitd.F90
886 ./ICE/icethd_zdf_bl99.F90
461 ./ICE/iceupdate.F90
128 ./ICE/icethd_zdf.F90
694 ./ICE/icectl.F90
205 ./ICE/icethd_da.F90
188 ./ICE/icecor.F90
169 ./ICE/icedyn_adv.F90
144 ./ICE/icethd_ent.F90
856 ./ICE/icedyn_adv_pra.F90
1048 ./ICE/icevar.F90
442 ./SAO/nemogcm.F90
1998 ./SAO/obs_fbm.F90
81 ./SAO/sao_data.F90
58 ./SAO/sao_intp.F90
173 ./SAO/sao_read.F90
88 ./TOP/TRP/trczdf.F90
235 ./TOP/TRP/trcsink.F90
195 ./TOP/TRP/trcldf.F90
109 ./TOP/TRP/trctrp.F90
295 ./TOP/TRP/trcrad.F90
215 ./TOP/TRP/trcsbc.F90
279 ./TOP/TRP/trcnxt.F90
991 ./TOP/TRP/trdmxl_trc.F90
125 ./TOP/TRP/trdtrc.F90
243 ./TOP/TRP/trcadv.F90
102 ./TOP/TRP/trcbbl.F90
163 ./TOP/TRP/trdtrc_oce.F90
386 ./TOP/TRP/trcdmp.F90
210 ./TOP/TRP/trdmxl_trc_rst.F90
597 ./TOP/trcsub.F90
203 ./TOP/PISCES/P2Z/p2zopt.F90
70 ./TOP/PISCES/P2Z/p2zsms.F90
492 ./TOP/PISCES/P2Z/p2zbio.F90
154 ./TOP/PISCES/P2Z/p2zsed.F90
255 ./TOP/PISCES/P2Z/p2zexp.F90
70 ./TOP/PISCES/par_pisces.F90
194 ./TOP/PISCES/sms_pisces.F90
93 ./TOP/PISCES/trcnam_pisces.F90
43 ./TOP/PISCES/SED/sedmodel.F90
138 ./TOP/PISCES/SED/sedwri.F90
257 ./TOP/PISCES/SED/sedmbc.F90
56 ./TOP/PISCES/SED/oce_sed.F90
36 ./TOP/PISCES/SED/sed_oce.F90
97 ./TOP/PISCES/SED/sedstp.F90
```

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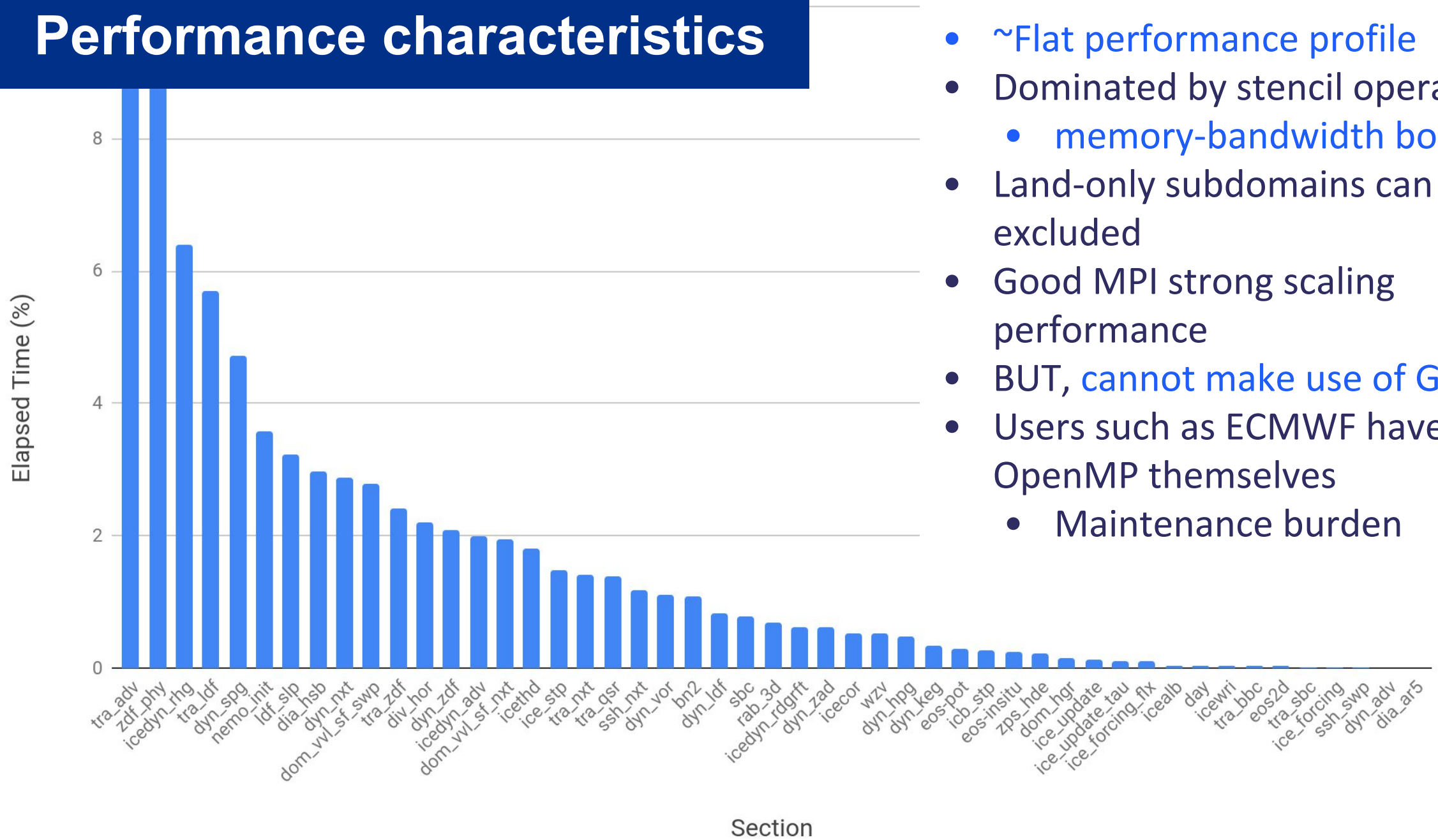
Performance characteristics



- ~Flat performance profile
- Dominated by stencil operations
  - memory-bandwidth bound
- Land-only subdomains can be excluded
- Good MPI strong scaling performance
- BUT, cannot make use of GPUs
- Users such as ECMWF have added OpenMP themselves
  - Maintenance burden

```
zwx(:,:,jpk) = 0.e0    ;    zwy(:,:,jpk) = 0.e0

DO jk = 1, jpk-1
   DO jj = 1, jpj-1
      DO ji = 1, jpi-1
         zwx(ji,jj,jk) = umask(ji,jj,jk) * ( mydomain(ji+1,jj
         zwy(ji,jj,jk) = vmask(ji,jj,jk) * ( mydomain(ji,jj+1
      END DO
   END DO
END DO

zslpx(:,:,jpk) = 0.e0    ;    zslpy(:,:,jpk) = 0.e0

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) =                          ( zwx(ji,jj,jk)
         &              * ( 0.25d0 + SIGN( 0.25d0, zwx(ji,jj,jk)
         zslpy(ji,jj,jk) =                          ( zwy(ji,jj,jk)
         &              * ( 0.25d0 + SIGN( 0.25d0, zwy(ji,jj,jk)
      END DO
   END DO
END DO

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) = SIGN( 1.d0, zslpx(ji,jj,jk) ) * MIN(    ABS( zslpx(ji  ,jj,jk) ),   &
         &                                                          2.d0*ABS( zwx  (ji-1,jj,jk) ),   &
         &                                                          2.d0*ABS( zwx  (ji  ,jj,jk) ) )
         zslpy(ji,jj,jk) = SIGN( 1.d0, zslpy(ji,jj,jk) ) * MIN(    ABS( zslpy(ji,jj  ,jk) ),   &
         &                                                          2.d0*ABS( zwy  (ji,jj-1,jk) ),   &
         &                                                          2.d0*ABS( zwy  (ji,jj  ,jk) ) )
      END DO
   END DO
END DO
```

Large code base, but:

- Fairly homogeneous (stencils)
- Apply same/similar optimisations everywhere
- Strict coding standards
- Have domain-specific knowledge, e.g.:
  - Loops over longitude, latitude and vertical levels
  - Tracers
  - Run-time constants
  - Temporary variables

DSL front-ends

Unmodified existing code

Constrained existing code

High-level domain-specific language

Unconstrained environment

Constrained environment

Performance limitations

High Performance

Supports evolution

Requires revolution

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DSL front-ends

NEMO

LFRic

High-level domain-specific language

Unconstrained environment

Constrained environment

Performance limitations

High Performance

Supports evolution

Requires revolution

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Strategy

- Jeremy Appleyard (NVIDIA) previously obtained good performance using just OpenACC KERNELS (v3.4 of NEMO)
- Extend PSyclone such that we can replicate his results
  - without manual code modification (ideally)
  - on ***any*** NEMO configuration
- Use NVIDIA's 'managed-memory' option to deal with data movement between CPU/GPU
- Extend PSyclone with functionality to introduce more tailored OpenACC directives as required

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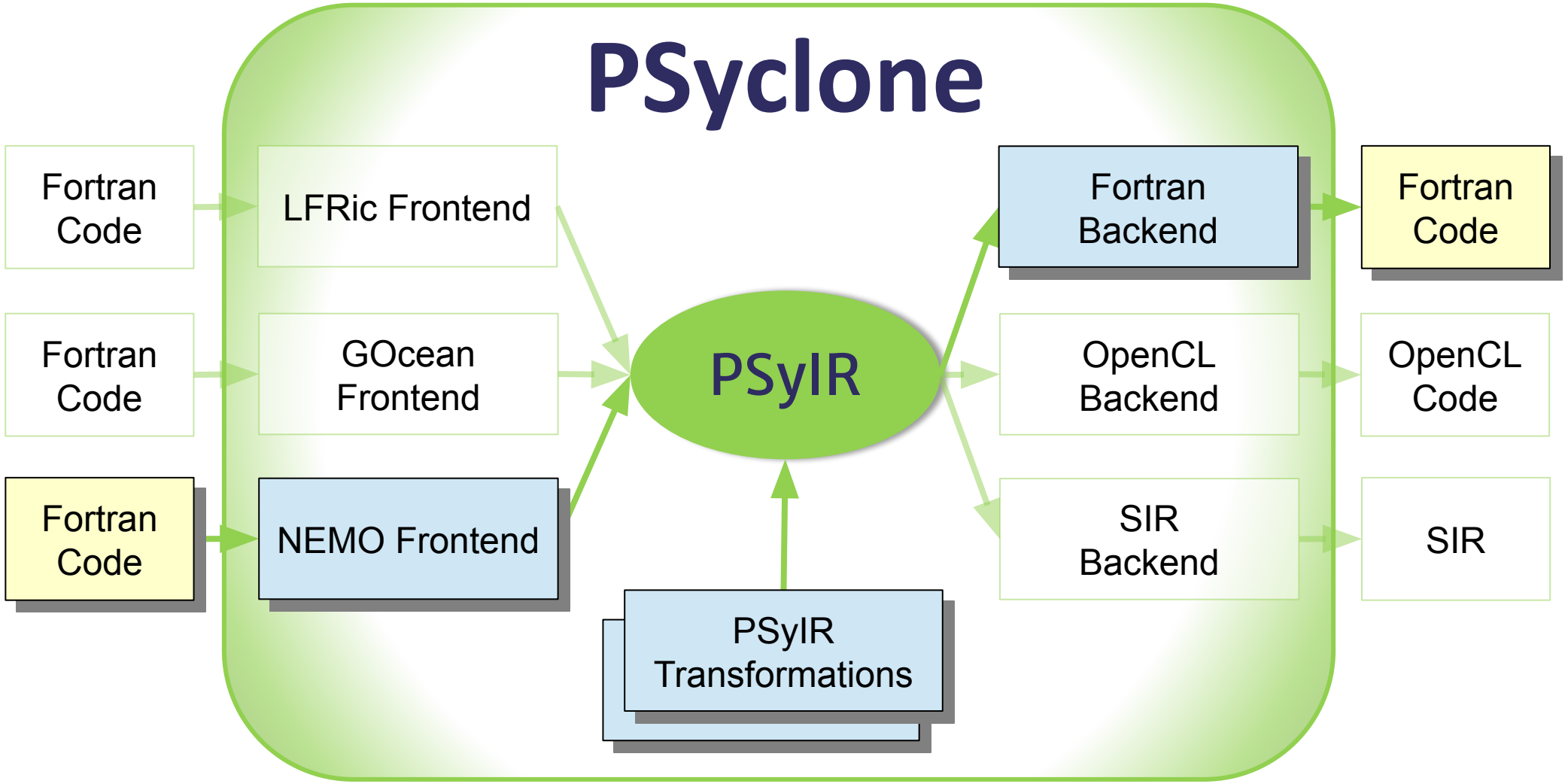

(PSyIR: PSyclone Internal Representation)

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Understanding the PSyIR of NEMO code

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PSyIR for array assignments (implicit loops)

```
zwx(:,:,jpk) = 0.e0    ;    zwy(:,:,jpk) = 0.e0

DO jk = 1, jpk-1
   DO jj = 1, jpj-1
      DO ji = 1, jpi-1
         zwx(ji,jj,jk) = umask(ji,jj,jk) * ( mydomain(ji+1,jj,jk) - mydomain(ji,jj,jk) )
         zwy(ji,jj,jk) = vmask(ji,jj,jk) * ( mydomain(ji,jj+1,jk) - mydomain(ji,jj,jk) )
      END DO
   END DO
END DO

zslpx(:,:,jpk) = 0.e0    ;    zslpy(:,:,

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) =
         &                 * ( 0.25d0 + SIGN
         zslpy(ji,jj,jk) =
         &                 * ( 0.25d0 + SIGN
      END DO
   END DO
END DO

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) = SIGN( 1.d0,
         &
         &
         zslpy(ji,jj,jk) = SIGN( 1.d0,
         &
         &
      END DO
   END DO
END DO
```

```
1: Assignment[]
    ArrayReference[name:'zwx']
        Range[]
            BinaryOperation[operator:'LBOUND']
                Reference[name:'zwx']
                Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            BinaryOperation[operator:'UBOUND']
                Reference[name:'zwx']
                Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Range[]
            BinaryOperation[operator:'LBOUND']
                Reference[name:'zwx']
                Literal[value:'2', Scalar<INTEGER, UNDEFINED>]
            BinaryOperation[operator:'UBOUND']
                Reference[name:'zwx']
                Literal[value:'2', Scalar<INTEGER, UNDEFINED>]
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
        Reference[name:'jpk']
    Literal[value:'0.e0', Scalar<REAL, SINGLE>]
2: Assignment[]
    ArrayReference[name:'zwy']
        Range[]
```

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PSyIR for explicit loops

```
zwx(:,:,jpk) = 0.e0    ;    zwy(:,:,jpk) = 0.e0

DO jk = 1, jpk-1
   DO jj = 1, jpj-1
      DO ji = 1, jpi-1
         zwx(ji,jj,jk) = umask(ji,jj,jk) * ( mydomain(ji+1,jj,jk) - mydomain(ji,jj,jk) )
         zwy(ji,jj,jk) = vmask(ji,jj,jk) * ( mydomain(ji,jj+1,jk) - mydomain(ji,jj,jk) )
      END DO
   END DO
END DO

zslpx(:,:,jpk) = 0.e0    ;    zslpy(:,:,jpk) = 0.e0

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) =                          ( zwx(
         &               * ( 0.25d0 + SIGN( 0.25d0, zwx
         zslpy(ji,jj,jk) =                          ( zwy(
         &               * ( 0.25d0 + SIGN( 0.25d0, zwy
      END DO
   END DO
END DO

DO jk = 1, jpk-1
   DO jj = 2, jpj
      DO ji = 2, jpi
         zslpx(ji,jj,jk) = SIGN( 1.d0, zslpx(ji,jj,j
         &
         &
         zslpy(ji,jj,jk) = SIGN( 1.d0, zslpy(ji,jj,j
         &
         &
      END DO
   END DO
END DO
```

```
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Schedule[]
        0: Loop[type='lat', field_space='None', it_space='None']
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            BinaryOperation[operator:'SUB']
                Reference[name:'jpj']
                Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Schedule[]
                0: Loop[type='lon', field_space='None', it_space='None']
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    BinaryOperation[operator:'SUB']
                        Reference[name:'jpi']
                        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Schedule[]
                        0: InlinedKern[]
                            Schedule[]
                                0: Assignment[]
                                    ArrayReference[name:'zwx']
                                        Reference[name:'ji']
                                        Reference[name:'jj']
                                        Reference[name:'jk']
                                    BinaryOperation[operator:'MUL']
                                        ArrayReference[name:'umask']
                                            Reference[name:'ji']
                                            Reference[name:'jj']
                                            Reference[name:'jk']
                                        BinaryOperation[operator:'SUB']
                                            ArrayReference[name:'mydomain']
                                                BinaryOperation[operator:'ADD']
                                                    Reference[name:'ji']
                                                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                                                Reference[name:'jj']
                                                Reference[name:'jk']
```

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PSyIR with CodeBlock

```
OPEN(unit = 4, file = 'output.dat', form='formatted')

DO jk = 1, jpk-1
   DO jj = 2, jpj-1
      DO ji = 2, jpi-1
         write(4,*) mydomain(ji,jj,jk)
      END DO
   END DO
END DO

CLOSE(4)
```

```
13: Loop[type='levels', field_space='None', it_space='None']
    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    BinaryOperation[operator:'SUB']
        Reference[name:'jpk']
        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
    Schedule[]
        0: Loop[type='lat', field_space='None', it_space='None']
            Literal[value:'2', Scalar<INTEGER, UNDEFINED>]
            BinaryOperation[operator:'SUB']
                Reference[name:'jpj']
                Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
            Schedule[]
                0: Loop[type='lon', field_space='None', it_space='None']
                    Literal[value:'2', Scalar<INTEGER, UNDEFINED>]
                    BinaryOperation[operator:'SUB']
                        Reference[name:'jpi']
                        Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Literal[value:'1', Scalar<INTEGER, UNDEFINED>]
                    Schedule[]
                        0: CodeBlock[[<class 'fparser.two.Fortran2003.Write_Stmt'>]]
```

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Tracer-advection mini-app

- Hands-on sessions will all use the Tracer-advection mini-app
  - Developed by CMCC
  - Basis of the 'NEMO Dwarf' (ESCAPE Project)
- Based on a tracer-advection routine from NEMO
  - Always high in performance profile (see earlier)
- Outer loop over tracer species becomes an 'iteration' loop
- Representative of majority of code base
- No MPI
- 288 lines of Fortran
- No inputs required - generates synthetic data

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Hands-on and questions...

```
$ git clone --recursive https://github.com/stfc/PSyclone.git
$ cd PSyclone
$ pip install .
$ cd tutorials/practicals/nemo/1_nemo_psyir
```

https://github.com/stfc/PSyclone/tree/master/tutorial/practicals/nemo/1_nemo_psyir

Questions on Slack: https://join.slack.com/t/meteoswiss-group/shared_invite/zt-j7ry1st0-4TW0D9B_auq7tDa4zylrqQ

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