is-enes
INFRASTRUCTURE FOR THE EUROPEAN NETWORK FOR EARTH SYSTEM MODELLING

NEMO: improving computational performance

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The IS-ENES3 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 824084

NEMO: computational performance community

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NEMO improvements

- Single core performance
  - Tiling
  - Loop fusion
  - Mixed precision
- Communication
  - Neighborhood collective communications
  - Extended halo size
- Macro task parallelization
- Multigrid refinement optimization
- I/O
  - Improving read/write with XIOS
  - Online diagnostics
- Support for different architectures
  - GPU
  - DSL
- Containerization

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Single core performance
Loop fusion

- Efficient exploitation of memory hierarchies and hardware peak performance
- **Loop fusion technique** aims at better exploiting the cache memory by fusing DO loops together

```
DO j=1, n-1
   DO i=1, n
      b (i,j) = in(i,j+1) - in(i,j)
   END DO
END DO

DO j=2, n-1
   DO i=1, n
      out (i,j) = b(i,j) - b(i,j-1)
   END DO
END DO
```

```
DO j=2, n-1; DO i=1, n
      b_0  = in(i,j+1) - in(i,j  ) ! correspond to b(i,j)
      b_m1 = in(i,j  ) - in(i,j-1) ! correspond to b(i,j-1)

      out(i,j) = b_0 - b_m1
END DO; END DO
```

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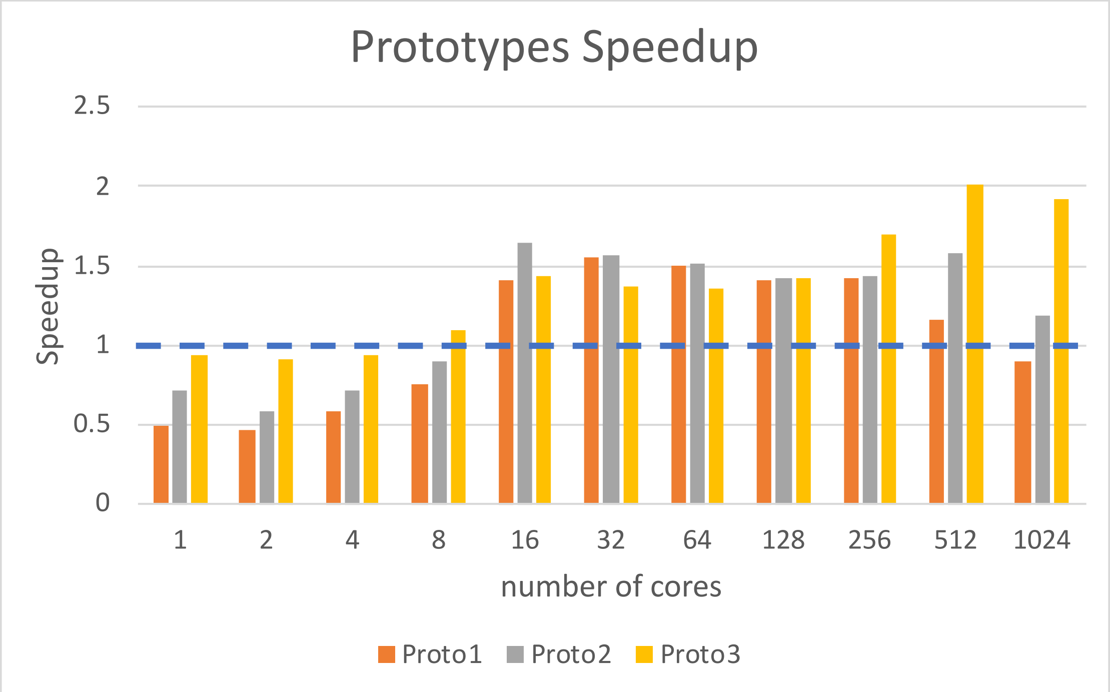
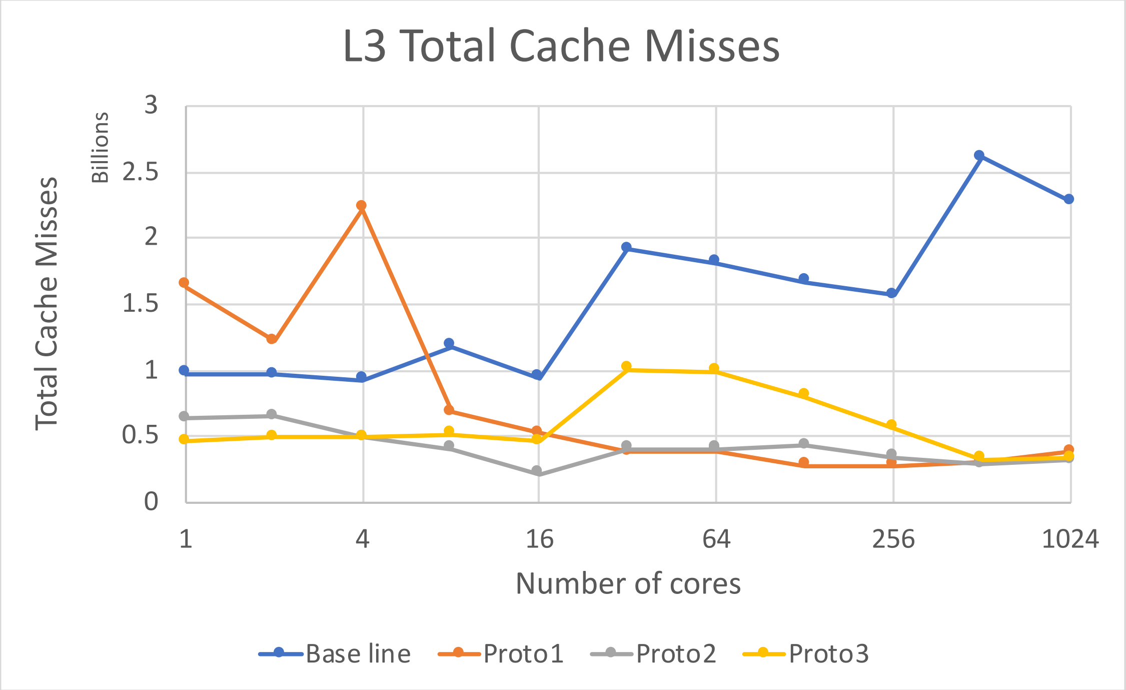
IS-ENES3 1st General Assembly
25-27th March 2020

Single core performance
Loop fusion

- Three different levels of fusion have been implemented
- proto1: has the maximum level of fusion with redundant operations
- proto2: introduces the buffers rotation in the outer loop
- proto3: uses the buffers rotation in the outer and middle loop





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Single core performance
Tiling

- Tiling allows us to divide the calculation into chunks of work that can remain cache-resident for as long as possible.
- The technique leaves the tile size and shape as tunable parameters, which can be tuned appropriately for cache sizes on any platform.
- Preliminary tests established that the CPU time taken by some typical 3D routines within NEMO using current configurations could be reduced by at least a factor of 2 by 3D tiling

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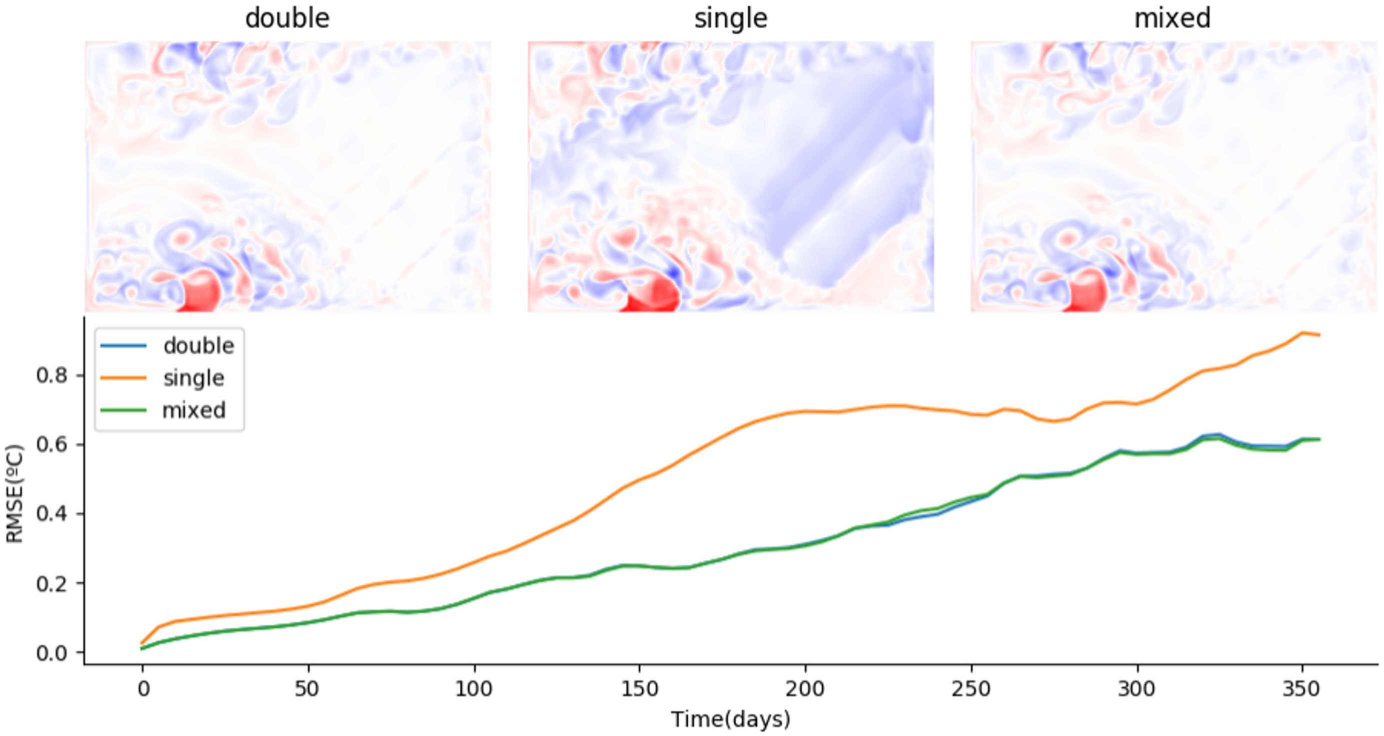
Single core performance Mixed Precision

Impact of precision on sea-surface temperature in NEMO4:
comparison of GYRE1/9º simulations using different precisions



Mixed-precision approaches can provide performance benefits while keeping the accuracy of the results.
In implementation phase this 2020.

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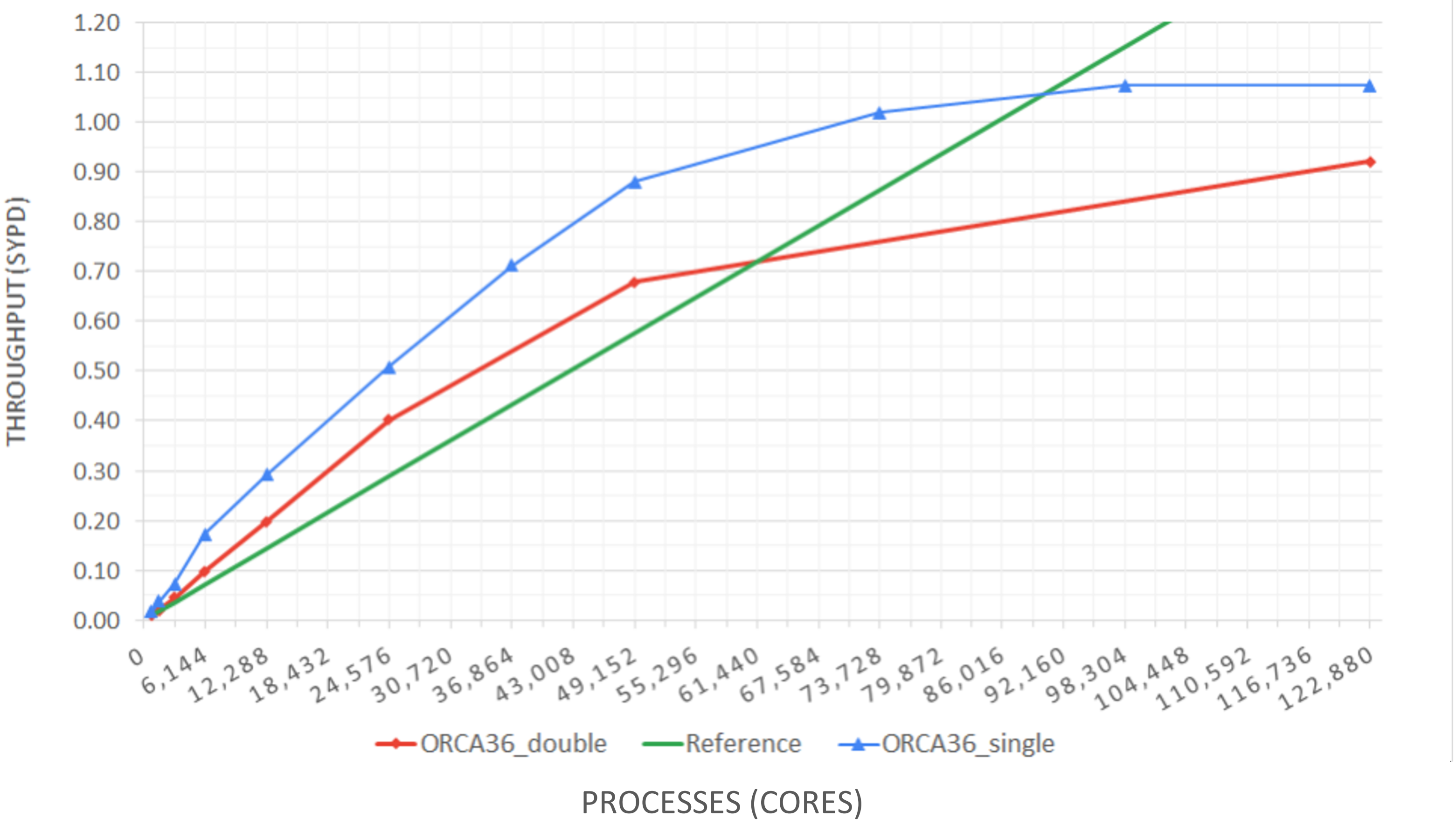
Single core performance
Mixed Precision

ORCA36 scalability – Double vs Single precision – Grand challenge



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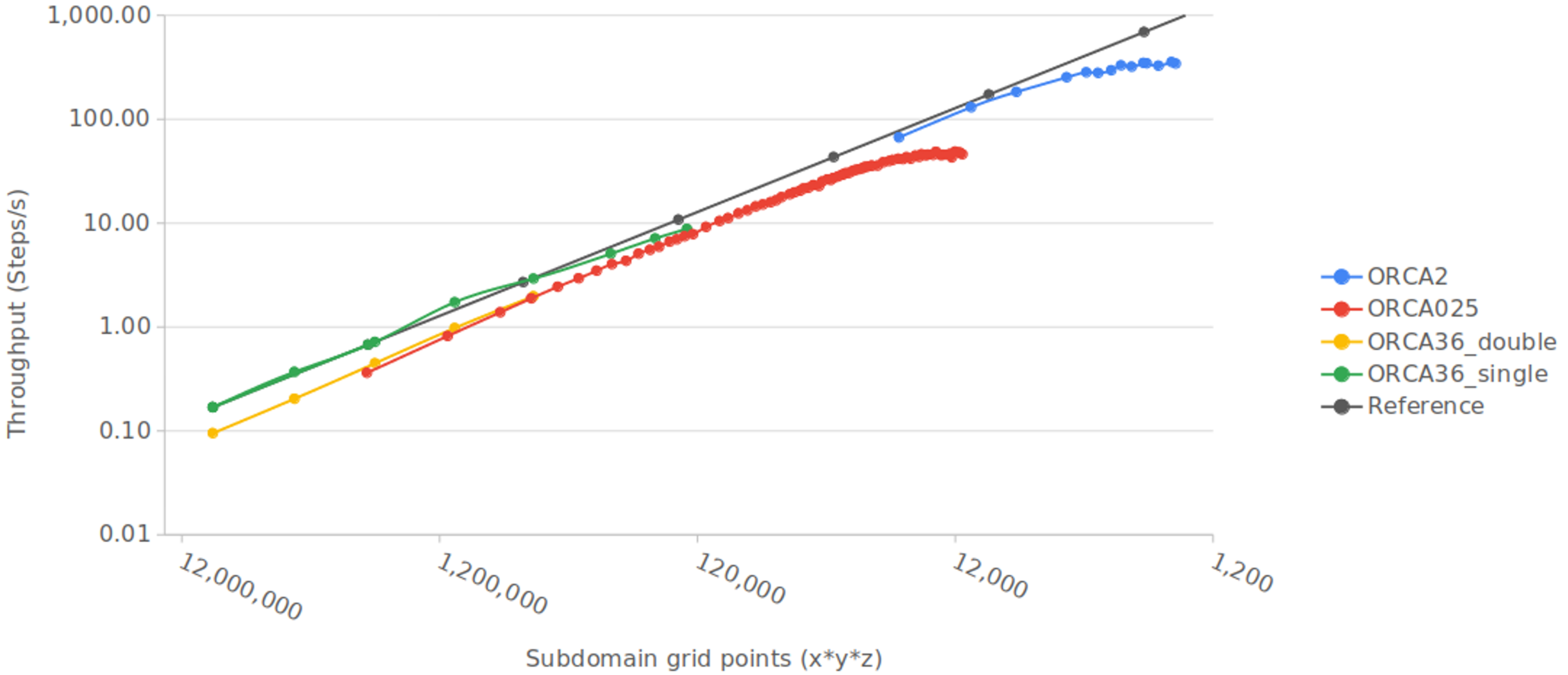
Single core performance Mixed Precision

ORCA2, ORCA025 and ORCA36 scalability



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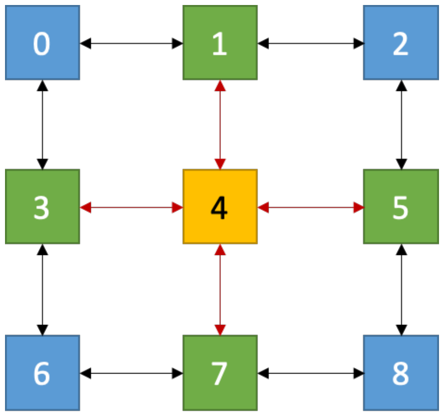
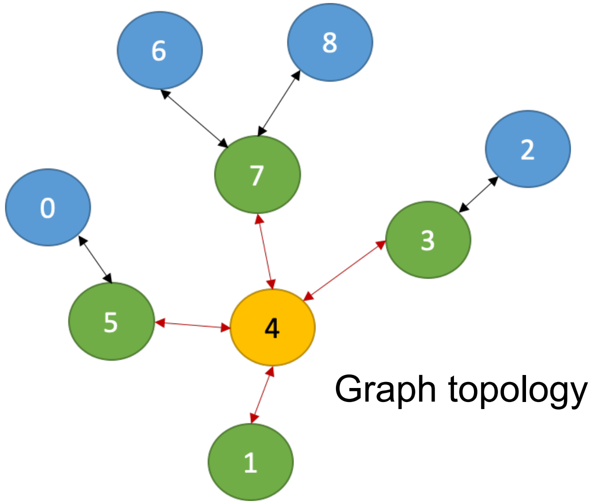
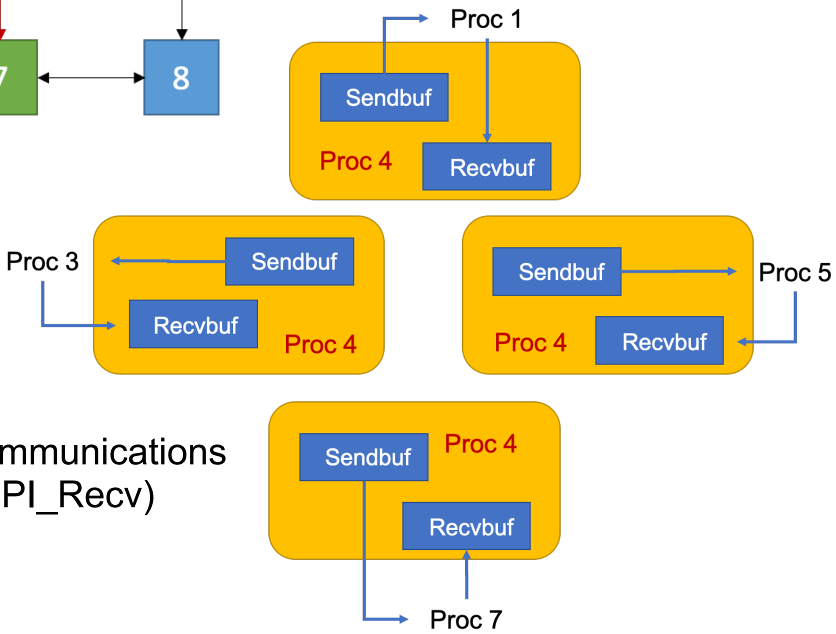
MPI Communication
Neighborhood collectives

Cartesian topology



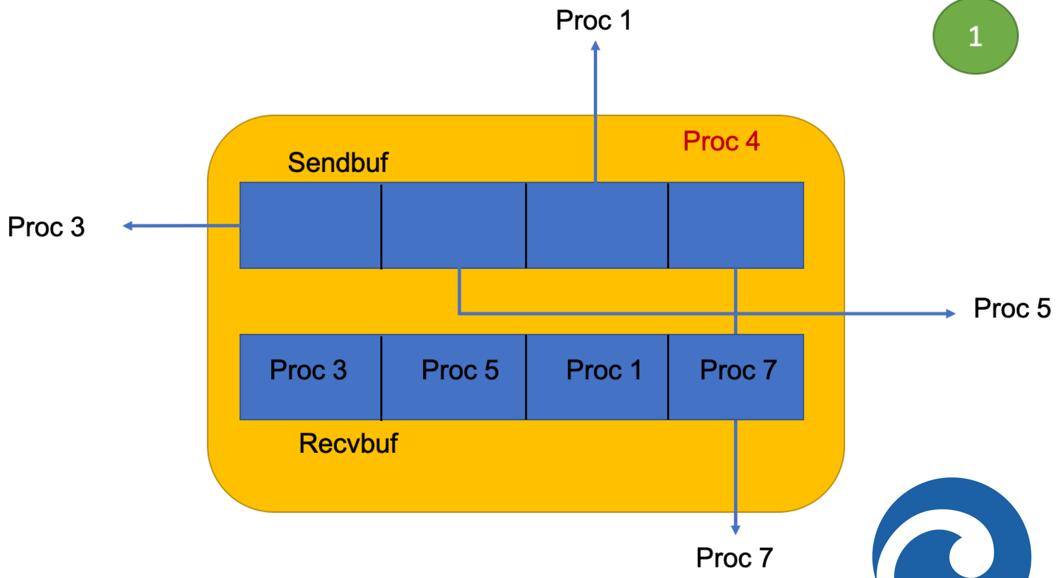


Graph topology



4 Point-2-Point communications
(MPI_Send/MPI_Recv)

1 collective communication
(MPI_Neighbor_alltoall)



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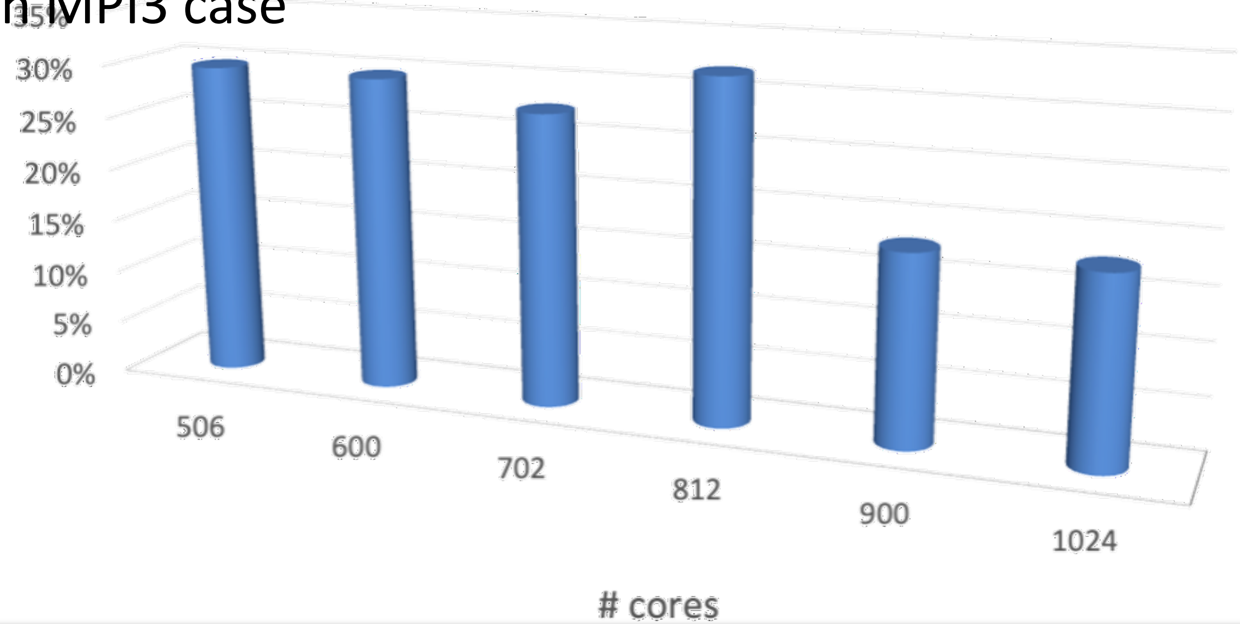
MPI Communication Neighborhood collectives

- Extension of LBC (Lateral Boundaries Condition) module to support MPI3 Neighborhood Collectives:
  - New Cartesian communicator
  - Ranks reordering to match NEMO processes order
  - Data buffer handling
  - Implementation of multi field exchange in MPI3 case

- Test on the advection scheme
  - GYRE_PISCES configuration (nn_GYRE=200 → ~6000x4000x31 grid resolution)
  - Communication time improved within a range of 18%-32%



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MPI Communication Extended halo

- The halo management support has been introduced to provide the developer with a tool for specifying different halo sizes for different NEMO Kernels.
- As an example, in the surface pressure gradient kernel it could be convenient to enlarge the halo region (up to 5 lines or more) to reduce the communication steps in the time sub-stepping loop. In all of the other kernels the halo size could be 2 lines
- A wider halo size reduces the frequency of message exchanges whilst increases the message size at each exchange.

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Macro Task Parallelism

- Parallelize OPA (ocean module) and TOP-PISCES (tracer advection biogeochemistry -BGC- module) into two executables and ensure 3D coupled fields exchange via the community coupler OASIS.
  - Strategy can be decomposed in 6 steps:
  - Set-up of an up-to-date TOP-PISCES stand-alone version
  - Identification of the exchanged coupling fields
  - Duplication of the existing surface (atmosphere) interface (sbccpl)
  - OASIS parameter and input file building
  - Validation of the coupled simulation by comparison with a similarly lasting simulation led with the standard online NEMO-TOP-PISCES configuration
  - Load balancing and performance measurement

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I/O optimization through XIOS

- Improvement on I/O reading initial conditions and reading regridding weights using XIOS
- the XIOS support has also been adopted for reading and writing of the restart files in the SI3 (sea ice model).

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Online diagnostics – GPU based

- The rationale of this activity is to improve the NEMO computational performance by offloading the computations for diagnostics on GPU.
- The ocean global heat content, salt content and volume conservation diagnostics (`dia_hsb`) has been chosen as starting point because it is the most expensive.
- The code itself is executed 50x faster than in a single CPU but the data transfer to and from GPU is the main bottleneck.
- Pinned Memory and GPU Directly Attached to the host can be used to mitigate the data transfer penalty

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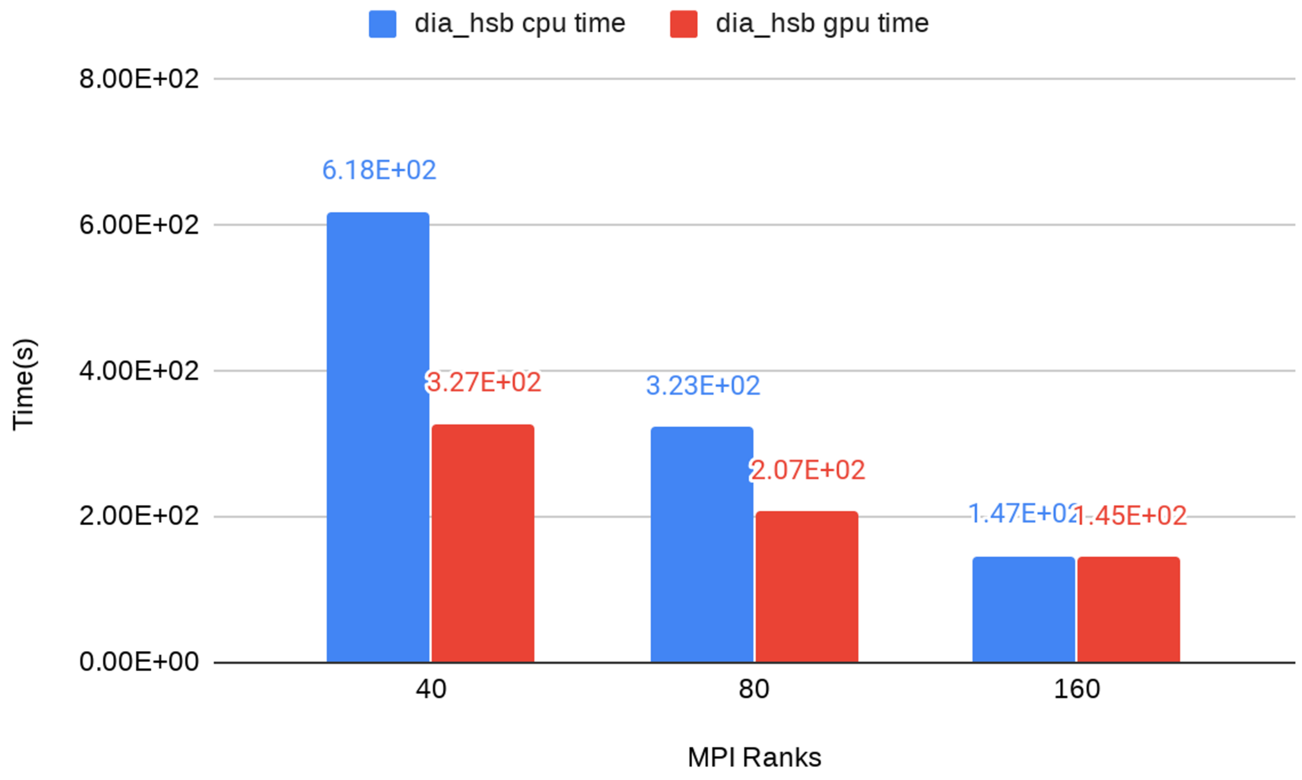
Online diagnostics – GPU based

`dia_hsb` scalability



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Online diagnostics – HPDA based

- The Ophidia High Performance Data Analytics (HPDA) framework has been used for offloading model diagnostics from NEMO to additional parallel cores.
- The Ophidia software architecture decouples the analytics phase from the underlying storage features via simple API, with the aim of supporting different storage devices.
- a diagnostic concerning the Potential Density has been developed in order to compute three different related metrics:
    - the potential 3D density referred to the surface;
    - the mean 3D density over a given time period;
    - the calculation of the 27.8 density isopycnic.

Centro Euro-Mediterraneo sui Cambiamenti Climatici

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Multigrid capability

- The support for nested multigrid in NEMO is implemented in the AGRIF component
- In realistic configuration, AGRIF is not optimized and lacks an efficient load balancing
- NEMO model has been updated to provide an estimation of the computational cost of each grid; a new load balancing policy can be implemented in AGRIF

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NEMO on GPU

- Investigate NEMO performance on GPUs
- Identify parts of the code preventing efficient execution on GPUs
- Use PSyClone to automatically insert OpenACC directives into the code
- The Met Office GO8: 1 deg. NEMO configuration (362x332x75 points) is used for tests; no MPI
- This configuration (without SI3) is running on 1 GPU 4 times faster than on 1 core; with SI3 the code on GPU is only slightly faster than on 1 core.

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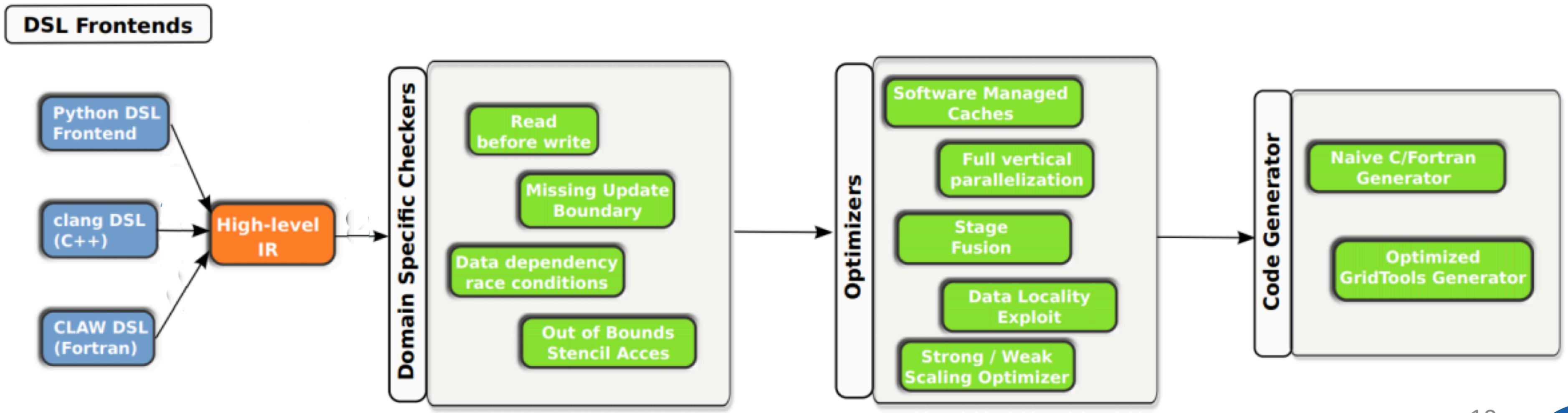
DSL GTClang for NEMO

- Domain Specific Language GTClang has being enhanced to support NEMO requirements (i.e. regular grid, numerical integration schema, computational kernels)
- Preliminary evaluation of GTClang through porting of specific “dwarf” which represent the advection schema (MUSCL) used in NEMO



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DSL GTClang for NEMO

```
DO jk = 1, jpkm1
 DO jj = 1, jpjm1
  DO ji = 1, fs_jpim1
   zwx(ji,jj,jk) = umask(ji,jj,jk) * ( ptb(ji+1,jj,jk,jn) - ptb(ji,jj,jk,jn) )
  END DO
 END DO
END DO

DO jk = 1, jpkm1              !-- Slopes
 DO jj = 2, jpj-1
    DO ji = 2, jpi-1
    zslpx(ji,jj,jk) = zwx(ji,jj,jk) + zwx(ji-1,jj,jk)
    END DO
 END DO
END DO

DO jk = 1, jpkm1                 !-- Horizontal advective fluxes
 DO jj = 2, jpj-2
    DO ji = 2, jpi-2
    zu  = pun(ji,jj,jk) / ( e1u(ji,jj) * e2u(ji,jj) * fse3u(ji,jj,jk) )
    zflux(ji,jj,jk) = pun(ji,jj,jk) * ( ptb(ji+1,jj,jk,jn) + zu * zslpx(ji+1,jj,jk) )
    END DO
 END DO
END DO

DO jk = 1, jpkm1                 !-- Tracer advective trend
 DO jj = 3, jpj-2
    DO ji = 3, jpi-2
    zu = 1. / ( e1t(ji,jj) * e2t(ji,jj) * fse3t(ji,jj,jk) )
    pta(ji,jj,jk,jn) = pta(ji,jj,jk,jn) - zu * ( zflux(ji,jj,jk) - zflux(ji-1,jj,jk) )
  END DO
 END DO
END DO
```

```
stencil advection_MUSCL {
  do {
    vertical_region (k_start, k_end - 1) {
      zwx = u_mask * (ptb(i+1) - ptb);
    }
      //-- Slopes of tracer
    vertical_region (k_start, k_end - 1)
      zslpx = zwx + zwx(i-1);
    }
      //-- Horizontal advective fluxes
    vertical_region (k_start, k_end - 1) {
      zu = pun / (e1u * e2u * fse3u);
      zflux = pun * (ptb(i+1) + zu * zslpx(i+1));
    }
      // Tracer advective trend
    vertical_region (k_start, k_end - 1) {
      zu = 1.0 / (e1t * e2t * fse3t)
      pta = pta - zu * (zflux - zflux(i-1));
    }
  }
}
```

Pros

- Easy code maintenance
- Improved code readability
- Seamless support for GPU
- Less error-prone code
- Fast and efficient technical support

Cons

- GTClang environment hard to compile and install
- No documentation
- No MPI support
- Lose of performance w.r.t. the original version

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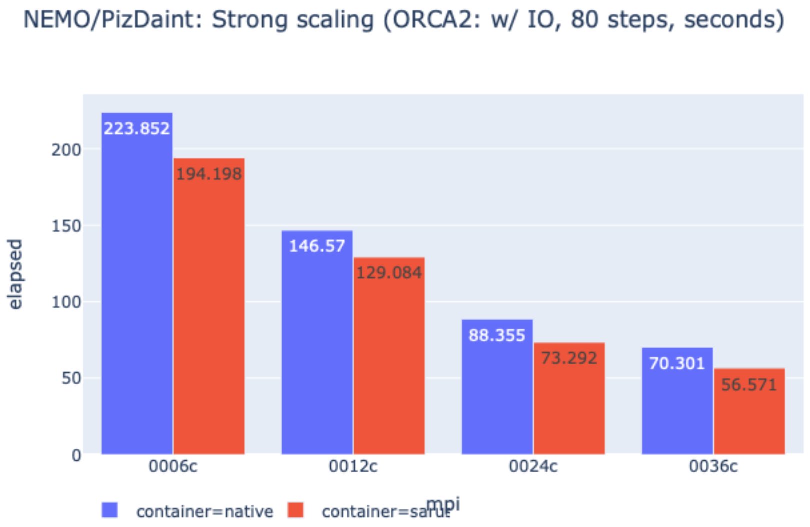
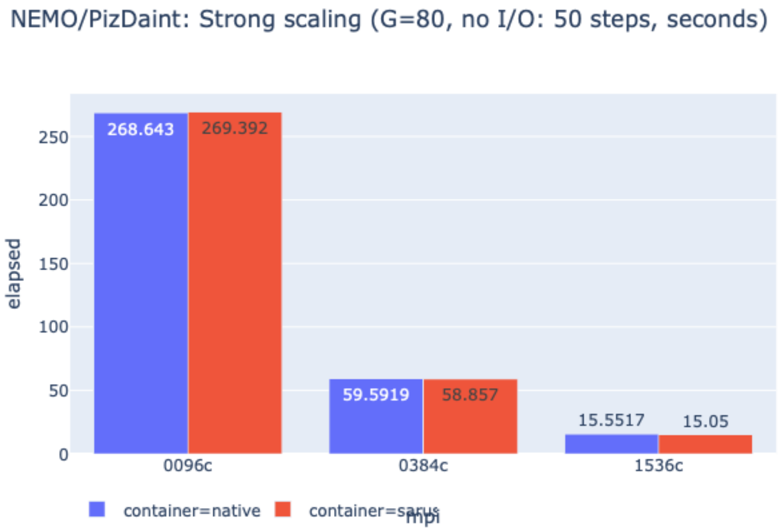
NEMO Containerization

- The aim is to build a self-contained installation of the NEMO which includes libraries, compilers and system settings
  - Configuration portability
  - Reproducibility of the same experiments on different machine, on different
- Container manager: SARUS (developed as CSCS)
- Two containers for two configurations were created and tested: GYRE, ORCA2





For more information: https://github.com/eth-cscs/ContainerHackathon

The Consortium

Coordinated by **CNRS-IPSL**, the IS-ENES3 project gathers **22 partners** in **11 countries**

with

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