NEMO: improving computational performance

ISENES3 – General Assembly – Oct, 4-6 2021

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

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IS-ENES3 2nd General Assembly
4-6th October 2021

NEMO: computational performance community

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NEMO improvements

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

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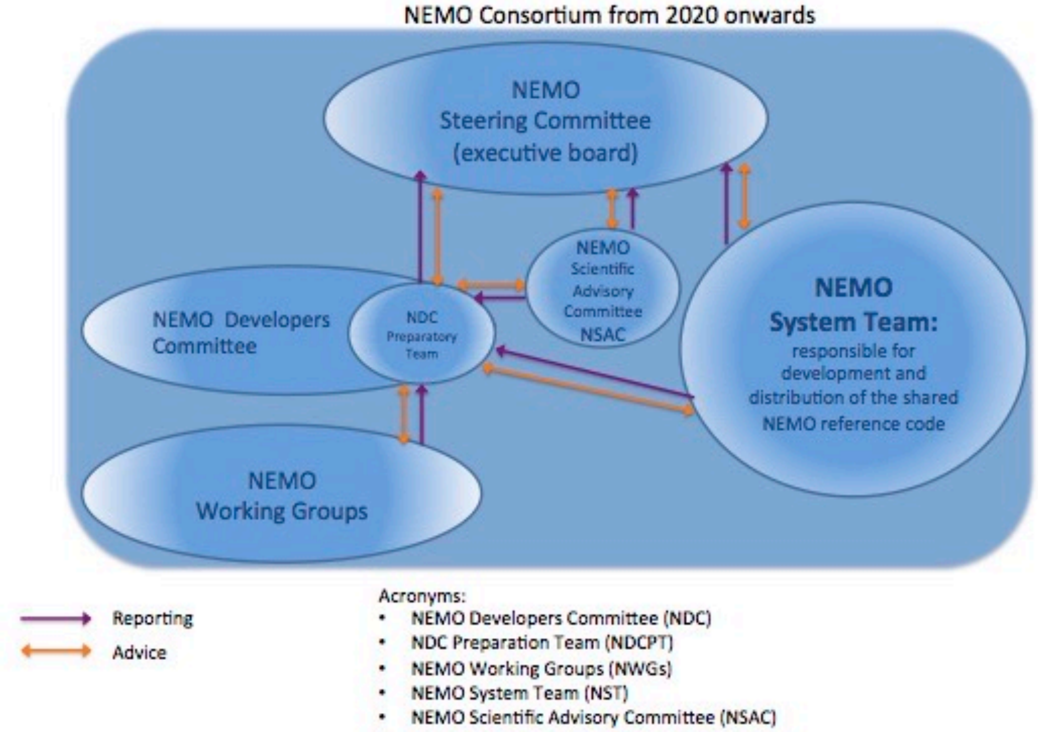
NEMO Consortium organization

- NEMO System Team (NST) is responsible for development and distribution of the NEMO reference code
  - New actions are defined in the annual WorkPlan
- NEMO Working Groups articulate and coordinate the exploration of options for development of the NEMO reference code
  - NEMO HPC-WG aims at evaluating solutions to improve the computational performance of the NEMO code.



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Loop fusion and Tiling

- Efficient exploitation of memory hierarchies and hardware peak performance
- **Loop fusion technique** aims at better exploiting the cache memory by fusing DO loops together
- **Tiling** the calculation is divided into chunks of work that can remain cache-resident for as long as possible.
  - tile size and shape can be tuned appropriately for cache sizes on any platform

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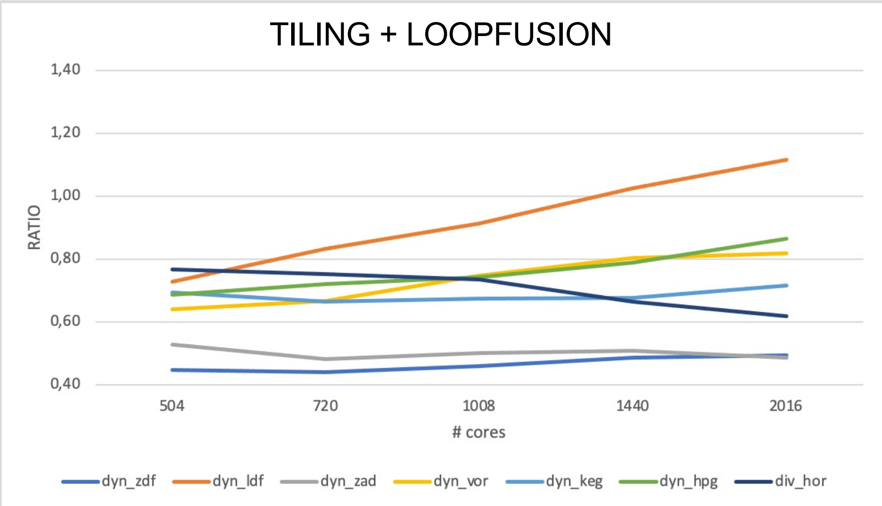
Loop fusion and Tiling



The ratio of the optimized code w.r.t. the baseline is reported changing the number of cores for the key routines of ocean dynamics. Ratio < 1 is good

- LoopFusion and Tiling applied only to the Ocean Dynamics and Ocean Tracer
- On average a speedup of 1.4x can be achieved
- The impacts of this optimization strongly depends by the platform and by the configuration

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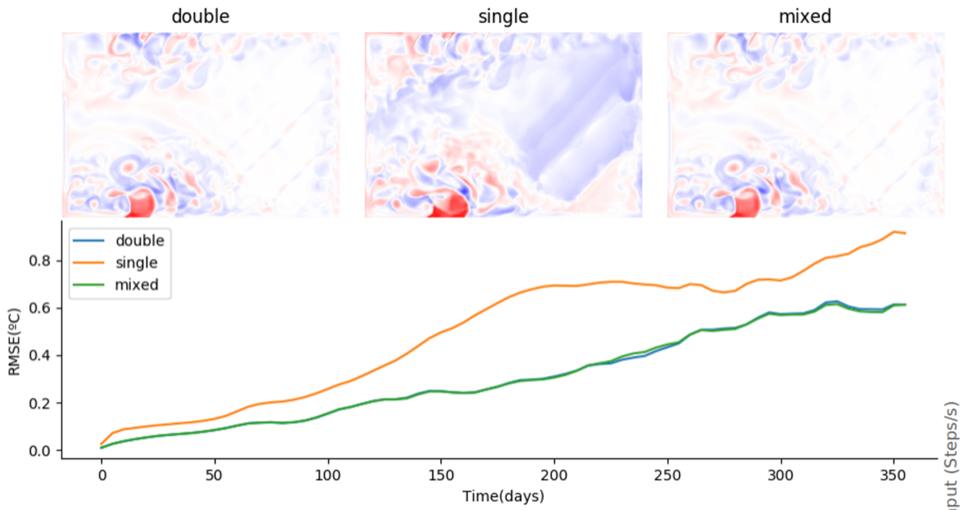
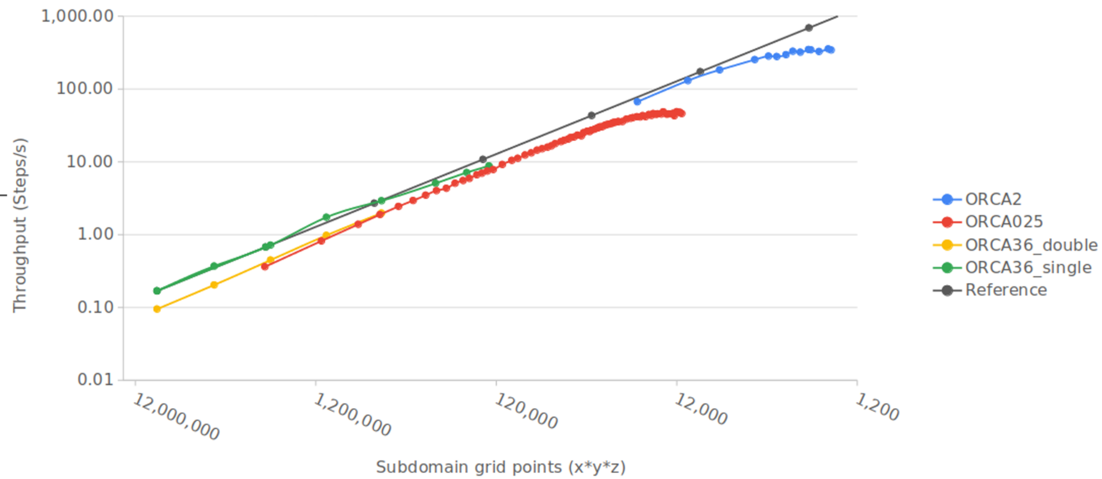
Mixed Precision

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.

- With an appropriate tuning of the variabiles in SP vs those in DP, the results accuracy of the mixed precision version is preserved
- The mixed precision approach considerably improve the parallel scalability
- Mixed precision support is under evaluation to be included in the official NEMO release



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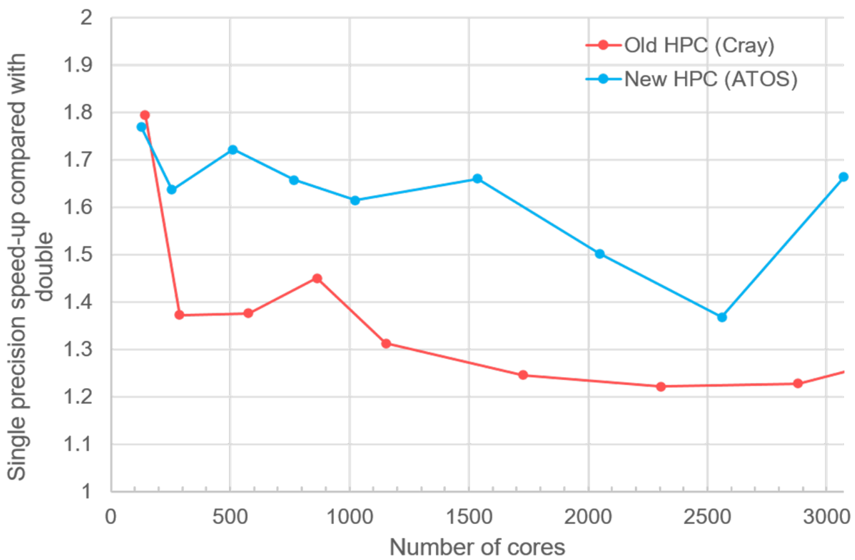
Single Precision at ECMWF



- Fully single-precision coupled atmosphere-wave-ocean forecasts now possible, **including NEMO**
- Tested with eORCA1 ocean and compared with operational reference (DP NEMO) in extended range forecasts
- Mostly skill neutral change
- Speed-up from using single precision in NEMO measured on old (Cray) and new (ATOS) HPC at ECMWF
- Final speed-up depends on I/O server → integration of NEMO with ECMWF I/O server MultIO underway

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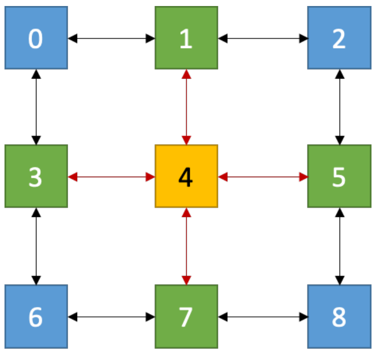
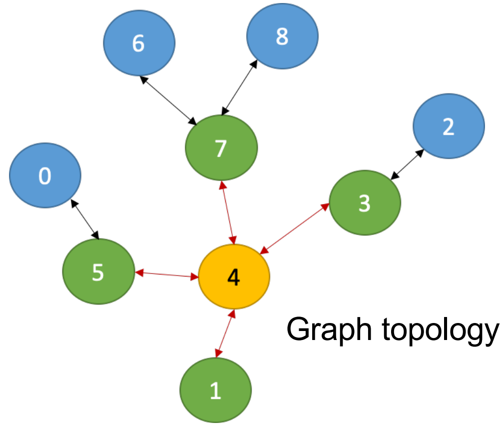
MPI Communication Neighborhood collectives

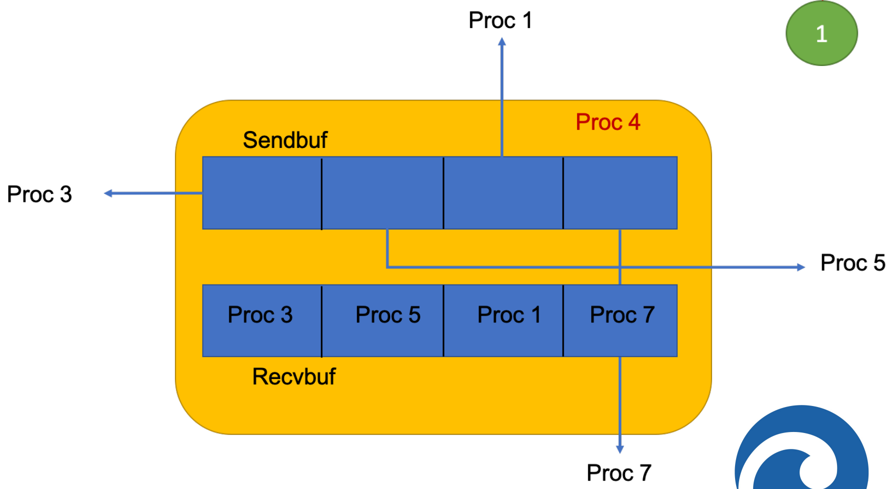
Cartesian topology

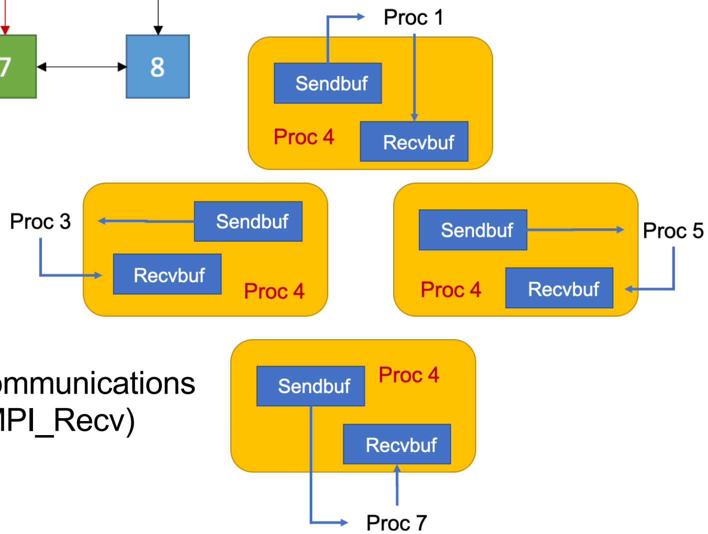




Graph topology

1 collective communication
(MPI_Neighbor_alltoall)





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

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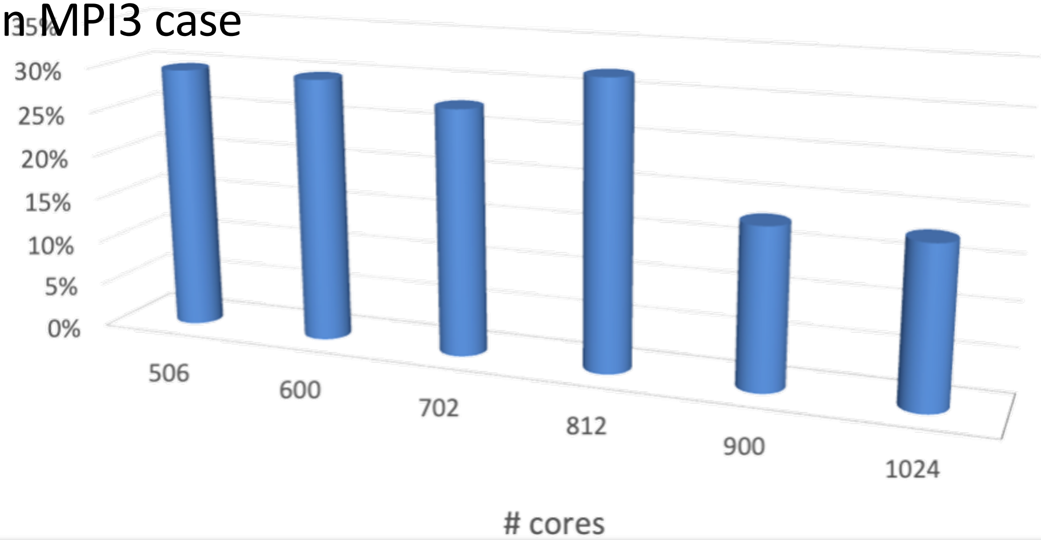
MPI Communication Neighborhood collectives

- 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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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.
  - The ocean-BGC coupled model exhibits an improvement of computing performance when the subdomain decomposition leads to computations/communications ratio that put the performance just below the scalability limit
  - The coupling cost, caused by OASIS coupling extra cost and load imbalance between components is non negligible (around 20% in our case) but can be reduced
  - This contrasted result suggests that the only clear performance gain can only be ensured with the radical cost lowering of the most time consuming component, the BGC model (coarsening)

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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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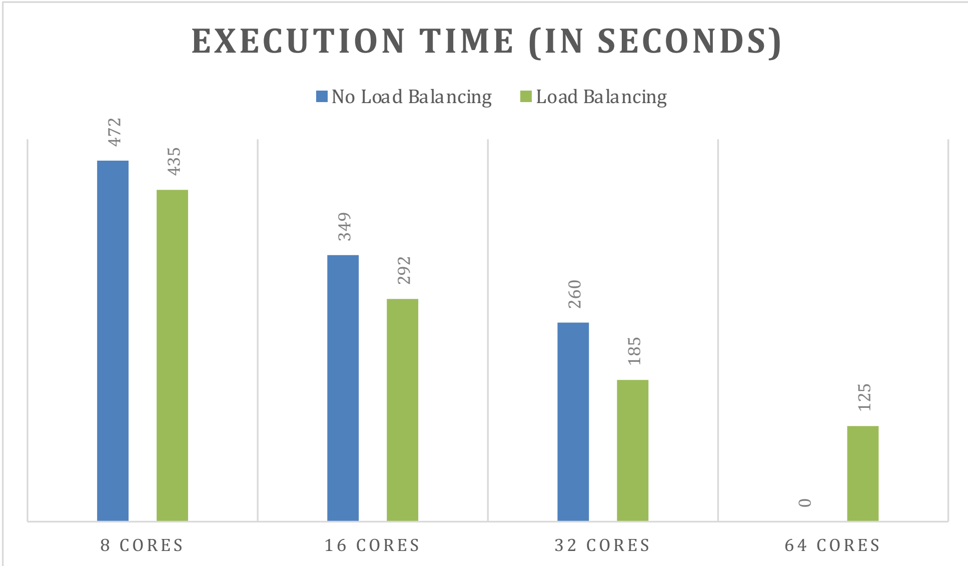
Multigrid capability

- The support for nested multigrid in NEMO is implemented in the AGRIF component
- NEMO model has been updated to provide an estimation of the computational cost of each cell grid; a new load balancing policy has been implemented in AGRIF
- Achieved 1.4x speedup on average



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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
- Asynchronal communications and a memory buffer approach reduce significantly the data transfer penalty

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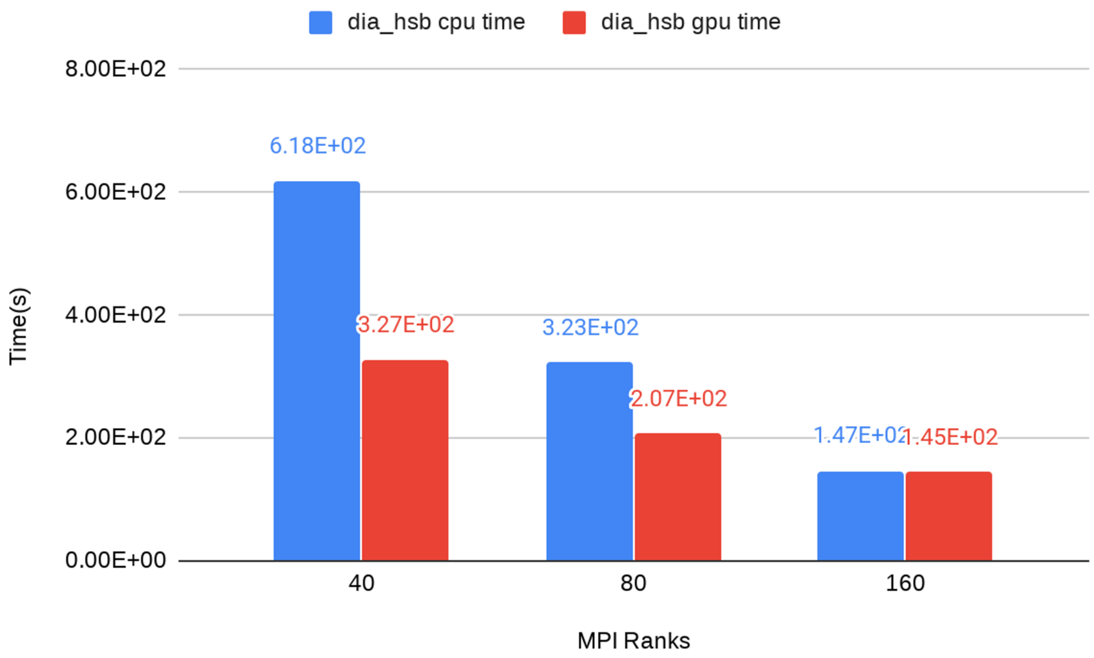
Online diagnostics – GPU based

`dia_hsb` scalability



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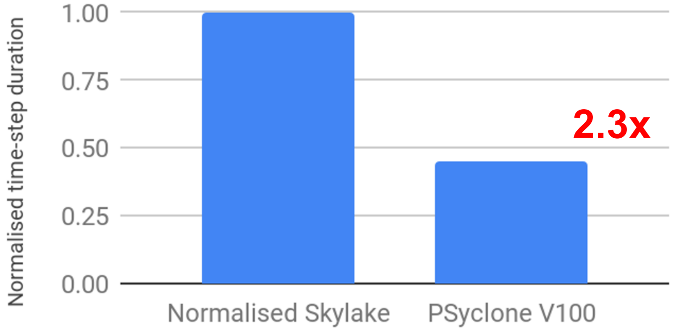
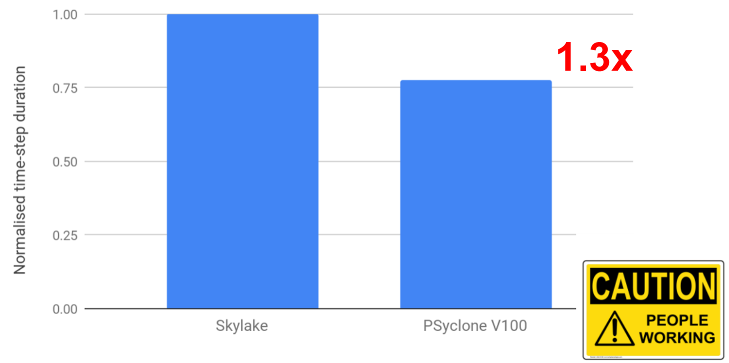
NEMO on GPU

- Use PSyclone to automatically insert OpenACC directives into the code

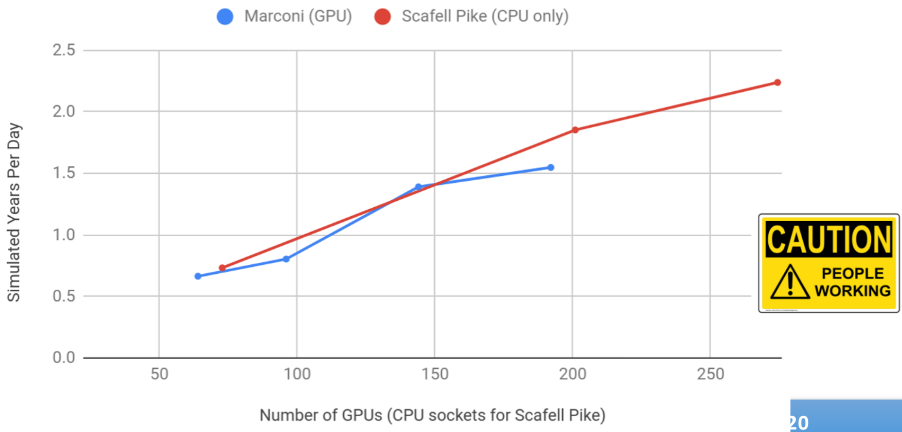
ORCA1 ocean, GPU



ORCA1 ocean+sea ice, GPU



ORCA12 ocean, GPU + MPI



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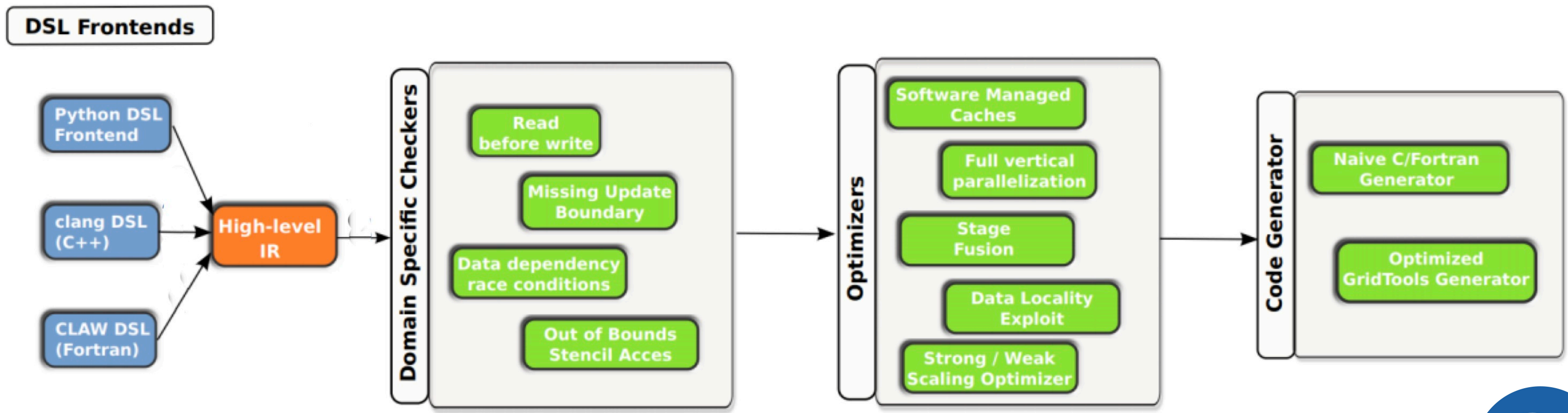
DSL GTClang for NEMO

- 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

```fortran
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
```

```cpp
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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The Consortium

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

CNRS with CEA, Sorbonne Université
National Centre for Atmospheric Science
Met Office
DKRZ
BSC
CERFACS
CMCC
Koninklijk Nederlands Meteorologisch Instituut
SMHI
UK Research and Innovation
Universidad de Cantabria
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