The webinar will start very soon !

Please check that your microphone is muted and your camera off !

Please only use the chat for practical questions, and use the Google doc for the 15-minutes slot dedicated to questions at the end of the webinar.

Sophie Valcke

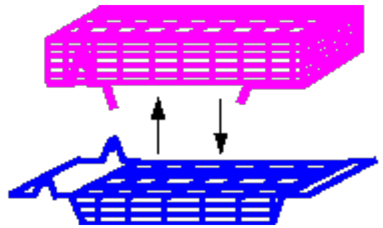
Outline

Introduction

1. Global performance & technical solutions
    - sequential vs concurrent coupling
    - integrated coupling framework vs coupler approach
2. Few coupling software
    - Earth System Modeling Framework (ESMF)
    - NCAR coupling framework Cpl7
    - Flexible Modeling System (FMS)
    - OASIS3-MCT
3. New in OASIS3-MCT_5.0 (12/2021)

Conclusions and perspectives

Why couple ocean, atmosphere, land, ocean, sea-ice models?



- Of course, to treat the Earth System globally

What does "coupling of codes" imply?

- Exchange and transform information at the code interface
- Manage the execution and synchronization of the codes

What are the constraints?

- ✓ Coupling should be easy to implement, flexible, efficient, portable
- ✓ Coupling algorithm dictated by science (sequ. vs conc. coupling)
- ✓ Start from existing and independently developed codes
- ✓ Global performance and load balancing issues are crucial
- ✓ Platform characteristics (OS, CPU, message passing efficiency, ...)

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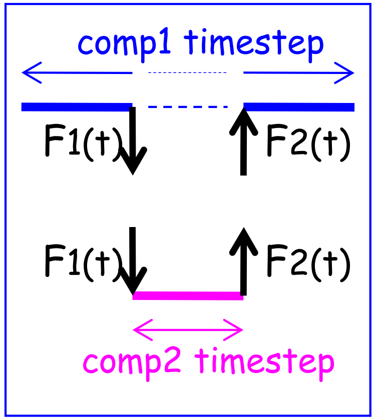
Conclusions and perspectives

The questions to ask yourself to optimise the performances of your coupled system:

- Do you want to optimise the throughput of your coupled model in term of Simulated Years Per (real) Day (SYPD)?
- Do you want to optimise your use of resources in terms of Simulated Years per CPU-hour?
- How do you have to layout the processes of your coupled components on the computing resources (CPUs) available? Is your coupling sequential or concurrent or a mix of both?

Global performance & technical solutions

Sequential coupling :

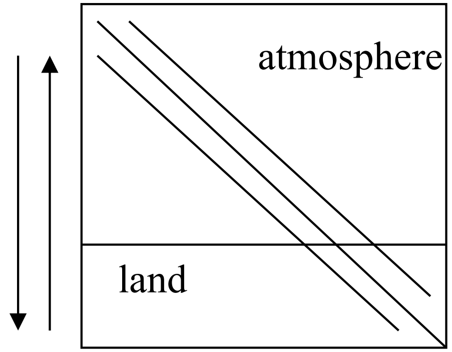


Implicit resolution of heat diffusion equation from the top of the atmosphere to the bottom of the land

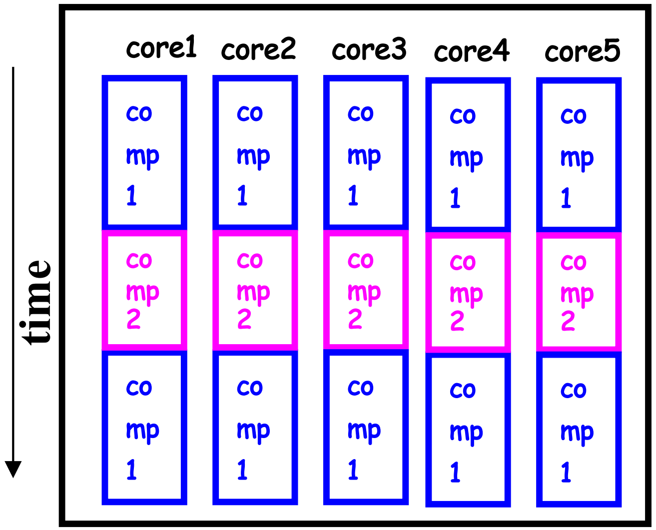
$$\partial T / \partial t = K \, \partial^2 T / \partial z^2$$

$$\frac{T_k^{n+1} - T_k^n}{\Delta t} = K \frac{T_{k+1}^{n+1} + T_{k-1}^{n+1} + 2T_k^{n+1}}{\Delta z^2}$$

$$AT^{n+1} = T^n$$



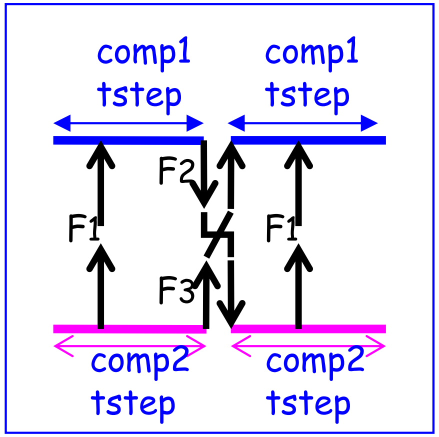
=> sequential execution on the same set of cores in one executable

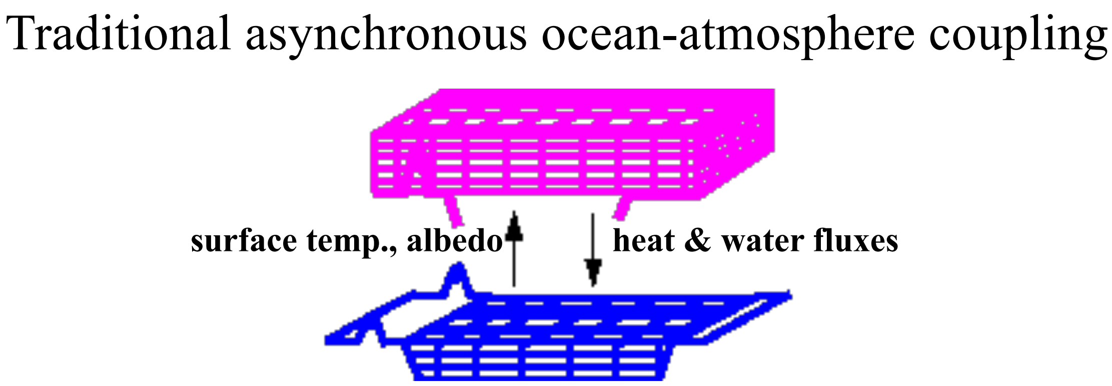


- ☺ Efficient coupling exchanges through the memory
- ☺ Optimal for load balancing if components can run efficiently on same number of cores
- ☹ Possible conflicts as components are merged in one executable (I/O, units, internal comm, etc.)
- ☹ No flexibility in coupling algorithm; no "in-place" exchanges

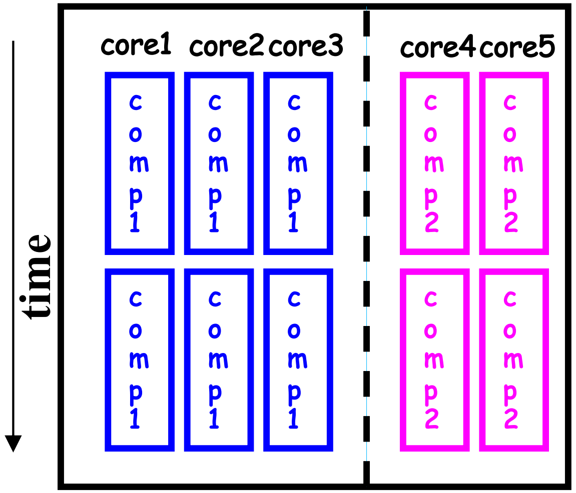
Global performance & technical solutions

Concurrent coupling:





=> concurrent execution on different sets of cores within one or separate executables



- ☺ Additional level of parallelism
- ☺ Flexible coupling algorithm (« in-place » exchanges within the timestep)
- ☹ Possible conflicts if components are merged in one executable (I/O, units, internal comm, etc.)
- ☹ Less efficient coupling exchanges as components may be on different nodes (no shared memory)
- ☹ Harder load balancing

1. merging the codes:

```
program prog1
…
call sub_prog2(data)
…
end prog1
```

→

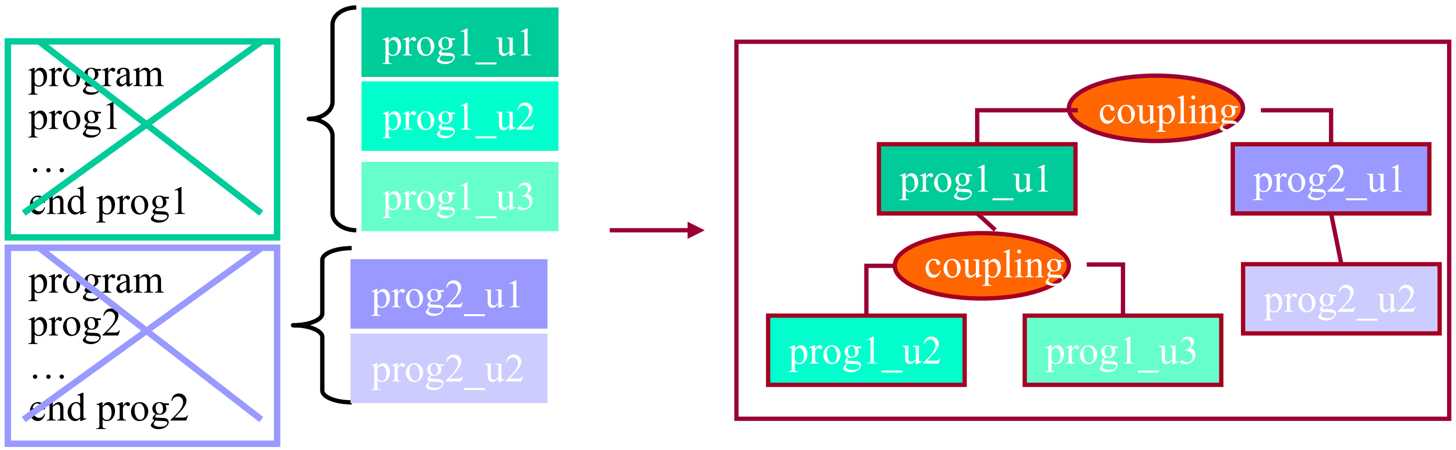
```
program prog2   (struck through)
subroutine sub_prog2(data)
…
end prog2
```

- ☺ efficient (memory exchange)
- ☺ as portable as the codes
- ☺ one executable: easier to debug, easier for the OS
- ☺ sequential execution of the components

- ☹ not easy to implement with existing codes (splitting, conflicts in namespaces and I/O)
- ☹ not flexible (coupling algorithm hard coded)
- ☹ no use of generic transformations/interpolations

2. integrated coupling framework

- Split code into elemental units
- Write or use coupling units
- Use the framework to build a hierarchical merged code
- Adapt code data structure and calling interface

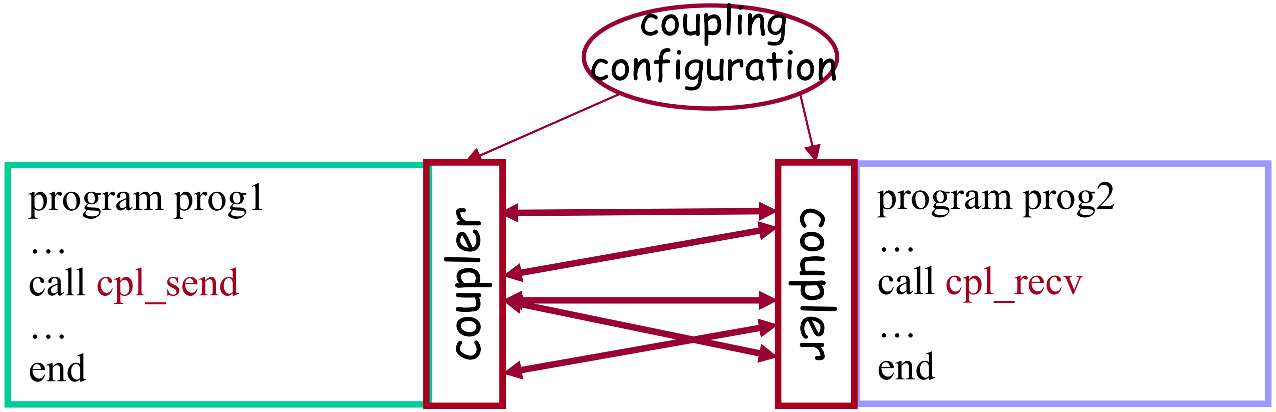


☺ efficient
☺ sequential and concurrent components
☺ use of generic utilities (parallelisation, regridding, time management, etc.)

☹ existing codes
😐 (easy)

→ probably best solution in controlled development environment

3. external coupler or coupling library

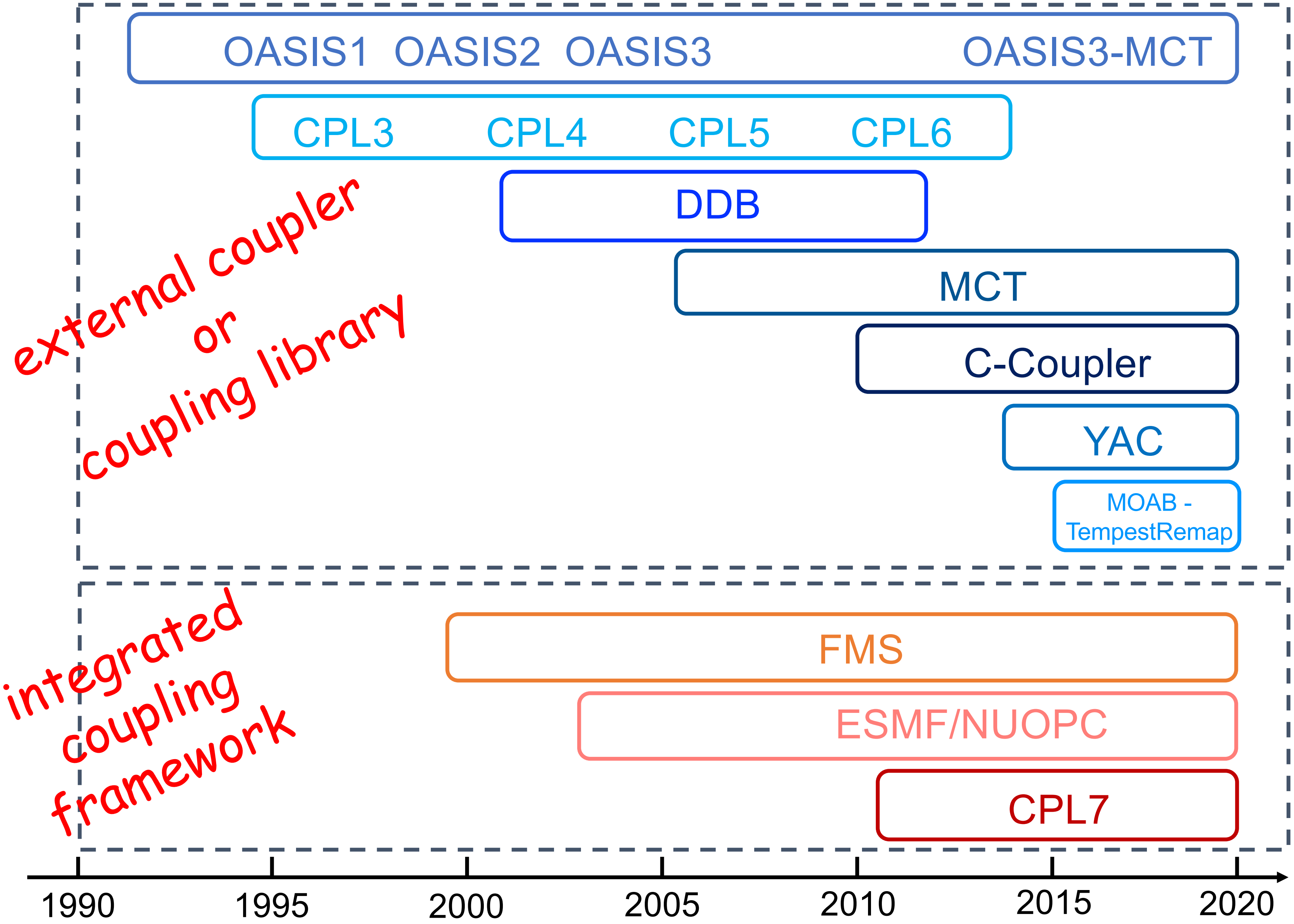


- ☺ existing codes
- ☺ use of generic transformations/regridding
- ☺ concurrent coupling (parallelism)

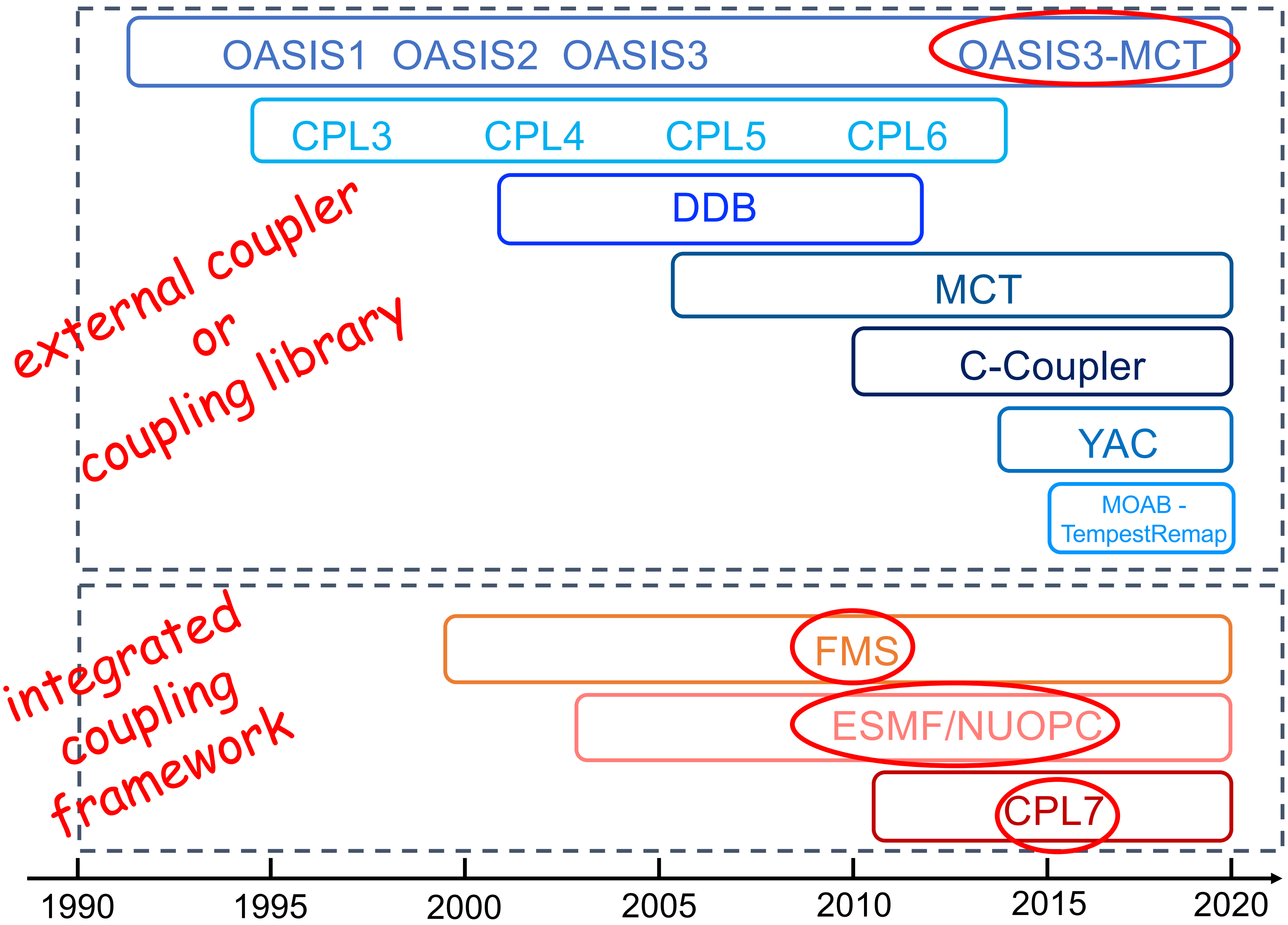
- ☹ efficient
- ☹ multi-executable: more difficult to debug; harder to manage for the OS

→ probably best solution to couple independently developed codes

Global performance & technical solutions



Global performance & technical solutions



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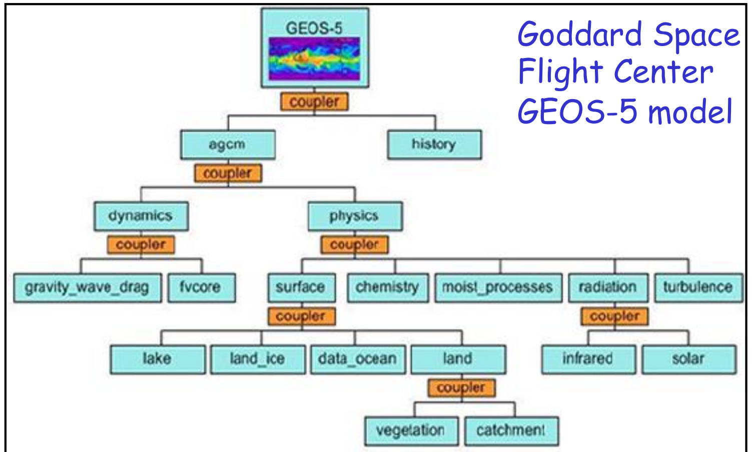
Conclusions and perspectives

The Earth System Modeling Framework

Open source software for building Earth Science applications based on components developed in different modeling centers

- NSF, NASA, DoD, NOAA with many other partners
- 37 different ESMF/NUOPC components listed (probably ~100 not declared)
- ESMF "Infrastructure" (e.g. calendar, parallelization) & "Superstructure" (component wrappers with standard interfaces for coupling)



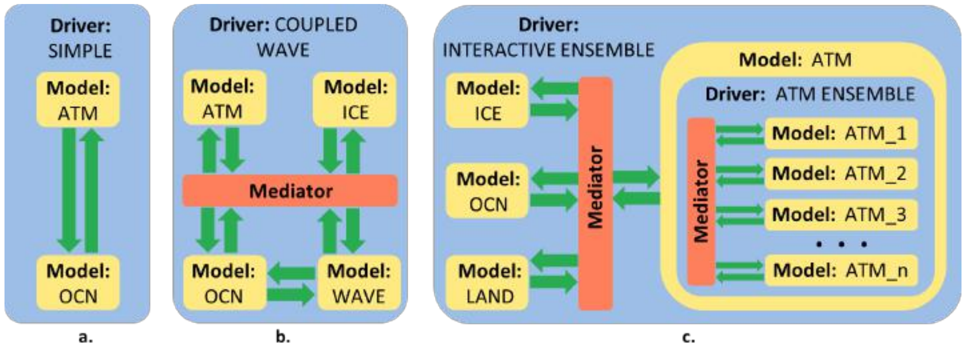
Goddard Space Flight Center GEOS-5 model

Component = well-defined function & calling interface

- Gridded Components: scientific code
- Coupler Components: data transformation/transfer
  - ➢ user builds a model as hierarchy of components
  - ➢ can be run sequentially, concurrently, in mixed mode
  - ➢ **integrated coupling framework** : single executable

NUOPC Interoperability layer:

- ➢ Conventions and templates for driver and components for better interoperability

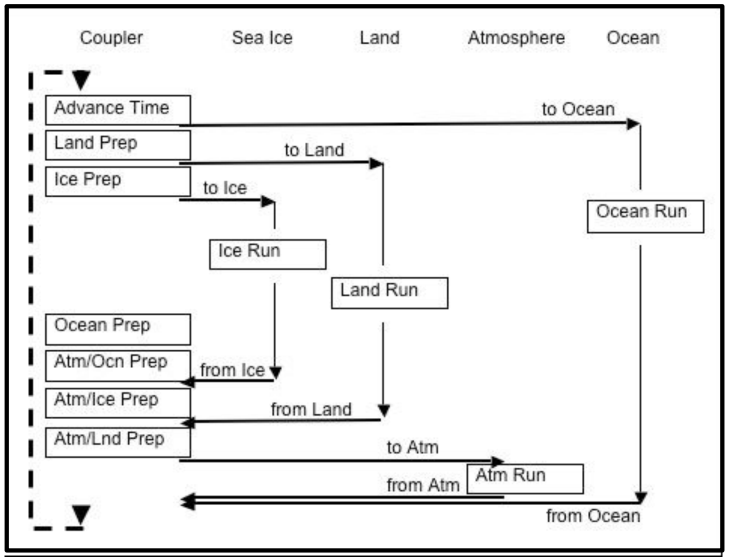


The NCAR coupling framework CPL7

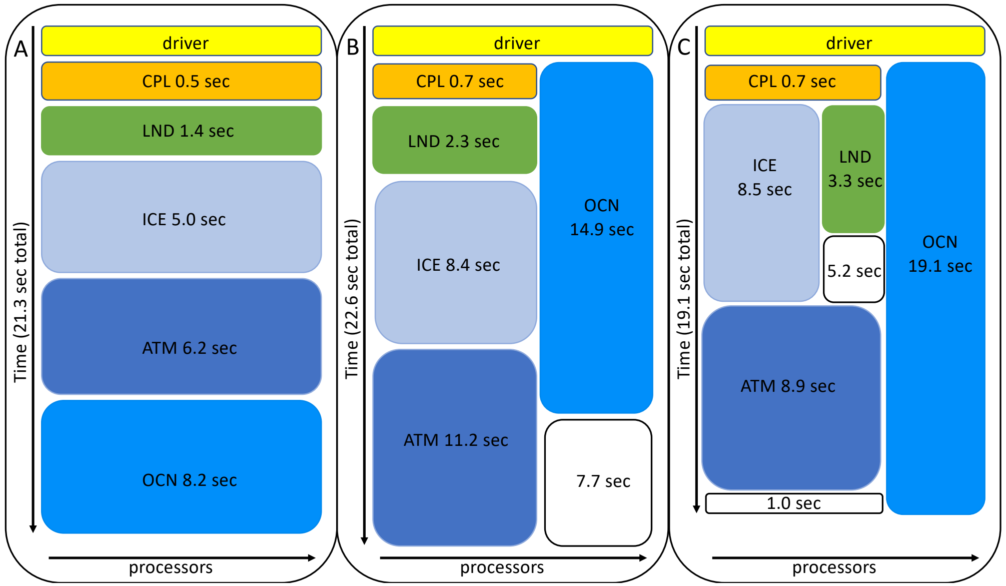
Software top-level layer (driver), that calls a coupler component and atmosphere, ocean, land and sea ice codes in sequence or in parallel

- Developed by NCAR Earth System Laboratory, used in CCSM4 and CESM1
- From coupler (cpl6) to **integrated coupling framework** (one executable)
- Use MCT internally with compatibility for ESMF-compliant components

Driver Loop Sequencing



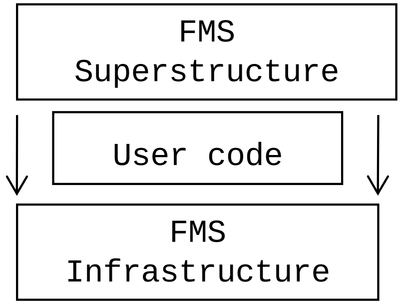
The driver can launch the different components following different layouts



The Flexible Modeling System (FMS)

Software to assemble a climate model with domain-specific "slots" for atmosphere, ocean, ocean surface including sea ice and land surface

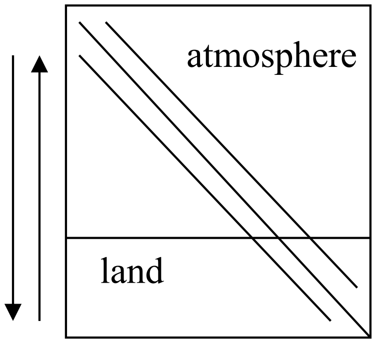
- Active for over a decade at GFDL; GFDL-CM4 and GFDL-ESM4 for CMIP6
- FMS shown to be scalable with up to O(10000) pes
- FMS "Infrastructure" (e.g. I/O, parallelization) & "Superstructure", i.e. standard interfaces to build **single-executable coupled model**



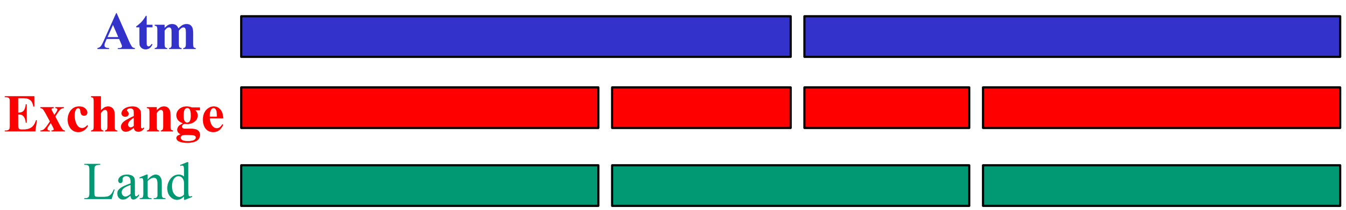
$$\partial T / \partial t = K \, \partial^2 T / \partial z^2$$

$$\frac{T_k^{n+1} - T_k^{n}}{\Delta t} = K \frac{T_{k+1}^{n+1} + T_{k-1}^{n+1} + 2T_k^{n+1}}{\Delta z^2}$$

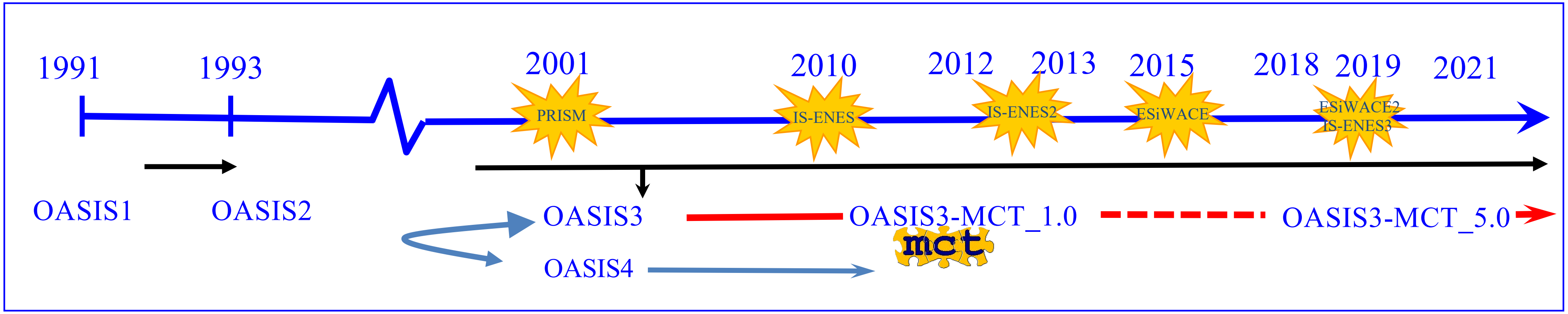
$$AT^{n+1} = T^n$$



- Implicit calculation of vertical diffusive fluxes over the whole column
- Up-down sweep for tridiagonal matrix resolution through the **exchange grid**

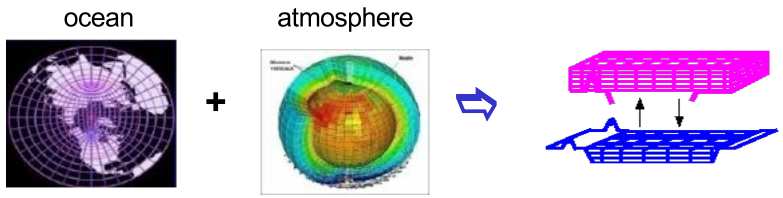


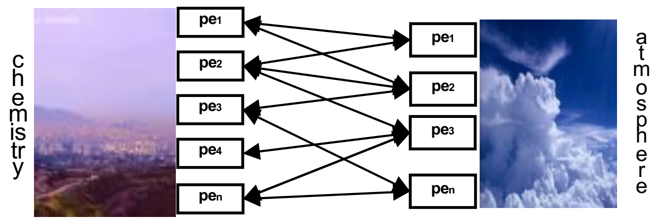
OASIS3-MCT



- OASIS1 -> OASIS2 -> OASIS3:
  2D ocean-atmosphere coupling
  low frequency, low resolution :
  → Flexibility, 2D interpolations

- OASIS4 / OASIS3-MCT:
  2D/3D coupling of high-resolution parallel components
  →Parallelism, performance





OASIS3-MCT community

OASIS3-MCT current users
2019 survey

67 climate modelling groups around the world use OASIS3-MCT …

…. to assemble more than 80 coupled applications !!

OASIS3-MCT is used in 5 of the 7 European ESMs in CMIP6

OASIS3-MCT: some generalities

- All sources are written in F90 and C
- Uses the Model Coupling Toolkit (MCT) from Argonne National Lab
- Open source product distributed under a LGPL license
- All external libraries used are public domain (MPI, NetCDF) or open source (LANL SCRIP, MCT)
- Current developers are:
  - 1 permanent FTE (CERFACS, CNRS)
  - 2 consultants : Anthony Craig (also CPL7 and ESMF), Andrea Piacentini

ESiWACE H2020 EU Centre of Excellence

- ESiWACE1 (2015-2019): 18 pm
- ESiWACE2 (2019-2022): 16 pms

IS-ENES EU FP7 project

- IS-ENES2 (2014-2017): 27 pm
- IS-ENES3 (2019-2022): 35 pms

IS-ENES3 and ESiWACE2 have received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 824084 & No 823988

OASIS3-MCT code interfacing

- Initialization: `call oasis_init_comp(...)`
- Local partition definition: `call oasis_def_partition (...)`
- Grid definition: `call oasis_write_grid (...)`
- Coupling field declaration: `call oasis_def_var (...)`
- End of definition phase: `call oasis_enddef (…)`
- Coupling field exchange:
  - in model time stepping loop

```
call oasis_put (…, date, var_array. …)
call oasis_get (…, date, var_array, …)
```

  - user defines externally the source or target
  - sending or receiving at appropriate time only
  - automatic averaging/accumulation if requested
  - automatic writing of coupling restart file at end of run
- Termination: `call oasis_terminate (…)`

OASIS3-MCT: interpolations & transformations

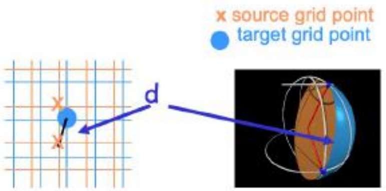
- on 2D or 3D scalar fields , bundles supported
- on different types of grids: lat-lon, rotated (logically rectangular), gaussian reduced, unstructured

❖ Transformations: statistics, addition/multiplication by scalar, global conservation

❖ Interpolations/regridding

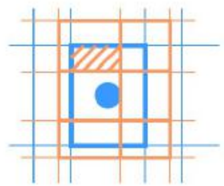
- offline with SCRIP, ESMF or XIOS using the unified regrid environment
- online with SCRIP (Jones, 1999)

new in OASIS3-MCT_5.0



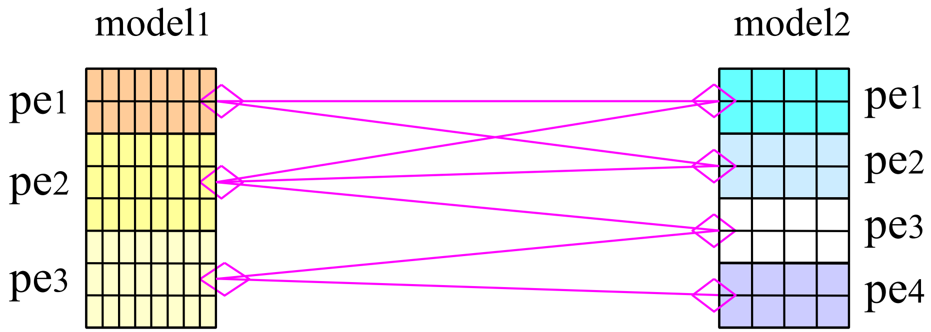
- Nearest-neigbour (SCRIP, ESMF):
  - closest point(s) on the source grid
- Bilinear (SCRIP, ESMF):
  - 4 enclosing neighbours on the source grid

- Higher-order non-conservative : bicubic (SCRIP) or patch (ESMF)
  - bicubic : as bilinear + gradients and cross-gradient at 4 enclosing neighbours
  - patch: average of multiple higher-order polynomial patches
- 1st order conservative (SCRIP, ESMF, XIOS)
  - use weighted sum of source cell values, the weight being proportional to the fraction of the target cell intersected by the source cell
- 2nd order conservative (SCRIP, ESMF, XIOS)
  - As 1st order + source field gradients in longitudinal and latitudinal directions



OASIS3-MCT parallel communication

- Fully parallel communication between parallel models based on Message Passing Interface (MPI)



Configuration of each coupling exchange in a **text** file *namcouple*

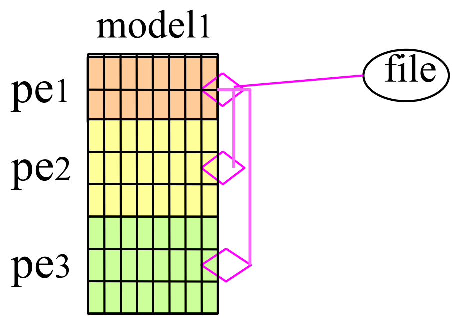
- source and target symbolic name (end-point communication)
- exchange period
- transformations/interpolations

Interpolation/regriddding weights and addresses can be calculated

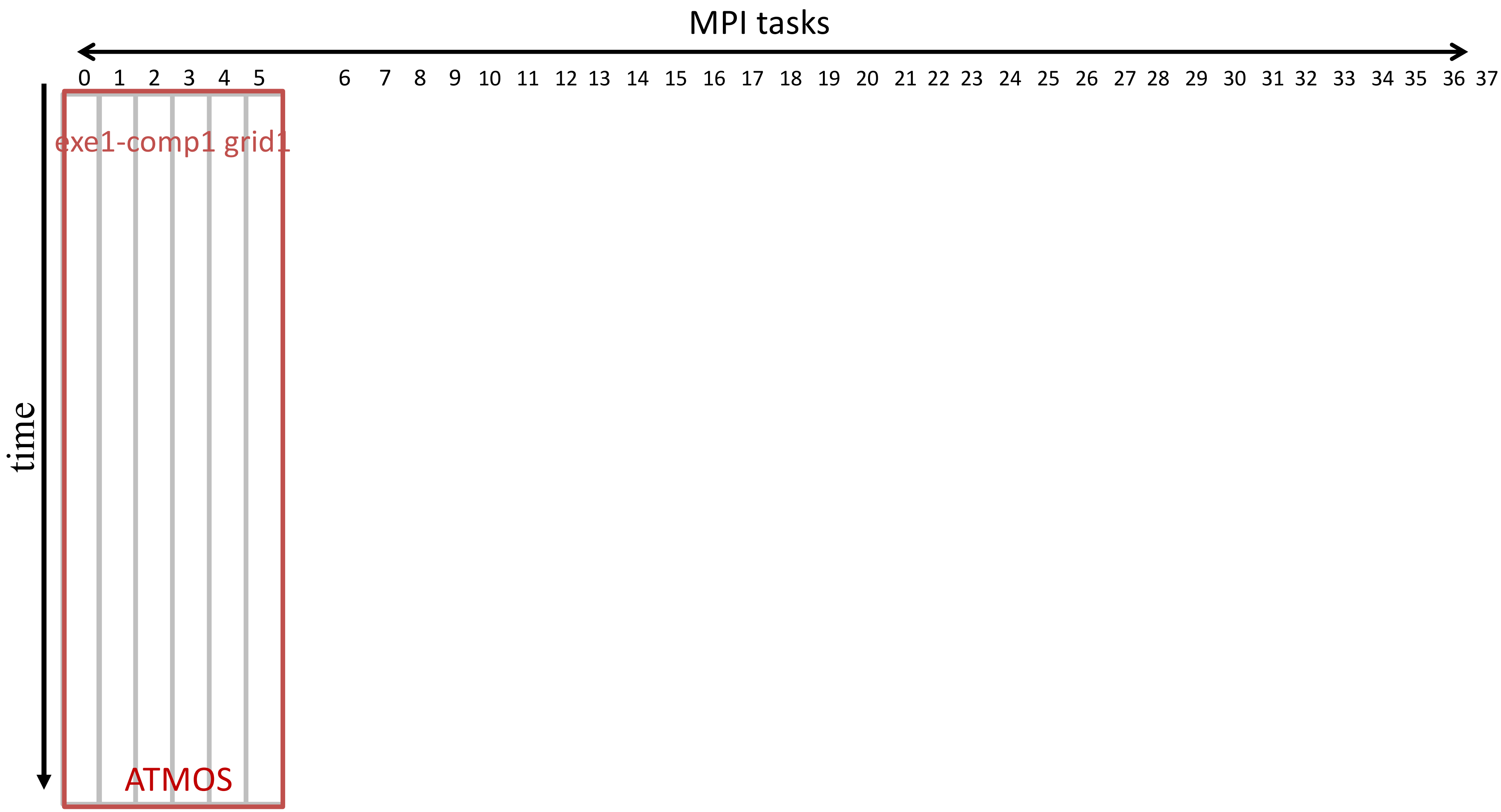
- offline with SCRIP, ESMF or XIOS in the unified environment
- online with SCRIP

new in OASIS3-MCT_5.0

- I/O functionality (switch between coupled and forced mode):

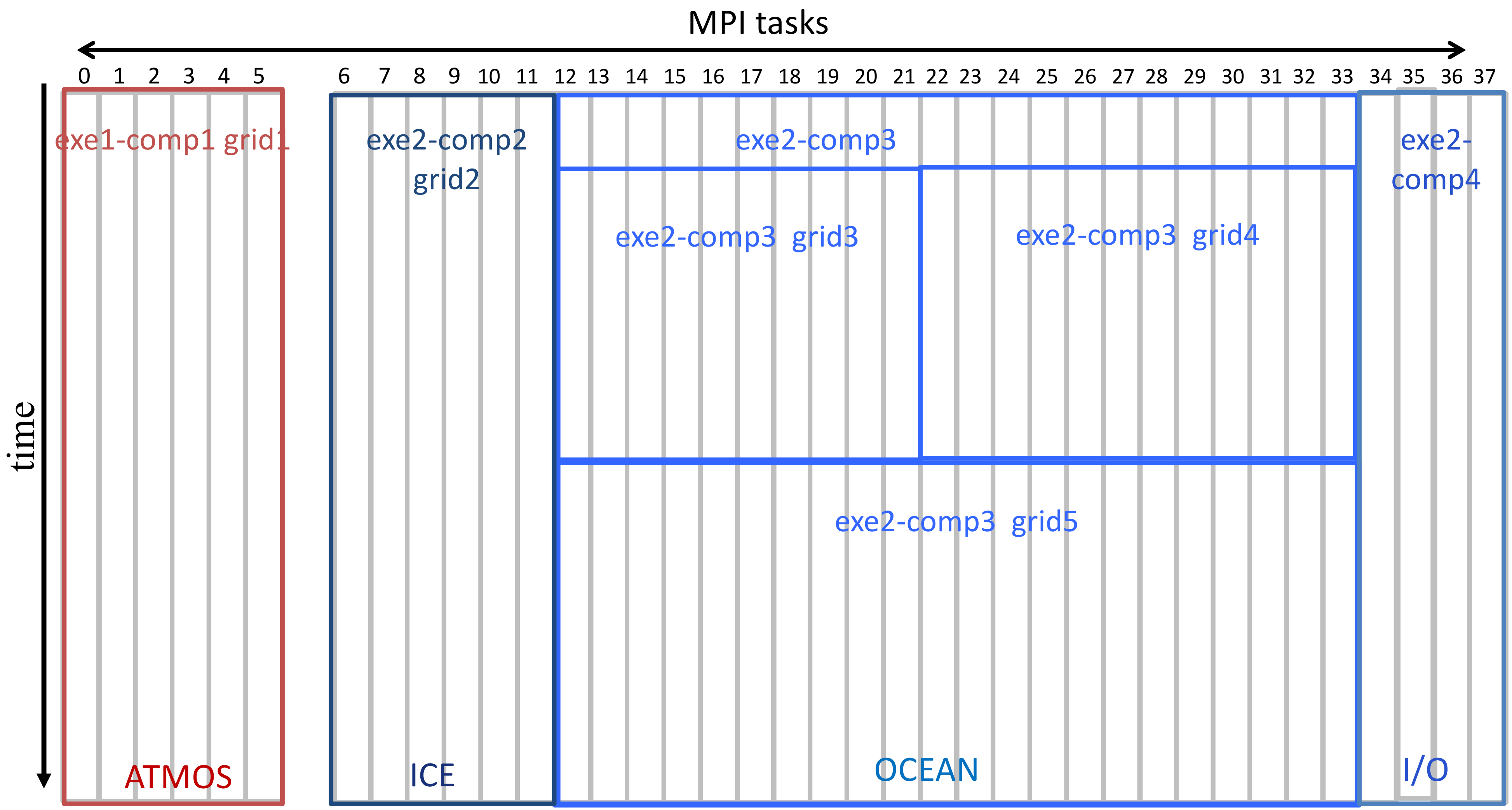


OASIS3-MCT parallel communication possible topologies of coupling exchanges



Executable 1 has 1 component comp1 that defines grid1

OASIS3-MCT parallel communication possible topologies of coupling exchanges

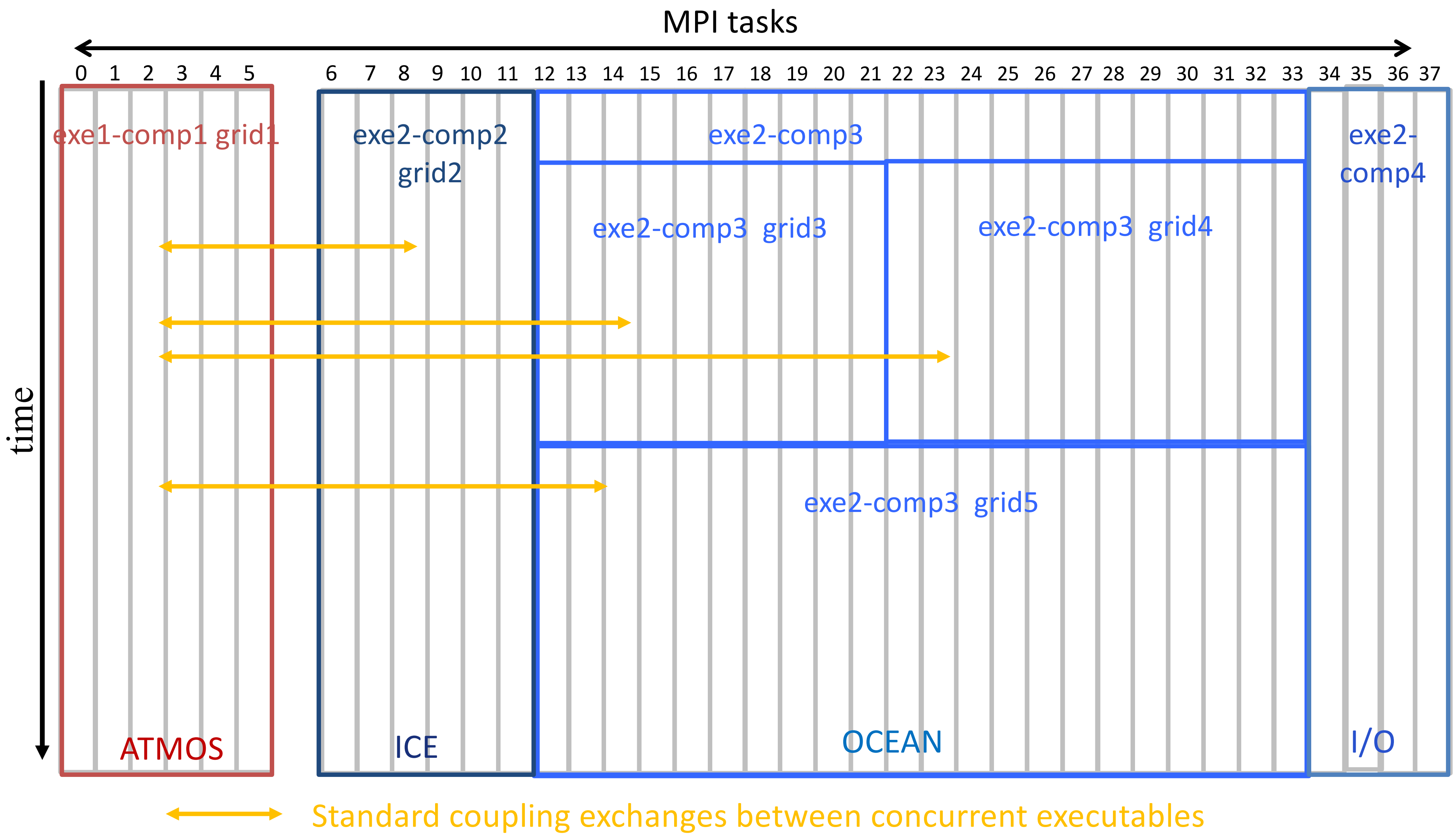


Executable 1 has 1 component comp1 that defines grid1

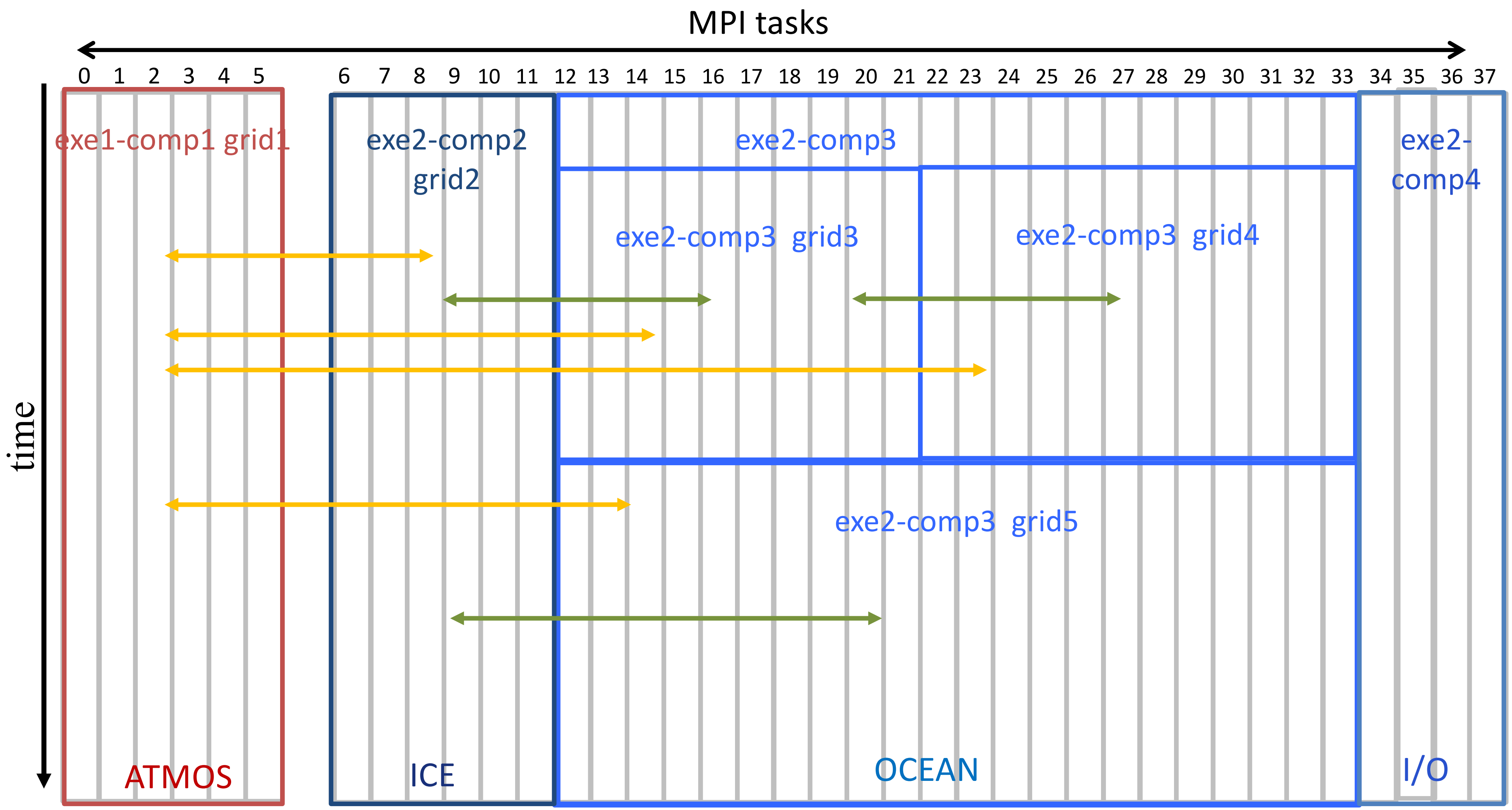
Executable 2 has 3 components;

- comp2 that defines grid2
- comp3 that 3 grids (grid3, grid4, grid5) on subset of processes
- comp4 that is not involved in the coupling

OASIS3-MCT parallel communication possible topologies of coupling exchanges



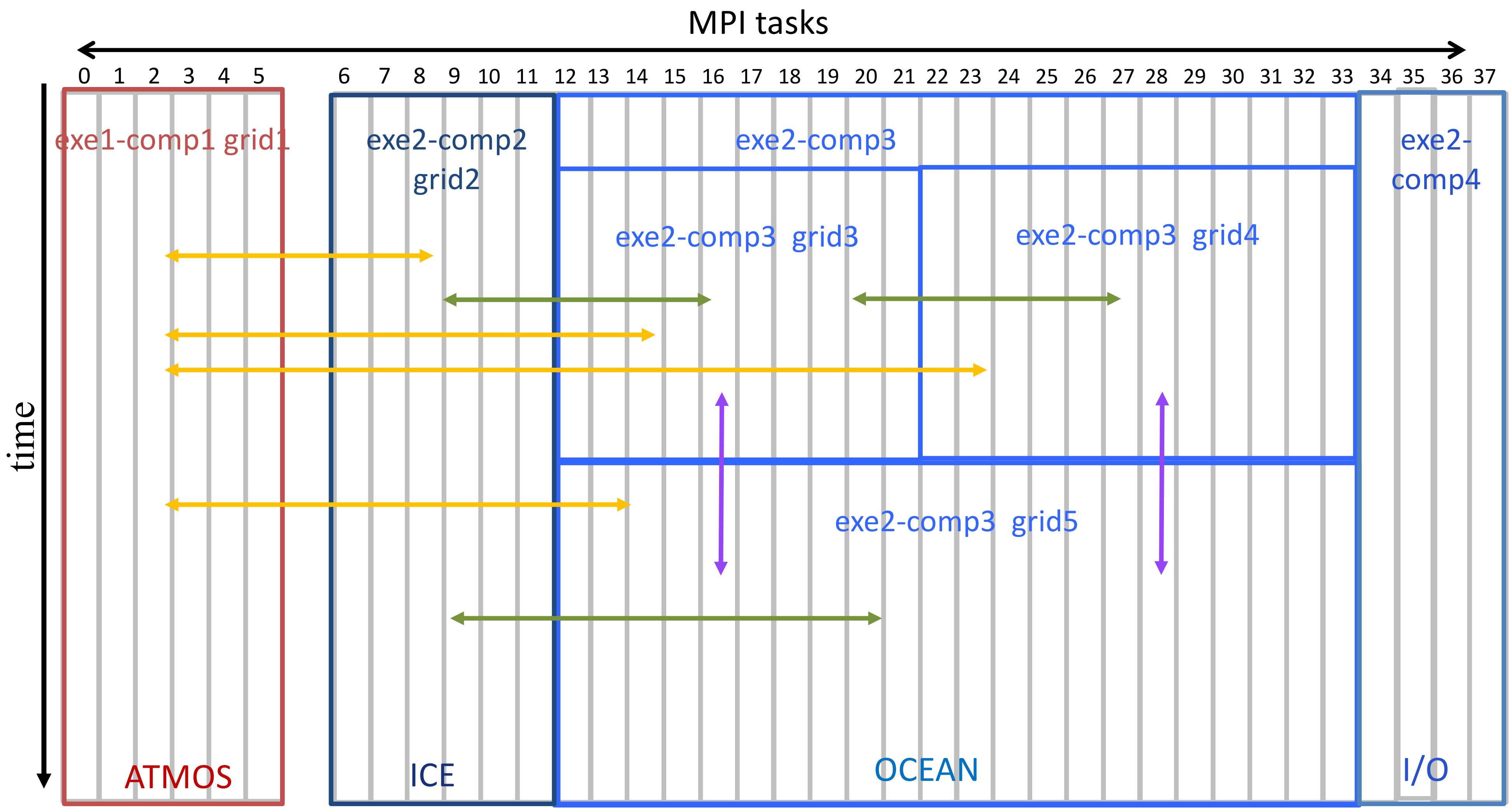
OASIS3-MCT parallel communication possible topologies of coupling exchanges



Standard coupling exchanges between concurrent executables

Coupling exchanges between concurrent components within one executable

OASIS3-MCT parallel communication possible topologies of coupling exchanges



Standard coupling exchanges between concurrent executables

Coupling exchanges between concurrent components within one executable

Coupling exchanges between sequential components within one executable

Extending the functionality, OASIS3-MCT "external coupling library" gets some characteristics of the "integrated coupling framework" approach

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3. New in OASIS3-MCT_5.0 (12/2021)

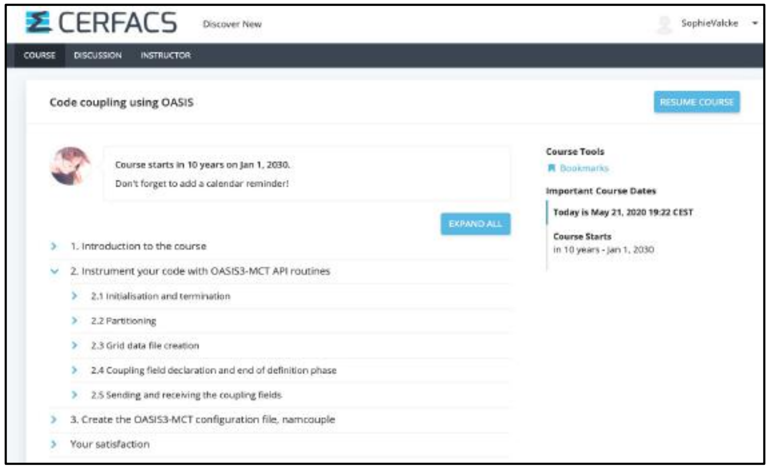
Conclusions and perspectives

New in OASIS3-MCT_5.0 (12/2021)

Source management and training

- Migration from SVN to GIT, full history
- New web site: https://oasis.cerfacs.fr/
- New Short Private Online Course (SPOC)
  - 20 hours on-line over 2 weeks: theory, videos, quizzes, hands-on with verification
  - instrument two toy models to set-up a coupled model exchanging one field in each direction
  - section on regridding/interpolation

✓ already 3 sessions, 22 participants, good overall feedback

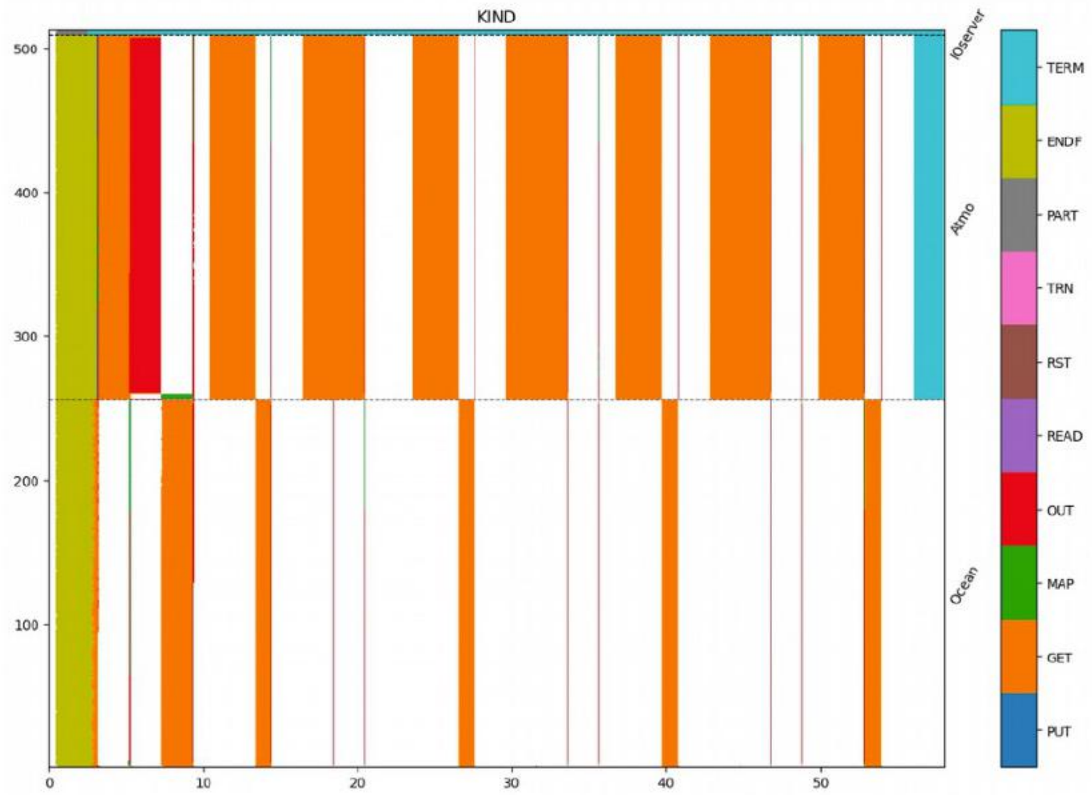


Tools / interface

- New Python, C & C++ bindings

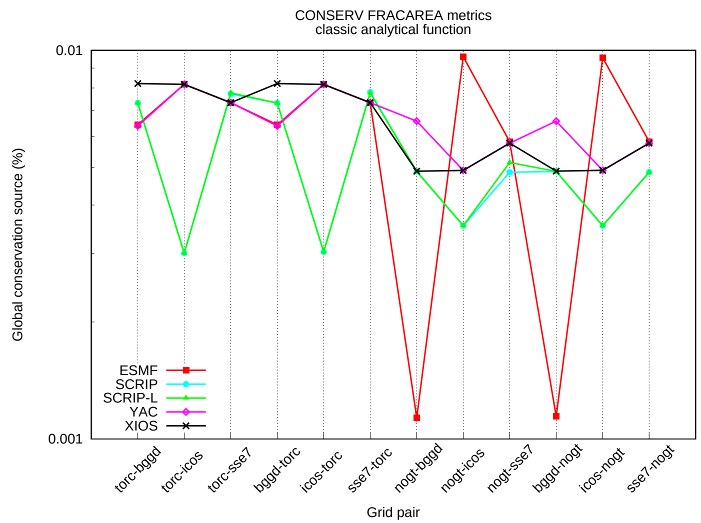
  in use at SMHI for standalone regridding weight computation tool

- New load balancing tool (ex lucia)



Regridding / interpolation / ensembles

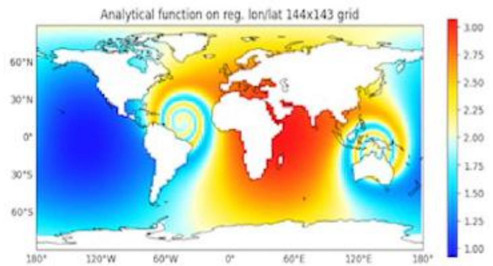
- Extension of oasis_get_intracomm for coupled models involving XIOS for ensemble simulations
- Locally-conservative runoff interpolation : no surface intersection, every source point needs a target neighbor (and not the opposite, as usual)
- Unified environment to use SCRIP, ESMF or XIOS offline to pre-calculate regridding weights
- Extensive benchmark of the regridding for SCRIP, ESMF, XIOS & YAC:
  - 5 algorithms (1st and 2nd order, conservative, …)
  - 4 different analytical functions
  - 6 grids used in real ocean or atmosphere models
  - metrics by the CANGA project



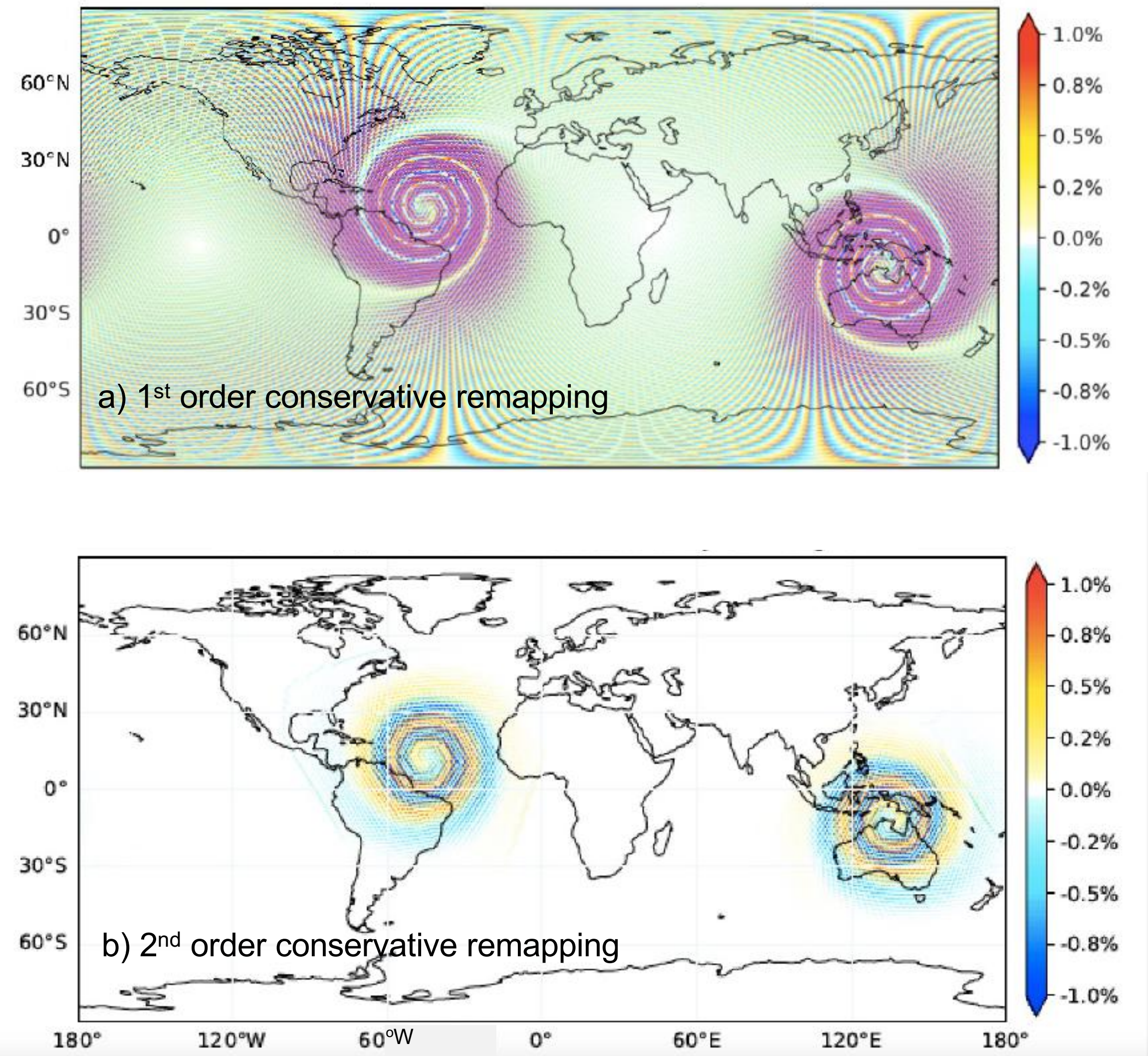
Valcke et al 2022, https://doi.org/ 10.3390/mca27020031
Valcke et al 2021, Cerfacs Tech Report, TR-CMGC-21-145

SCRIP, ESMF, XIOS, YAC regridding benchmark

Comparison between 1st and 2nd O conservative remapping error

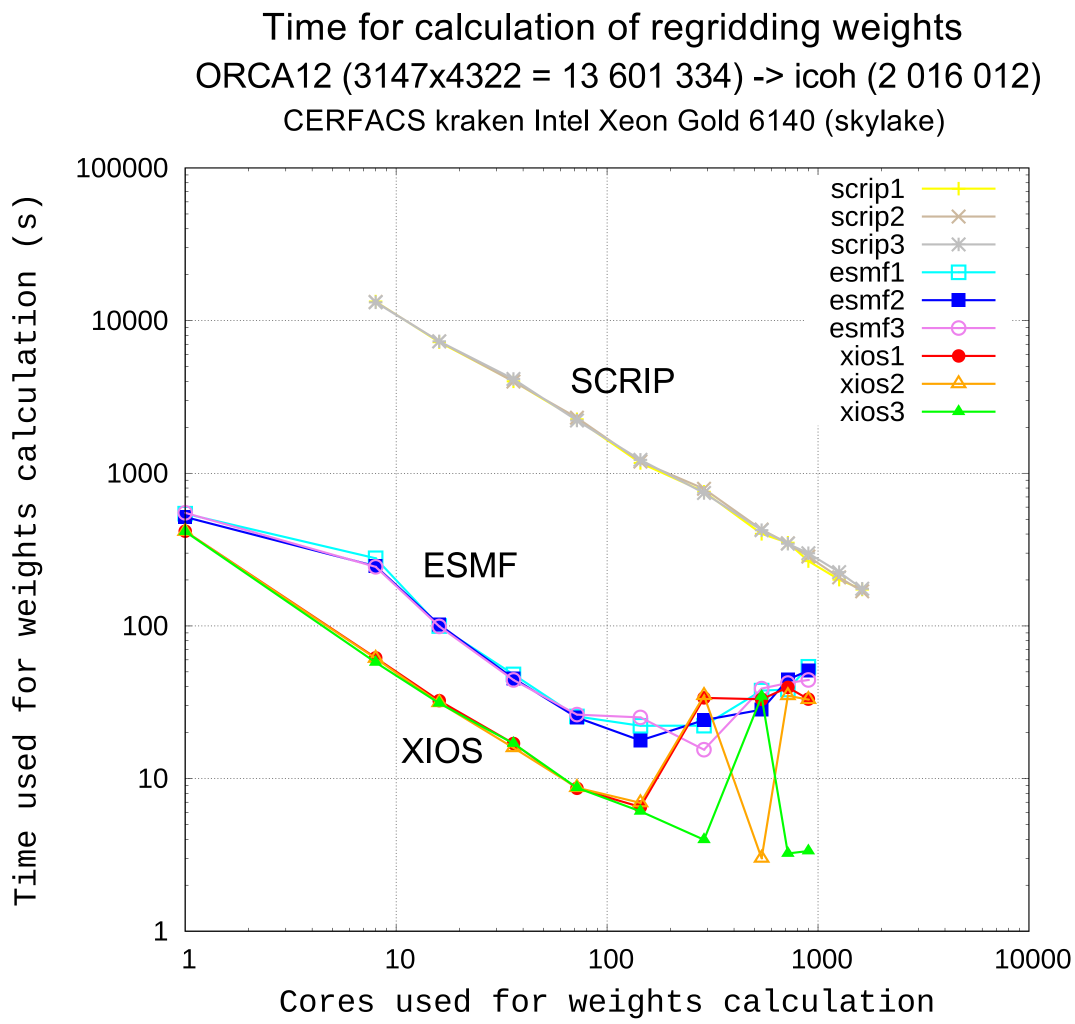


vortex function



Error (%) for FRACAREA a) 1st & b) 2nd order conservative remapping with YAC for the vortex function from low- to high-resolution icosahedral grid

SCRIP, ESMF & XIOS performance



- ESMF and XIOS show good performances (much more than the SCRIP)
- XIOS is more performant than ESMF but shows unstable behaviour for more than ~200 cores (to be investigated)
- On-line regridding for dynamic grids is becoming an option even for high-resolution coupled models

Conclusions and perspectives

1. Global performance and technical solutions

Importance of the layout of the coupled components on computing resources:

- Sequential or concurrent coupling or mix of both?
- Optimise the throughput (Simulated Years Per Day)?
- Optimise the use of resources (SYPC)?

Categorization of the different coupling software into two families: **"integrated coupling framework"** & **"external coupler or coupling library"**

2. Few coupling software

- integrated coupling framework : ESMF, cpl7, FMS
- coupler approach: OASIS3-MCT

➢ Extending the functionality of OASIS3-MCT to allow coupling between sequential components within a single executable, the OASIS3-MCT coupler gets some characteristics of the integrated coupling framework approach

3. New in OASIS3-MCT_5.0 :

- New Python, C & C++ bindings
- Short Private Online Course (SPOC)
- New load balancing tool
- Unified environment to pre-calculate regrid weights with SCRIP, ESMF or XIOS
- Regridding benchmark on SCRIP, ESMF, XIOS and YAC

Conclusions and perspectives

- OASIS3-MCT most likely provides a satisfactory solution for fully parallel coupling in our climate models at the resolutions targeted operationally for the next ~5 years.
- Support of grids with evolving masks under consideration, a first step toward dynamic coupling, i.e. grids evolving in time !!??
- Merging with the XIOS server developed at IPSL?

The end