

Dr2xml session

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and the XIOS Team!

Outline

1. Introduction

- Dr2xml, what's this?
- Brief history
- The CMIP6 Data Request

2. General features

- Utility
- Cautions
- Simple functional scheme
- The ping file

3. Usage

- Installation
- Configuration
- Execution
- Verification

4. Functionalities

- Basic functions
- Customisation
- Extended usage

1. Introduction

a) dr2xml, what's this?

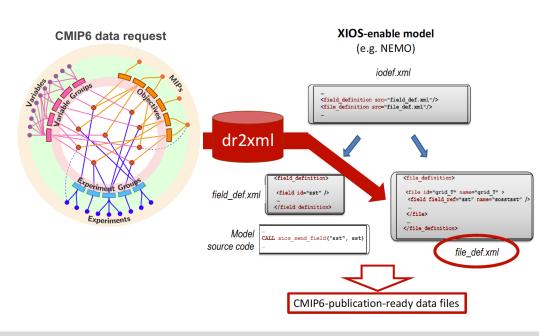
- Python tool
- XIOS file-def XML writer
 - o fields and attributes (« variable » in XIOS vocab) in file
 - Automatic implementation of XIOS spatial & temporal filters
 - Automatic NetCDF file handling (naming, time-splitting, metadata, append write...)

Useful for :

- XIOS-enabled models (output management)
- large number of fields to output
- standard data (format and content)
- adding a lot of mandatory attributes in the netCDF output files

CMIP6 production

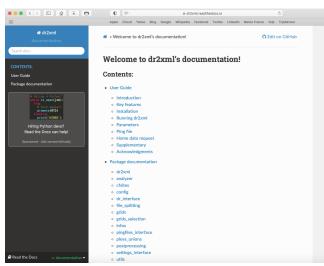
- Systematic production of CMIP6 compliant CF-netCDF files
- Satisfying the CMIP6 Data Request



1. Introduction

b) brief history

- Born with CMIP6 (Data Request)
- Development started in sept. 2016 (S. Sénési, CNRM + M.P Moine, Cerfacs)
- Now developed & maintained by G. Rigoudy, CNRM
- Developed in close collaboration with the XIOS-dev Team (a lot of functionalities introduced in XIOS for CMIP6/dr2xml needs)
- Used at IPSL and CNRM-CERFACS in climate models doing CMIP6
 - At CNRM-CERFACS: embedded in the modelling workflow (ECLIS)
 - At IPSL: used upstream of the modelling workflow (LibIGCM)
- All along the dev period, phasing with:
 - The CMIP6 Data Request versions
 - The CMIP6 Controlled vocabulary
- Stabilized version in July 2018 for CMIP6 (v1.13)
- Last evolutions:
 - Code modularization
 - New functionalities
 - Python 3 PEP8
- Sources on Github: https://github.com/rigoudyg/dr2xml
- ReadtheDocs documentation: https://dr2xml.readthedocs.io/en/documentation/ (not yet finalized)



1. Introduction

c) the CMIP6 Data Request

Big picture:

- Developed for CMIP6 by Martin Juckes since 2016 to...
- Meet the challenge of model/MIP objectives/experiment design complexity and exposing number/diversity of diagnosis requested by each MIP
- Fully enable the intercomparison:

« The thousands of diagnostics generated at each centre from hundreds of simulations should be produced and documented in a consistent manner to facilitate meaningful comparisons across models. Hence, for each experiment the MIPs have requested specific output to be archived and shared via the Earth System Grid Federation (ESGF), and the CMIP6 organisers have imposed requirements on file format and metadata »

Concretely:

- Is a data base with:
 - a python API (facilitates automated interrogation of the data base)
 - a browsable html interface
- That gives, for each CMIP6 simulation:
 - the variables that should be output (according to the selected priority)
 - on which grid/domain/levels
 - over which time period
 - at which frequency
 - with which netCDF attributes...
- CMIP6 DR python API is used by dr2xml

The CMIP6 Data Request (version 01.00.31)

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Abstract. The data request of the Coupled Model Intercomparison Project Phase 6 (CMIP6) defines all the quantities from CMIP6 simulations that should be archived. This includes both quantities of general interest needed from most of the CMIP6endorsed Model Intercomparison Projects (MIPs) and quantities that are more specialised and only of interest to a single endorsed MIP. The complexity of the data request has increased from the early days of model intercomparisons, as has the

CMIP6 Data Request http://clipc-services.ceda.ac.uk/dreg/index.html

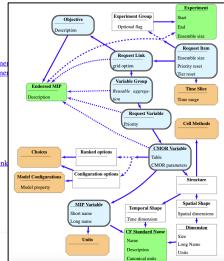
Data Request [01.00.31]

Overview tables and search

- · Overview: all variables and experiments
- · Overview: priority 1 variables, tier 1 experime
- · Overview: priority 1 variables, tier 1 experime
- · Search for variables
- · Search for experiments

Sections of the data request

- 1.1 Model Intercomparison Project [mip]
- 1.2 MIP Variable [var]
- 1.3 CMOR Variable [CMORvar]
- · 1.4 Request variable (carrying priority and lin
- 1.5 Experiments [experiment]
- 1.6 Scientific objectives [objective]
- 1.7 Specification of dimensions [grids]
- 1.8 CF Standard Names [standardname]
- 1.9 Experiment Group [exptgroup]
- 2.1 Spatial dimensions [spatialShape]
- · 2.2 Temporal dimension [temporalShape]



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World Meteorological Organization, Geneva, Switzerland

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a) dr2xml utility

Management of complex and various outputs, supporting:

- o all physical field shapes (1D, 2D, 3D, 4D, time-varying or constant)
- o all output frequencies (yearly, monthly, daily, 6-hourly, 3-hourly, 1-hourly, sub-hour)
- choice of sampling period
- on the fly diagnostic computation (ex. zonal means, interpolation on pressure levels, on observation sites...)
- allows multivariate diagnostics (computing a diagnostics depending on 2 or more model native variables)

Avoids time-consuming post-processing steps:

- no need to use CMOR
- o nor any other offline post-processing steps (even for diagnostic computation)
- o formatting/standardisation directly ensured (file names, global and local attributes, temporal axis)

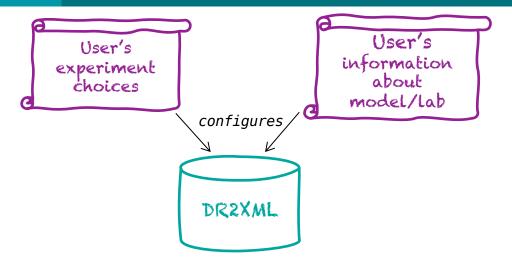
Reduced risk of errors

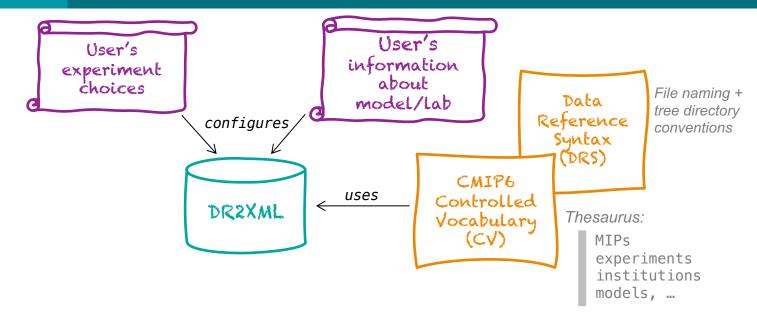
- "all included" and integrated post-processing
- one tool does all: XIOS!
- o homogeneity, coherence, reliability, robustness

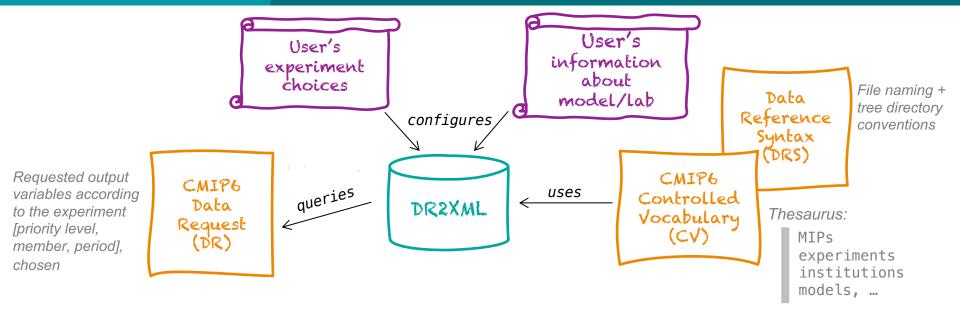
b) cautions

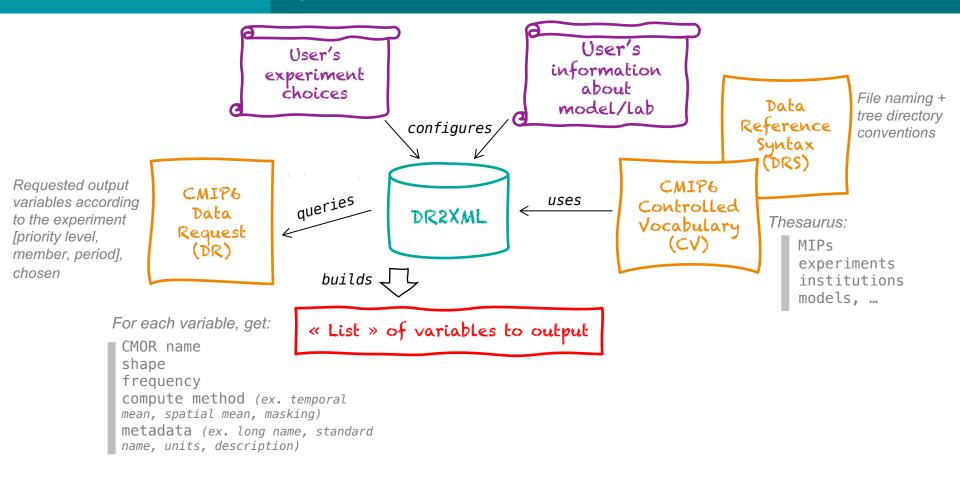
- One shot! which means...
 - no safety net once the production started
 - o all requested output and output you need must be there!
- Before running the whole simulation:
 - Dr2xml configuration must be carefully checked (a verbose log file enables to visualize the planned output variables)
 - It is highly recommended to perform a short test run and control/validate the output netCDF files, for e.g. with NCTIME and potentially PrePARE (if the simulation is a CMIP6 one)

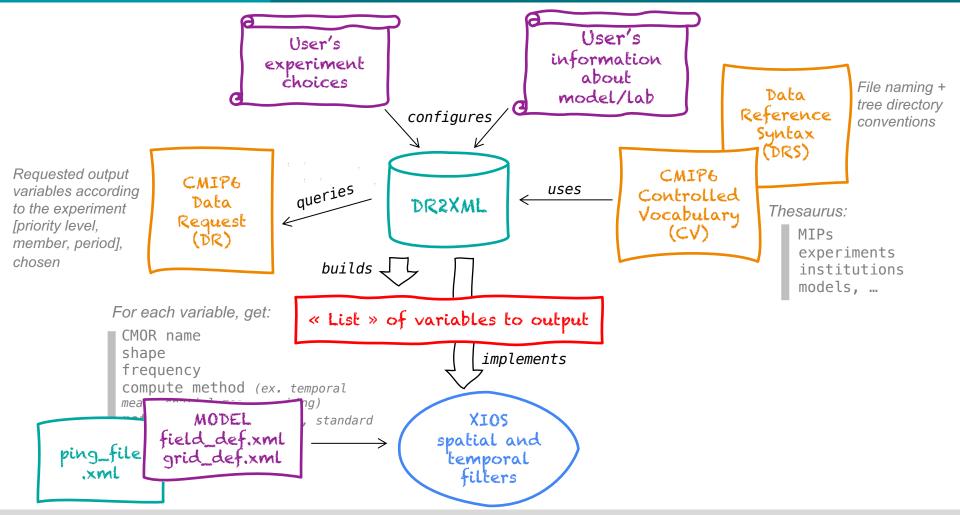


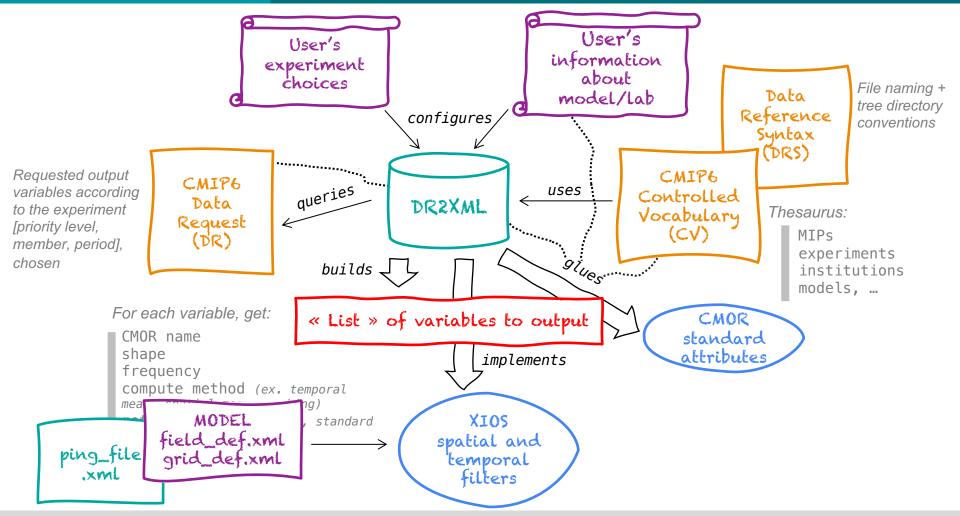


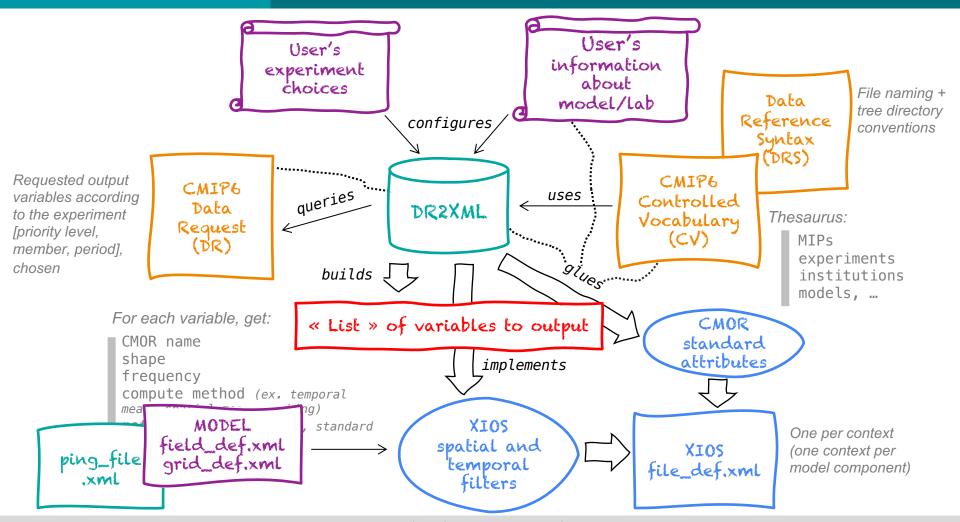








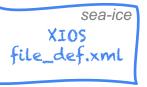


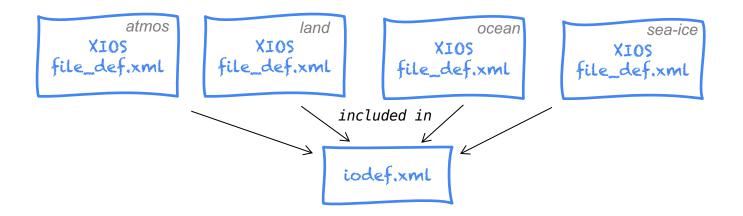


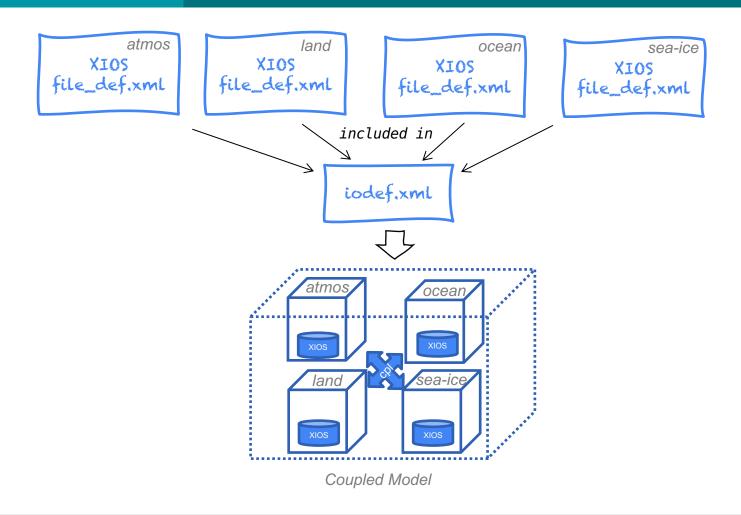


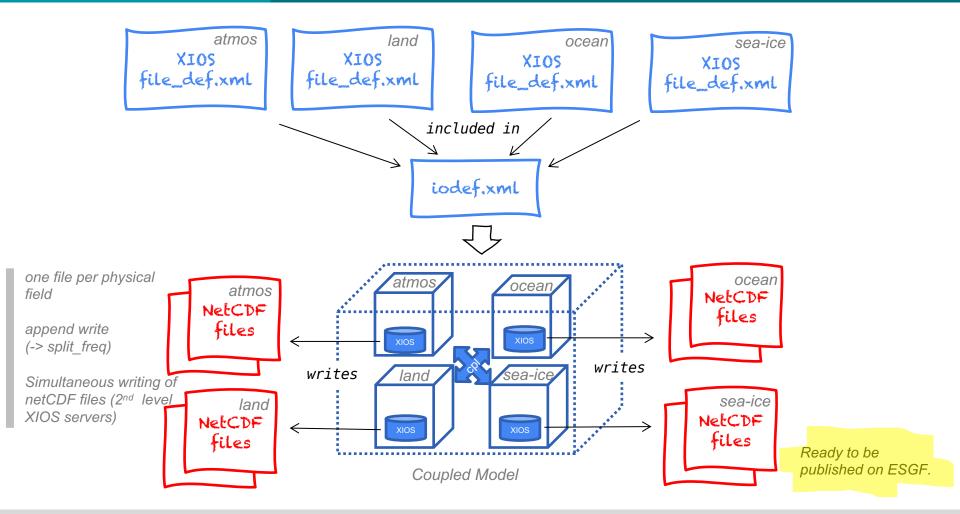








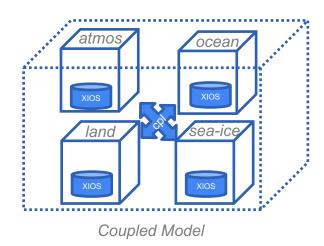




d) the ping files

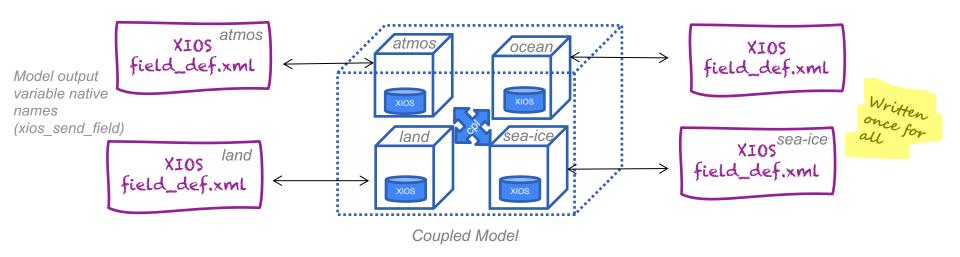


Standard variable names

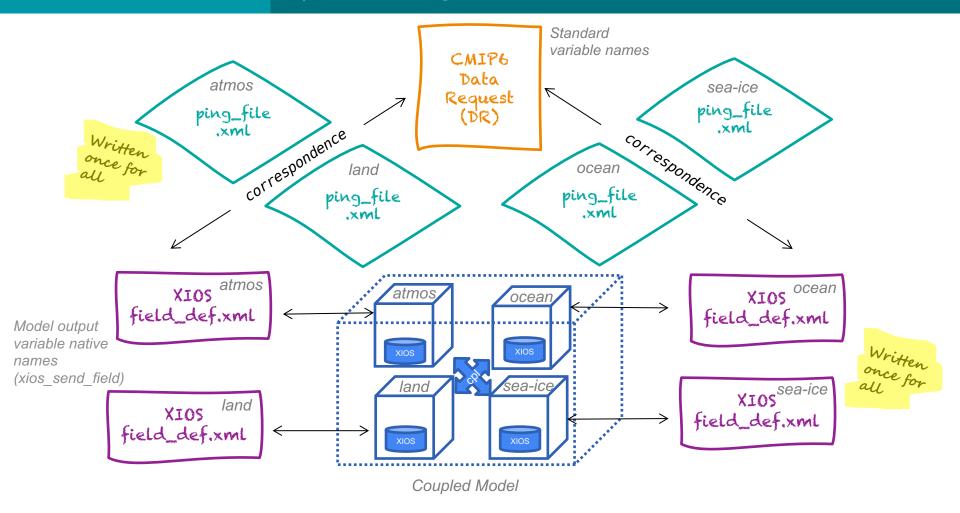


d) the ping files





d) the ping files



e) "sos_Omon" example (DR info.)

1.3 CMOR Variable: [sos] Sea Surface Salinity

•label : sos

•vid : [var] sos [74a9891bcab2667dbcb66574c6370c86]

title: Sea Surface Salinity

•defaultPriority: 1

modeling_realm : ocean

•type : real

•2.3 Dimensions and related information [stid]: <u>Temporal</u> mean, <u>Global field (single level) [XY-na] [amse-tmn] [str-a098]</u>

•processing: Report on native horizontal grid as well as on a spherical latitude/longitude grid.

frequency : monrowIndex : 22mipTable : Omon

•description: Sea water salinity is the salt content of sea water, often on the Practical Salinity Scale of 1978. However, the unqualified term 'salinity' is generic and does not necessarily imply any particular method of calculation. The units of salinity are dimensionless and the units attribute should normally be given as 1e-3 or 0.001 i.e. parts per thousand.

•[...]

1.2 MIP Variable: [sos] Sea Surface Salinity

•label : sos

•provmip : [mip] OMIP [OMIP]

prov : OMIP.dayunits : 0.001

•title : Sea Surface Salinity

•uid : 74a9891bcab2667dbcb66574c6370c86

•procnote : (",)
•procComment :

•1.8 CF Standard Names [sn]: <u>SeaSurfaceSalinity</u>

•description : [...]

1.8 CF Standard Names: [SeaSurfaceSalinity] Sea Surface Salinity

•units : 1e-3

•label : SeaSurfaceSalinity

•title : Sea Surface Salinity

ruid : <mark>sea_surface_salinity</mark>

•description :[...]

2.3 Dimensions and related information: [str-a098] Temporal mean, Global field (single level) [XY-na] [amse-tmn]

•label: str-a098

spid: [spatialShape] XY-na [a656047a-8883-11e5-b571-ac72891c3257]

•title: Temporal mean, Global field (single level) [XY-na] [amse-tmn]

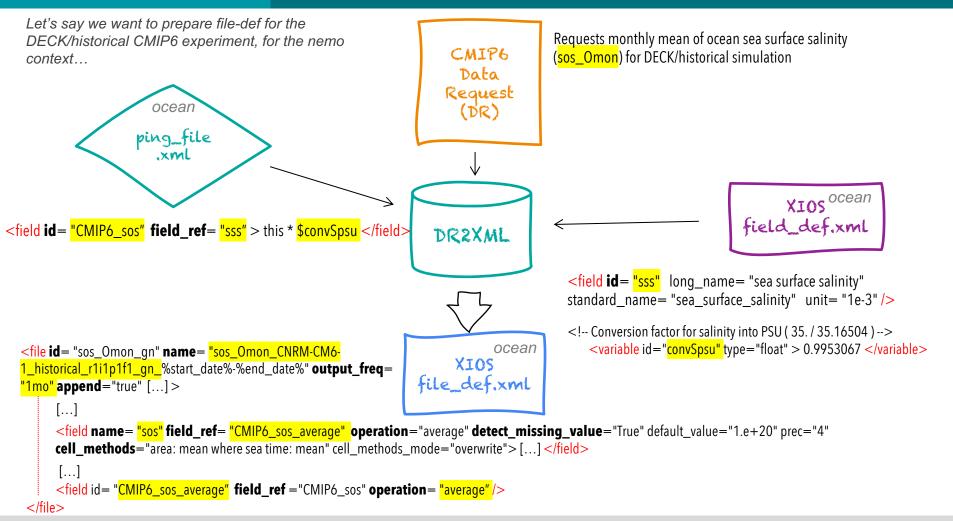
•cell_methods: area: mean where sea time: mean

•cell_measures : area: areacello

description: For time mean fields, it may be useful to add information about the sampling interval in the cell_methods string. The syntax is to append, in brackets, 'interval: *amount* *units*', for example 'area: time: mean (interval: 1 hr)'. The units must be valid UDUNITS, e.g. day or hr.

| ●[...]

e) "sos_Omon" example



ocean: Nemo 3.6 (eORCA1, tripolar primarily 1deg; 362 x 294 longitude/latitude; 75 levels; top grid cell 0-1 m)

e) "sos_Omon" example (cont.)

```
dr2xml_nemo.xml
       <file id="sos_0mon_gn" name="sos_0mon_CNRM-CM6-1_historical_r1i1p1f1_gn_%start_date%-%end_date%" output_freq="1mo" append="</pre>
                                                                                                                                                                                   ocean
       true" output_level="10" compression_level="4" split_freq="500y" split_freq_format="%y%mo" split_last_date="2014-- 00:00:00"
       time_units="days" time_counter_name="time" time_counter="exclusive" time_stamp_name="creation_date" time_stamp_format="
       %Y-%m-%dT%H:%M:%SZ" uuid_name="tracking_id" uuid_format="hdl:None/%uuid%" convention_str="CF-1.7 CMIP-6.2">
           <variable name="activity_id" type="string"> CMIP </variable>
           <variable name="data_specs_version" type="string"> 01.00.32 </variable>
           <variable name="dr2xml_version" type="string"> 2.2 </variable>
           <variable name="experiment_id" type="string"> historical </variable>
           <variable name="description" type="string"> CMIP6 historical </variable>
           <variable name="title" type="string"> CMIP6 historical </variable>
           <variable name="experiment" type="string"> all-forcing simulation of the recent past /variable>
                                                 <variable name="source_id" type="string"> CNRM-CM6-1 </variable>
           <variable name="external variables"</pre>
          <variable name="forcing_index" type</pre>
                                                 <variable name="source type" type="string"> AOGCM </variable>
           <variable name="frequency" type="st</pre>
                                                 <variable name="sub_experiment_id" type="string"> none </variable>
           <variable name="further_info_url" t</pre>
           CMIP6.CNRM-CERFACS.CNRM-CM6-1.histo
                                                 <variable name="sub_experiment" type="string"> none </variable>
           <variable name="grid" type="string"
<variable name="grid_label" type="s</pre>
                                                 <variable name="table_id" type="string"> Omon </variable>
                                                 <variable name="title" type="string"> CNRM-CM6-1 model output prepared for CMIP6 / CMIP historical </variable>
           <variable name="nominal_resolution"</pre>
           <variable name="history" type="stri</pre>
                                                 <variable name="variable_id" type="string"> sos </variable>
           <variable name="initialization inde</pre>
                                                 <variable name="variant_info" type="string"> none </variable>
           <variable name="institution_id" typ</pre>
           <variable name="institution" type="</pre>
                                                 <variable name="variant label" type="string"> r1i1p1f1 </variable>
           CERFACS (Centre Europeen de Recherc
                                                 <field name="sos" field ref="CMIP6 sos average" operation="average" detect missing value="True" default value="1.e+20"</pre>
           <variable name="license" type="stri</pre>
                                                 prec="4" cell_methods="area: mean where sea time: mean" cell_methods_mode="overwrite">
           Attribution-NonCommercial-ShareAlik
           https://pcmdi.llnl.gov/CMIP6/Terms0
                                                      <variable name="standard_name" type="string"> sea_surface_salinity </variable>
           proper acknowledgment. Further info
                                                      <variable name="description" type="string"> Sea water salinity is the salt content of sea water, often on the
           further_info_url (recorded as a glo
                                                      Practical Salinity Scale of 1978. However, the unqualified term 'salinity' is generic and does not necessarily imply
           warranty, either express or implied
           particular purpose. All liabilities
                                                      any particular method of calculation. The units of salinity are dimensionless and the units attribute should normally
           negligence) are excluded to the ful
                                                      be given as 1e-3 or 0.001 i.e. parts per thousand. </variable>
           <variable name="mip_era" type="stri</pre>
           <variable name="parent_experiment_i</pre>
                                                      <variable name="long name" type="string"> Sea Surface Salinity </variable>
           <variable name="parent_mip_era" typ</pre>
                                                      <variable name="history" type="string"> none </variable>
           <variable name="parent_activity_id"</pre>
          <variable name="parent_source_id" t</pre>
                                                      <variable name="units" type="string"> 0.001 </variable>
          <variable name="parent_time_units"</pre>
                                                      <variable name="cell methods" type="string"> area: mean where sea time: mean </variable>
           <variable name="parent_variant_labe</pre>
                                                      <variable name="cell measures" type="string"> area: areacello </variable>
           <variable name="branch_method" type</pre>
           <variable name="branch_time_in_chil</pre>
                                                      <variable name="interval_operation" type="string"> 1800 s </variable>
           <variable name="physics_index" type</pre>
           <variable name="product" type="stri</pre>
           <variable name="realization_index" </file>
           <variable name="realm" type="string"> ocean </variable>
           <variable name="source" type="string"> CNRM-CM6-1 (2017):
aerosol: prescribed monthly fields computed by TACTIC_v2 scheme
                                                                                                                                                 Arpege/Surfex: 28 758 lines!
atmos: Arpege 6.3 (T127; Gaussian Reduced with 24572 grid points in total distributed over 128 latitude circles (with 256 grid points
per latitude circle between 30degN and 30degS reducing to 20 grid points per latitude circle at 88.9degN and 88.9degS); 91 levels;
                                                                                                                           CNRM-CM6

→ Nemo/Gelato: 14 840 lines!

top level 78.4 km)
atmosChem: OZL_v2
                                                                                                                           coupled model
land: Surfex 8.0c
                                                                                                                                                 Trip: 383 lines
```

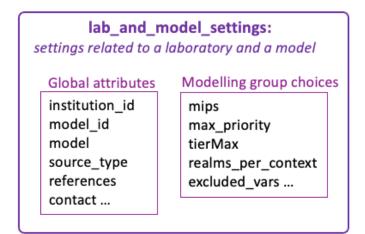
seaIce: Gelato 6.1 </variable>

a) installation

- Dr2xml (+ XIsXwritter, six)
 - \$ git clone https://github.com/rigoudyg/dr2xml.git
- dreqPy (the CMIP6 Data Request)
 - \$ pip install -upgrade [--user] dreqPy==01.00.32
 - \$ svn co http://proj.badc.rl.ac.uk/svn/exarch/CMIP6dreq/tags/01.00.32
- CMIP6_CVs
 - \$ git clone https://github.com/WCRP-CMIP/CMIP6_CVs

b) configuration

• 2 files of drzxml settings (python dictionaries)



```
simulation_settings:
settings related to an experiment
Global attributes & choices

experiment_id
activity
realization_index
initialization_index
physics_index
forcing_index
parent_experiment_id ...
```

- a set of model related XML files for XIOS: context, domains, field_defs
- additional XML files, the so-called "ping_files" (one per context)

c) execution

(file_def)

3. Usage

d) verification

```
Skipped variables (i.e. whose alias is not present in the pingfile):

>>> TABLE:

Ofx 03/09 ----> sftof(1) ugrid(1) volcello(1)

>>> TABLE:

SImon 01/20 ----> sirdgconc(1)

>>> TABLE:

Omon 03/37 ----> msftmz(1) msftmzmpa(1) vsf(1)
```

- 2 user-friendly views in dr2xml log file
- ...That does not exempt from looking carefully at the generated file-def!



a) basic functions

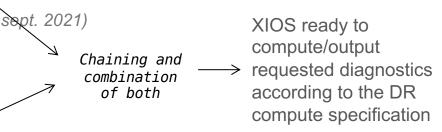
"basic functions": ordinated and optimised combination of XIOS filters automatically implemented according to the specifications of the data request.

Spatial:

- remapping on different grids
- regridding on pressure levels
- o regridding on height levels (in next version, sept. 2021)
- interpolation at observation sites
- meridional/zonal means

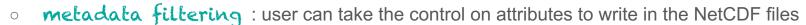
Temporal:

- sampling period
- time mean / time point
- diurnal cycle



b) customisation

- Filtering options:
 - curation: can filter out variables that are requested twice
 - selection:
 - filtering on experiment, on simulated year, or both
 - choosing the maximum priority level of variables to output
 - exclusion/inclusion: user can also provide lists of excluded/included...
 - variables (var)
 - tables (tbl)
 - pairs (var,tbl)
 - spatial shapes







b) customisation (cont.)

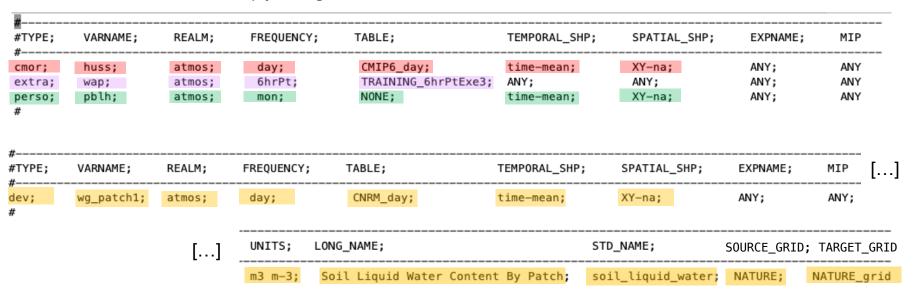
Add methods :

- o dr2xml allows to output additional variables = the so-called "home data request"
 - "cmor" variables: defined in the Data Request but not requested for this experiment
 - "extra" variables: defined through additional tables and which are not "cmor"
 - "perso" variables: to quicky output a model native variable, without caring about naming nor attributes (no need to be defined in the ping file)
 - "dev" variables: for development purpose: can be used to output variables with a minimal set of attributes (no need to be defined in the field_def xml)
- The "home data request" was used during CMIP6 production as a "safety net" to compensate DR potential lacks



b) "home data request"

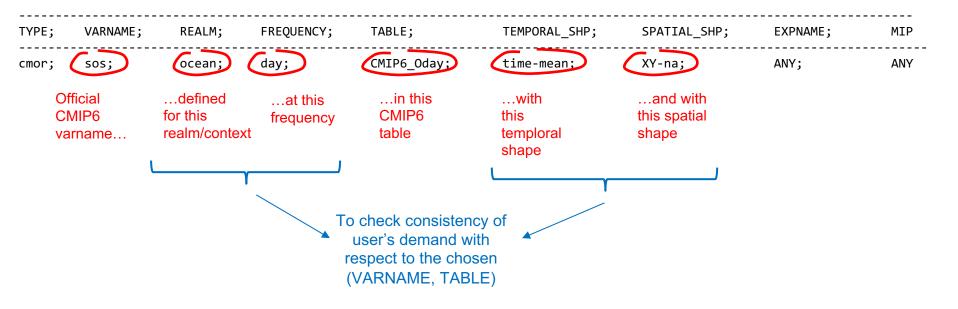
- The "home data request", brief user guide:
 - a simple text file
 - 3 header lines
 - one line per home variable
 - 8 [+5] columns, one per home variable parameter/attribute
 - parameter values are separated by ';'
 - no empty trailing lines



b) "home data request" (cont.)



Example 1 : adding a CMIP6 variable with all of its CMOR standard attributes



b) "home data request" (cont.)

```
Example 1 : addir
TYPE;
        VARNAME;
cmor;
```

Most of this information is mirrored in the CMIP6 Data Request

```
"Header": {
                                                      CMI6 Oday.json
    "data specs version": "01.00.30",
    "cmor_version": "3.4",
                                         a CMIP6/CMOR official table
    "table_id": "Table Oday",
    "realm": "ocnBgchem",
                                         (ison file) containing several
    "table date": "09 May 2019",
                                         variables.
    "missing value": "1e20",
    "int_missing_value": "-999",
    "product": "model-output",
    "approx interval": "1.00000",
    "generic_levels": "olevel",
    "mip era": "CMIP6",
    "Conventions": "CF-1.7 CMIP-6.2"
"variable entry": {
   "sos": {
        "frequency": "day",
        "modeling_realm": "ocean",
        "standard_name": "sea_surface_salinity",
        "units": "0.001".
        "cell_methods": "area: mean where sea time: mean",
        "cell measures": "area: areacello",
        "long_name": "Sea Surface Salinity",
        "comment": "Sea water salinity is the salt content of sea
         water, often on the Practical Salinity Scale of 1978 [...]",
        "dimensions": "longitude latitude time",
        "out name": "sos",
        "type": "real",
        "positive": ""
        "valid min": ""
        "valid max": ""
        "ok min mean abs":
        "ok max mean abs": ""
    },
```

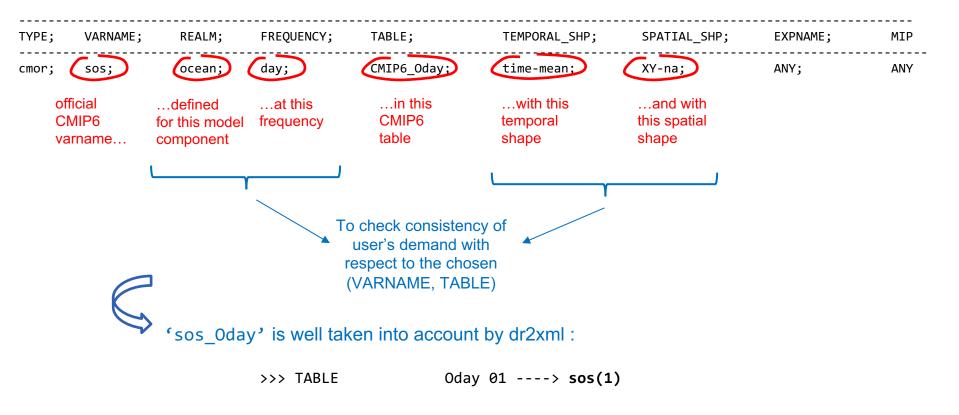
```
= CMOT
```

```
EXPNAME;
                 MIP
ANY;
                 ANY
```

b) "home data request" (cont.)



Example 1 : adding a CMIP6 variable with all of its CMOR standard attributes



b) "home data request" (cont.)

TYPE = extra

Example 2: adding all variables included in a user-defined external Table with CMOR-like attributes

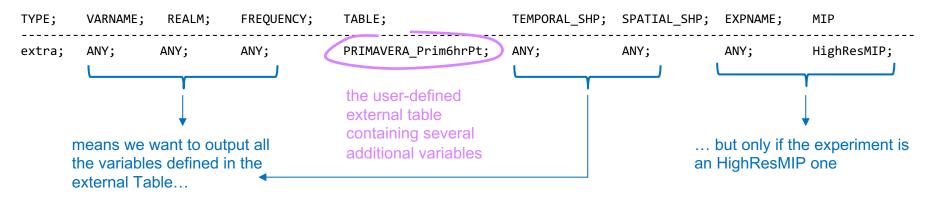
CMIP6 (CMOR) like attributes used by dr2xml to build XIOS instructions (output_freq, operation, ...) and to set XIOS variables (i.e. netCDF attributes)

```
"Header": {
                                           PRIMAVERA Prim6hrPt.json
        "data specs version": "01.00.13",
        "table id": "Table Prim6hrPt",
                                            a user-defined external table
        "realm": "land atmos ocean".
                                            (json file) containing several
        "cmor version": "3.2",
                                            additional variables.
        "table date": "12 July 2017",
        "missing value": "1e20",
        "product": "model-output",
        "approx interval": "0.250000",
        "generic levels": "",
        "mip era": "PRIMAVERA",
        "Conventions": "CF-1.7 CMIP-6.0"
    "variable entry": {
       "thetapv2": {
            "frequency": "6hr",
            "modeling_realm": "atmos",
            "standard_name": "theta_on_pv2_surface",
            "units": "K",
            "cell_methods": "time: point",
            "cell measures": "area: areacella".
            "long_name": "Theta on PV +/- 2 Surface",
            "comment": "",
            "dimensions": "longitude latitude time1",
            "out name": "thetapv2",
            "type": "real",
            "positive": "",
            "valid min": ""
            "valid max": "".
            "ok_min_mean_abs": "",
            "ok max mean abs": "",
            "primavera priority": "1"
```

b) "home data request" (cont.)



Example 2 : adding all variables included in a user-defined external Table with CMOR-like attributes

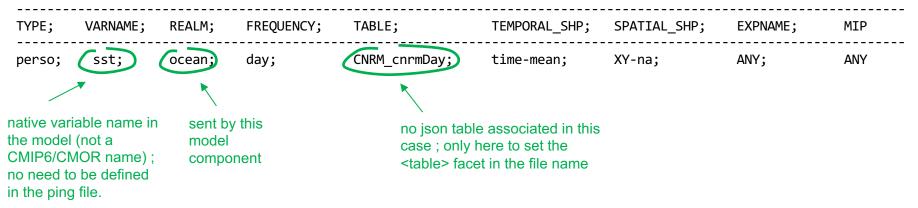




b) "home data request" (cont.)



<u>Example 3</u>: adding a non-CMIP6 (model native) variable without any specific attributes. The variable has not to be defined in field_def XML file but not in the ping file (keep the original name)





'sst' is well taken into account by dr2xml (without being defined in the ping file, only in the field def XML):

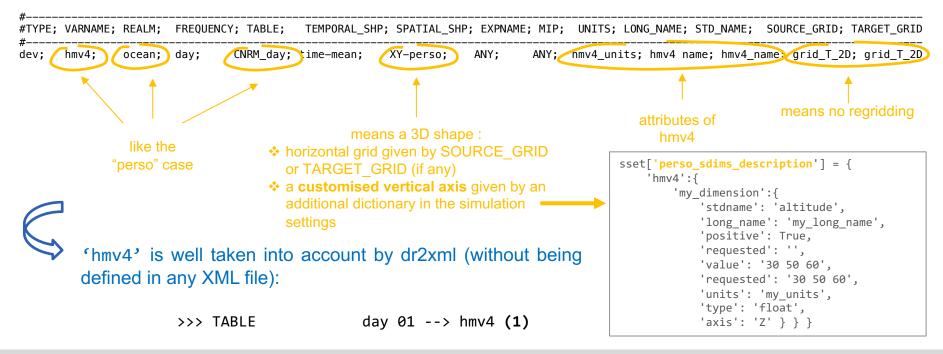
>>> TABLE

cnrmDay 01 --> sst(1)

b) "home data request" (cont.)



<u>Example 4</u>: adding a non-CMIP6 (model native) variable, defining "on the fly" the target grid and its attributes (units, standard name...). Avoid to have this variable defined in XIOS field_def XML file and/or to write an extra json table. Can be seen as an hybrid of the 'perso' and 'extra' type (for devel. purpose only)



c) extended usage

- Dr2xml for daily research production
 - discipline: Adopt the good practices using the CMOR/CMIP6 standards, even for non CMIP6 production
 - flexibility: The user can free somewhat or a great from the DR, choosing to:
 - make a new simulation with the same output variables as in a given CMIP6 experiment
 - ignore all of from the CMIP6 DR and only specify its own outputs via the "home data request"
- Adaptation to other projects like CORDEX
 - o new functionalities implemented (e.g. interpolation to altitude level)
 - o other needs to be instructed... (in IS-ENES3 framework)



summary

- DR-dr2xmL-XIOS pipeline is designed to facilitate the configuration of XIOS-enabled climate models contributing to CMIP exercises
- Is the best way to conform (as far as we can) to a data request as complex as the CMIP6 one
- Scraps the nightmare of a "by hand" model output configuration
- Dynamic analyse of the simulated period and adaptation of output configuration consequently
- Files written by XIOS configured by dr2xml are CMIP6-compliant
- Avoid the CMORisation step in the data production workflow
- Can be used as well for daily research simulations, benefitting (or not...) from the CMIP6 standards

Without CMIP6 and the Data Request dr2xml won't have existed, even less without XIOS, but now we've got it, sounds there is a life (for it) after CMIP6!

The End

Thanks to all for your participation!









Keep in touch!





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hands-on (notebooks)



- First, a quick demo notebook in plenary room, afterwards you will go in private rooms for the hands-on
- Before starting the hands-on, please update the dr2xml and dr2xml_training sources:

```
cd ~Dekstop/DR2XML/dr2xml ; git pull
cd ~Dekstop/DR2XML/dr2xml_training ; git pull
```

- Launch jupyter-notebook and start the exercises (1 to 4)
- There is nothing to seek by yourself, the solution is in, and the notebook cells are commented
- The objective is that you execute the cells step by step and understand what is done
- In order to have all onboard, the content of the two dr2xml setting files are imported in the notebooks and modified on the fly though notebook cells (python dictionary updating). You can have a look at these 2 files beforehand to get familiar with their content.

hands-on (notebooks)



Dr2xml_demo notebook

Purpose: Training notebook for a first contact with dr2xml: how to configure? how to run?

Exercice 1: Change the general configuration

Objective: Configure so as to run dr2xml for another:

- (a) context/realm
- (b) CMIP6 experiment
- (c) model version

Exercice 2: Customize the outputs (simple way)

Objective: Try various simple methods to customize the ouputs by using the **excluded/included** keys:

- (a) exclude one table
- (b) exclude pairs of variable/table
- (c) include only one variable from one table

Exercice 3: Customize the output (more flexible ways)

Objective: Try a more sophisticated method to customize the ouputs: the so-called "home_data_request"

- (a) requesting additional CMIP6 standard variables, already existing in a CMIP6 Table
- (b) requesting a CMIP6 standard variable but that do not exist in the predefined CMIP6 Table for the frequency we want
- (c) requesting a CMIP6 standard variable but that do not exist in the predefined CMIP6 Table for the shape we want
- (d) requesting a totally new variable, that is not defined in the CMIP6 standards (2 ways)
- (e)-(h) a flexible way to add variables for development purpose

Exercice 4: Run a non CMIP6 experiment

Objective: configure dr2xml for a non-cmip6 experiment