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Parallel Python Tools for Handling Big Climate Data

Sheri Mickelson

Kevin Paul

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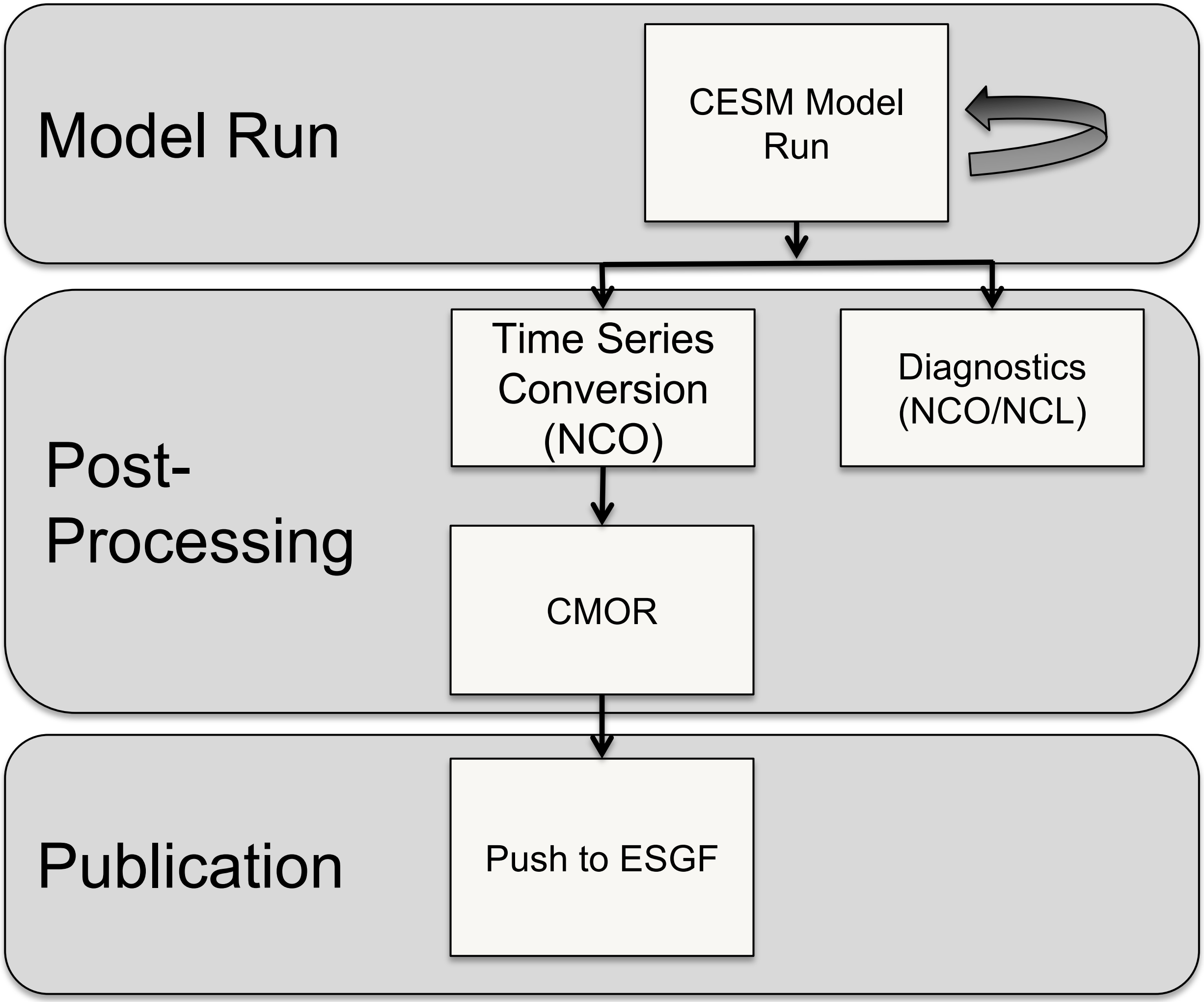
CESM's CMIP5 Workflow



Lessons We Learned From CMIP5

CESM was the first model to complete their simulations, but the last to complete publication.

Why?

- All of the post-processing was serial and it took a long time to run
- Workflow was error prone and was time consuming to debug
- Too much human intervention was needed between post-processing steps and time was wasted
- There was only one person who knew the status of all of the experiments

Motivating Factor
CMIP5 vs CMIP6

CMIP5

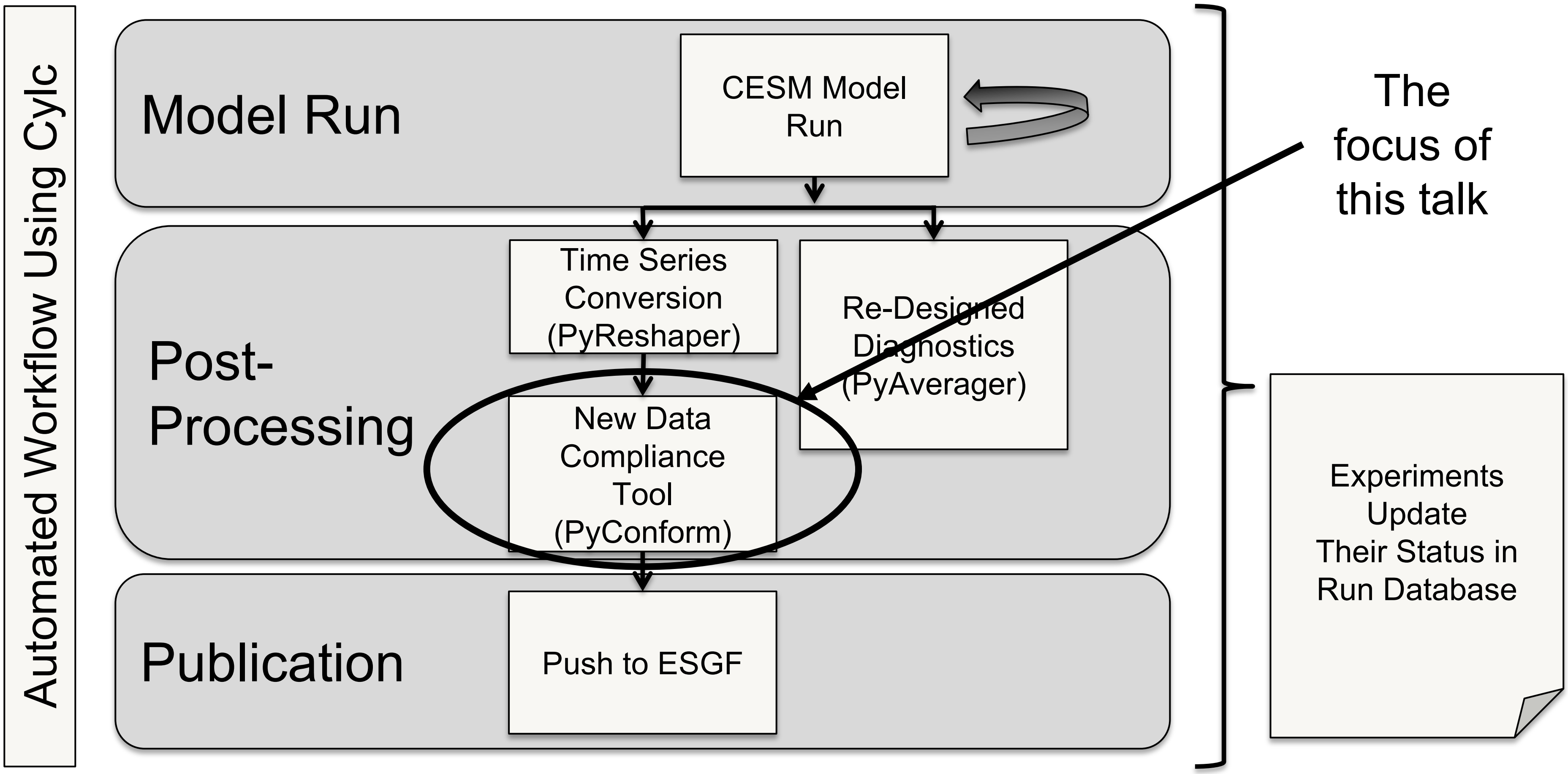
- 25 Experiments
- Timeline: 3 years
- Output size: 800TB
- Published size: 200TB

CMIP6

- 102 Experiments
- Timeline: 1 year
- Output size: 8PB (estimate)
- Published size: 2PB (estimate)

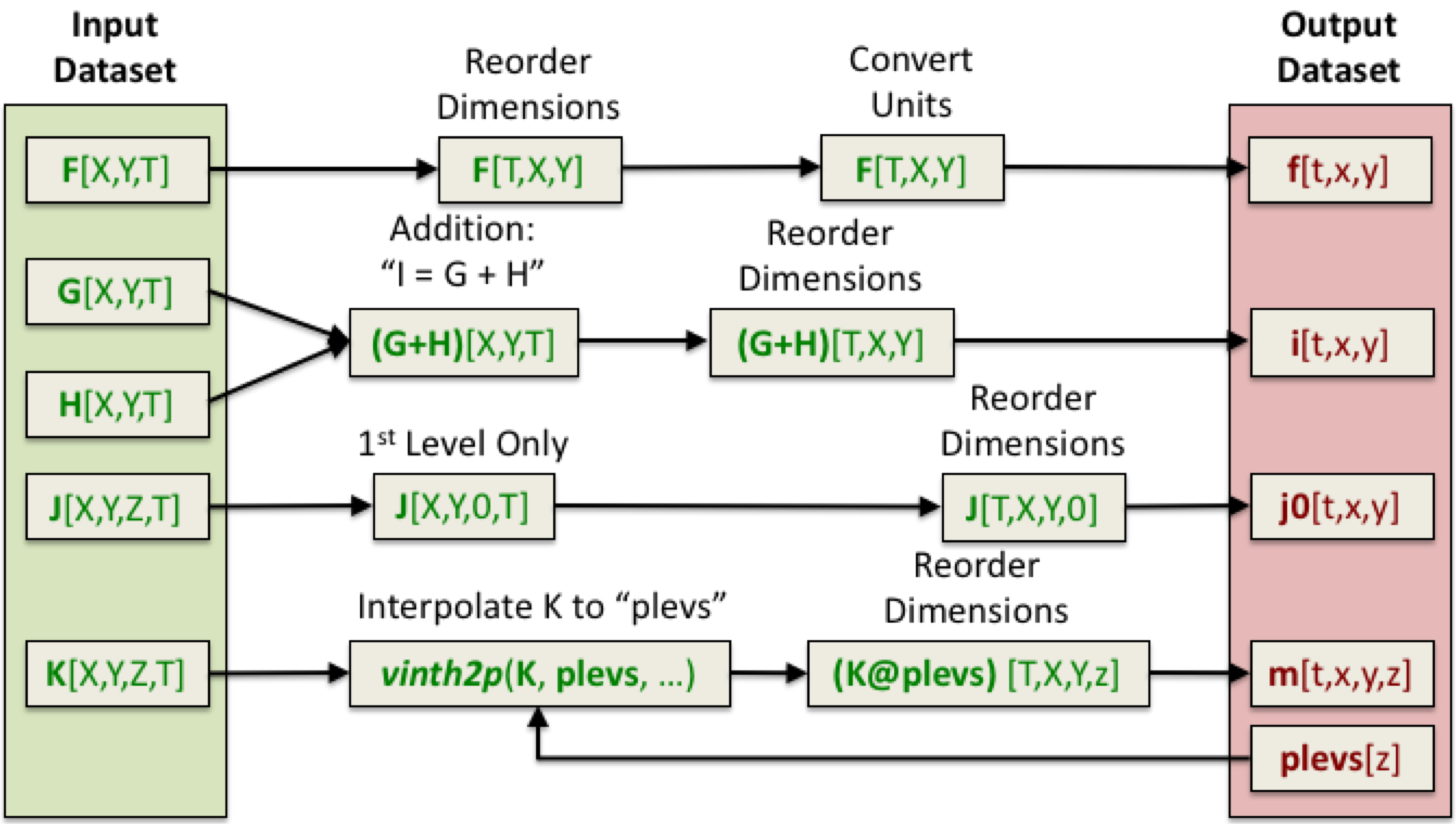
http://www.bbc.com/earth/story/20170510-terrifying-20m-tall-rogue-waves-are-actually-real

New CESM/CMIP6 Workflow



Data Compliance

Taking model output and processing it into experiment compliant data



Previous Version Used for CMIP5

- Used Fortran and CMOR to read in the raw output, do all conversions, and write out complaint files

- Serial, no parallelization

Slow
Rigid and Hard to Expand
Error Prone

PyConform: New Version Used for CMIP6

- Uses Python
    - netCDF4, numpy, dreqPy, cf_units, pyNGL
- Parallelization done with MPI4Py
- A three step process

Faster **(16x to 38x speedup over Fortran method)**
Flexible User Interface

First Step

Users need to create a text file with definitions that describe how to map model variables to requested variables

Examples:

```
cfc11global=f11vmr
ch4=vinth2p(CH4, hyam, hybm, plev, PS, P0)
mc=CMFMC+CMFMCDZM
siage=siage
```

Second Step

Then users run the iconform tool that matches the definitions to its variable information within the CMIP6 Data Request

The Data Request lists variable requirements:

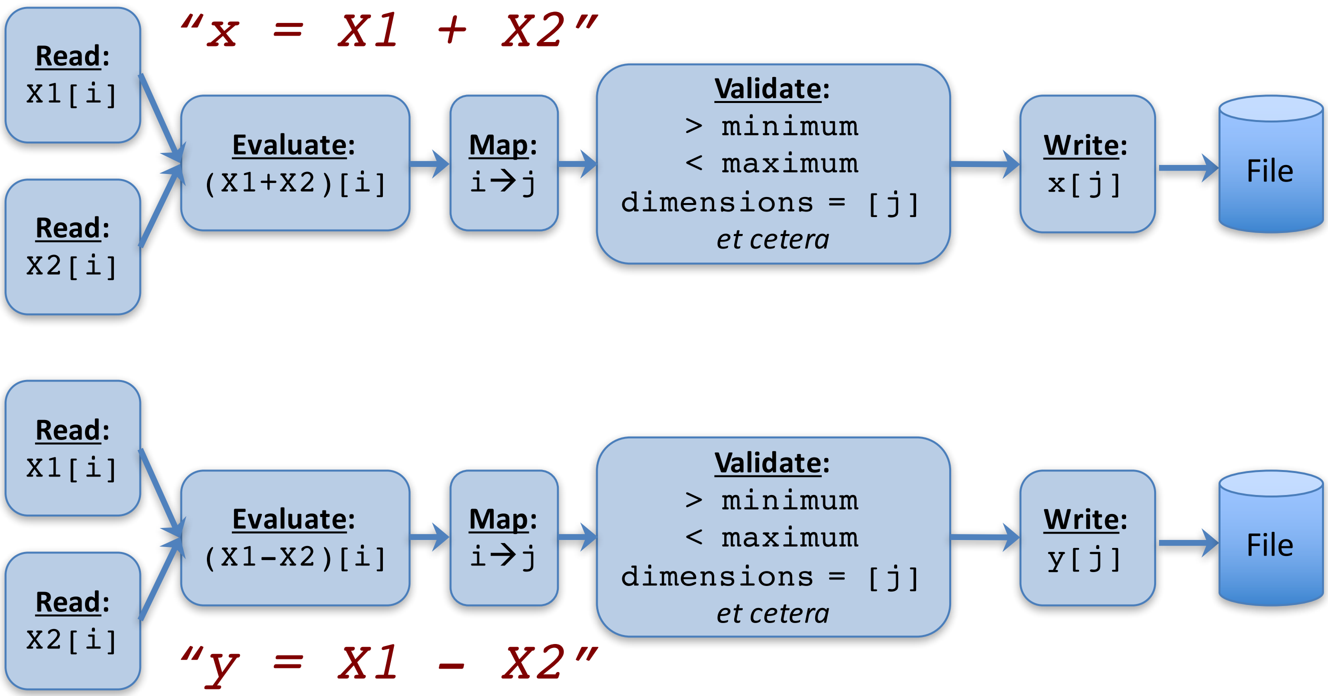
- Units
- Dimensions
- Descriptions
- Positive Attribute on Vertical Dimensions
- And a lot more …

Sample Portion of a PyConform Input File


```
"ua": {
    "attributes": {
        "_FillValue": "1e+20",

        "cell_measures": "area: areacella",

        "cell_methods": "time: mean",

        "comment": "\"Eastward\" indicates a
vector component which is positive when directed
eastward (negative westward). Wind is defined as a
two-dimensional (horizontal) air velocity vector,
with no vertical component. (Vertical motion in
the atmosphere has the standard name
upward_air_velocity.)",

        "description": "\"Eastward\" indicates
a vector component which is positive when directed
eastward (negative westward). Wind is defined as a
two-dimensional (horizontal) air velocity vector,
with no vertical component. (Vertical motion in
the atmosphere has the standard name
upward_air_velocity.)",

        "frequency": "mon",

        "id": "ua",

        "long_name": "Eastward Wind",

        "mipTable": "Amon",

        "out_name": "ua",

        "prov": "Amon ((isd.003))",

        "realm": "atmos",

        "standard_name": "eastward_wind",

        "time": "time",

        "time_label": "time-mean",

        "time_title": "Temporal mean",

        "title": "Eastward Wind",

        "type": "real",

        "units": "m s-1",

        "variable_id": "ua"
    },
    "datatype": "real",

    "definition": "vinth2p(U,hyam,hybm,plev,
                   PS,P0)",
```

Third Step

Then users run the xconform tool that generates requested variables based on the input specifications



Physarray Object

- Is a subclass of the maskedArray in NumPy
- Additional features that were needed above the masked array class:
  - Automatic Unit Conversion
  - Automatic Dimension Handling
  - Automatic Handling of the Positive Attribute

Physarray Object

Extra features we needed to generate the data correctly:
Automatic Unit Handling

"X = X1 + X2"

Units: K = Units: K + Units: K

"X" = Units: K

"X = X1 + X2"

Units: K = Units: K + Units: C

Convert to K before operation is performed

Units: K

"X" = Units: K + Units: K

"X = X1 * X2"

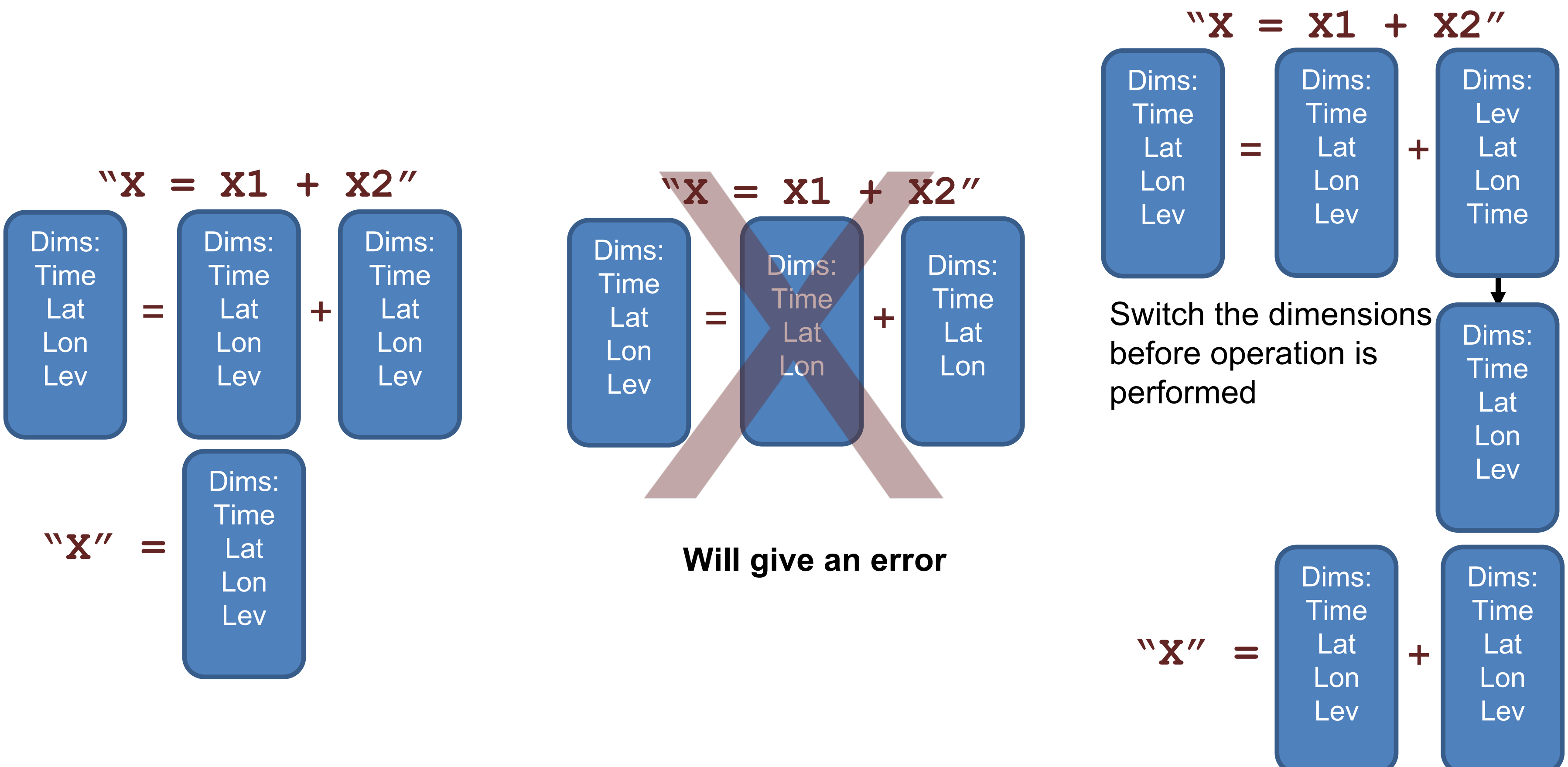
Units: kg m-2 = Units: kg * Units: m-2

"X" = Units: kg m-2

* Must be cf compliant units

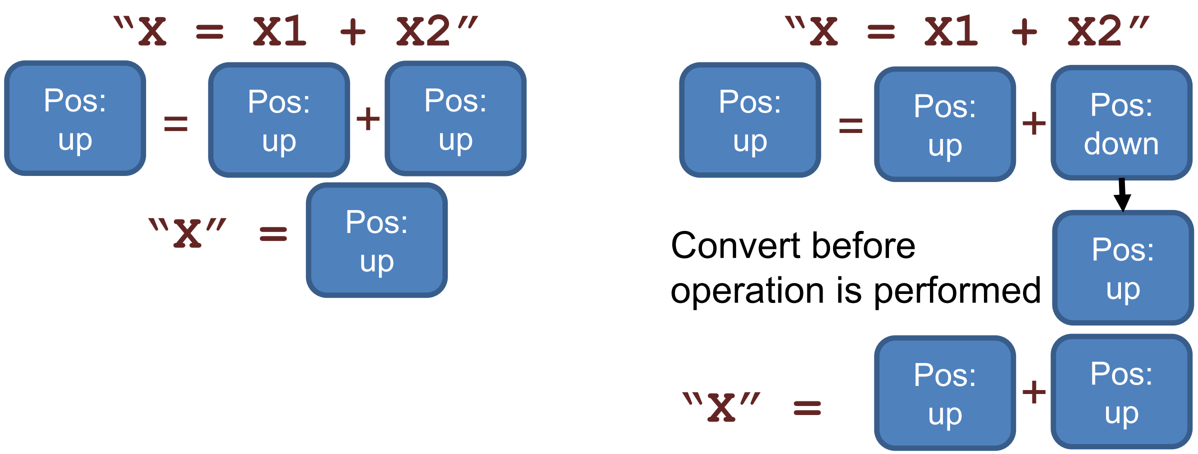
Physarray Object

Extra features we needed to generate the data correctly:
Automatic Dimension Handling



Physarray Object

Extra features we needed to generate the data correctly:
Automatic Handling of the Positive Attribute
(flipping the vertical dimension)



Switching to Xarray/Dask

- We are working on a new version that uses xarray
- While we no longer need the ability to handle dimension reordering, we still need functionality to handle the unit conversion and the flipping of the vertical dimension
- We will also need to evaluate the performance

Moving Forward ….

- We are currently using PyConform in its current form for our CMIP6 output

- We are looking at a redesign of the internal data structures to use new capabilities that didn't exist when we started the project

- Performance and usability are key for this tool and we will move in those directions

Questions

Contact: mickelso .at. ucar.edu
https://github.com/NCAR/PyConform

http://m.sweetclipart.com/halloween-pumpkin-pail-with-candy/