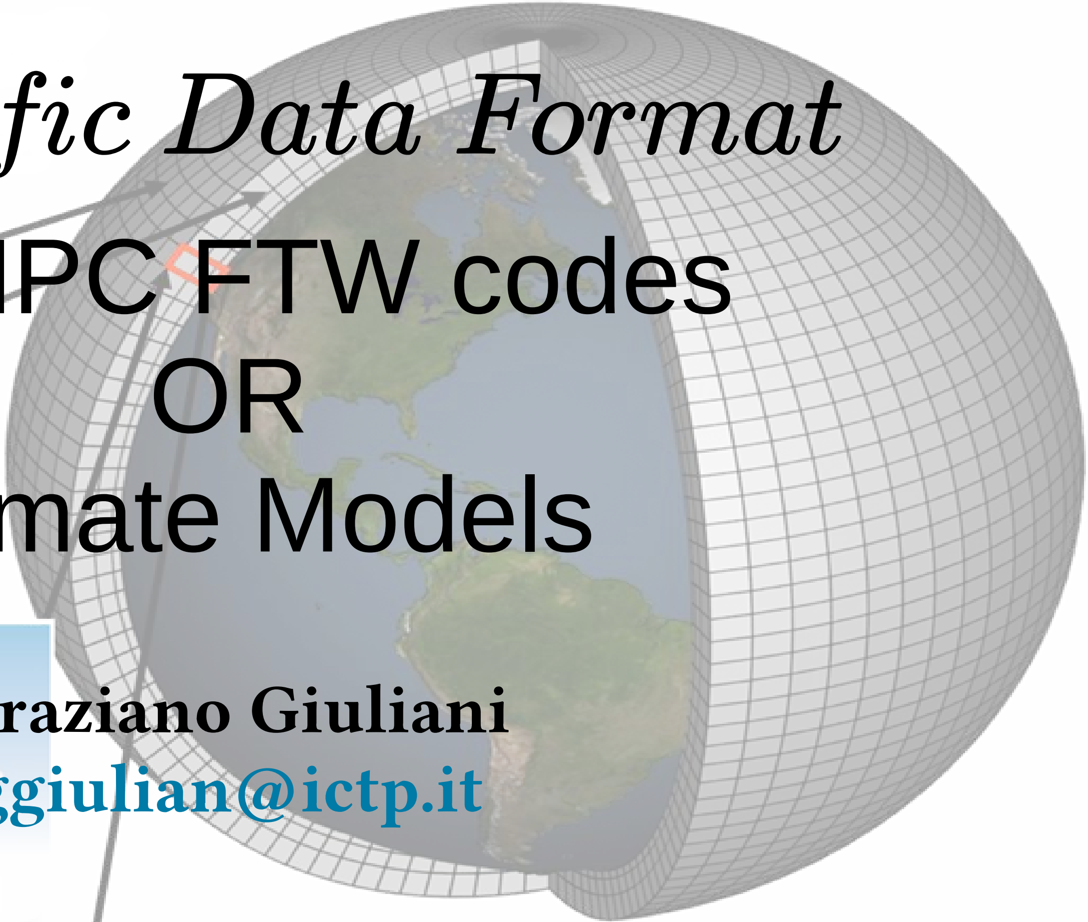
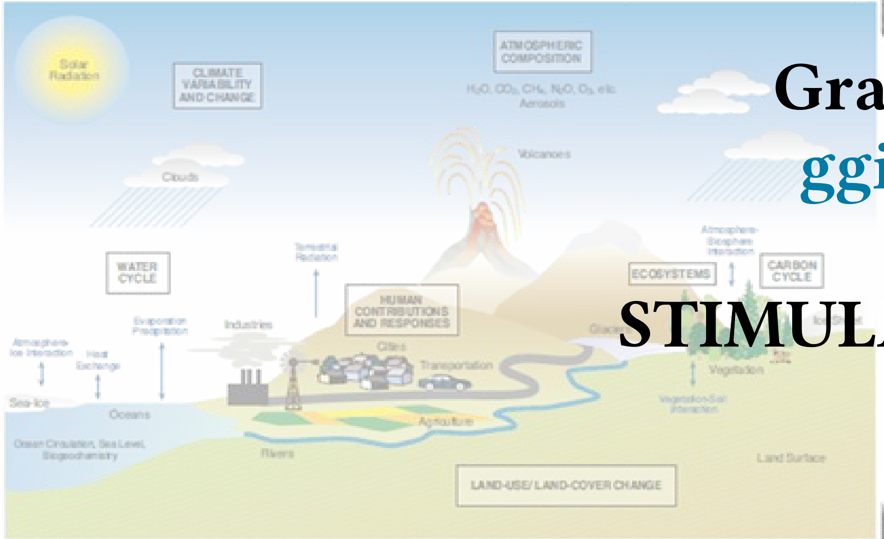
Scientific Data Format



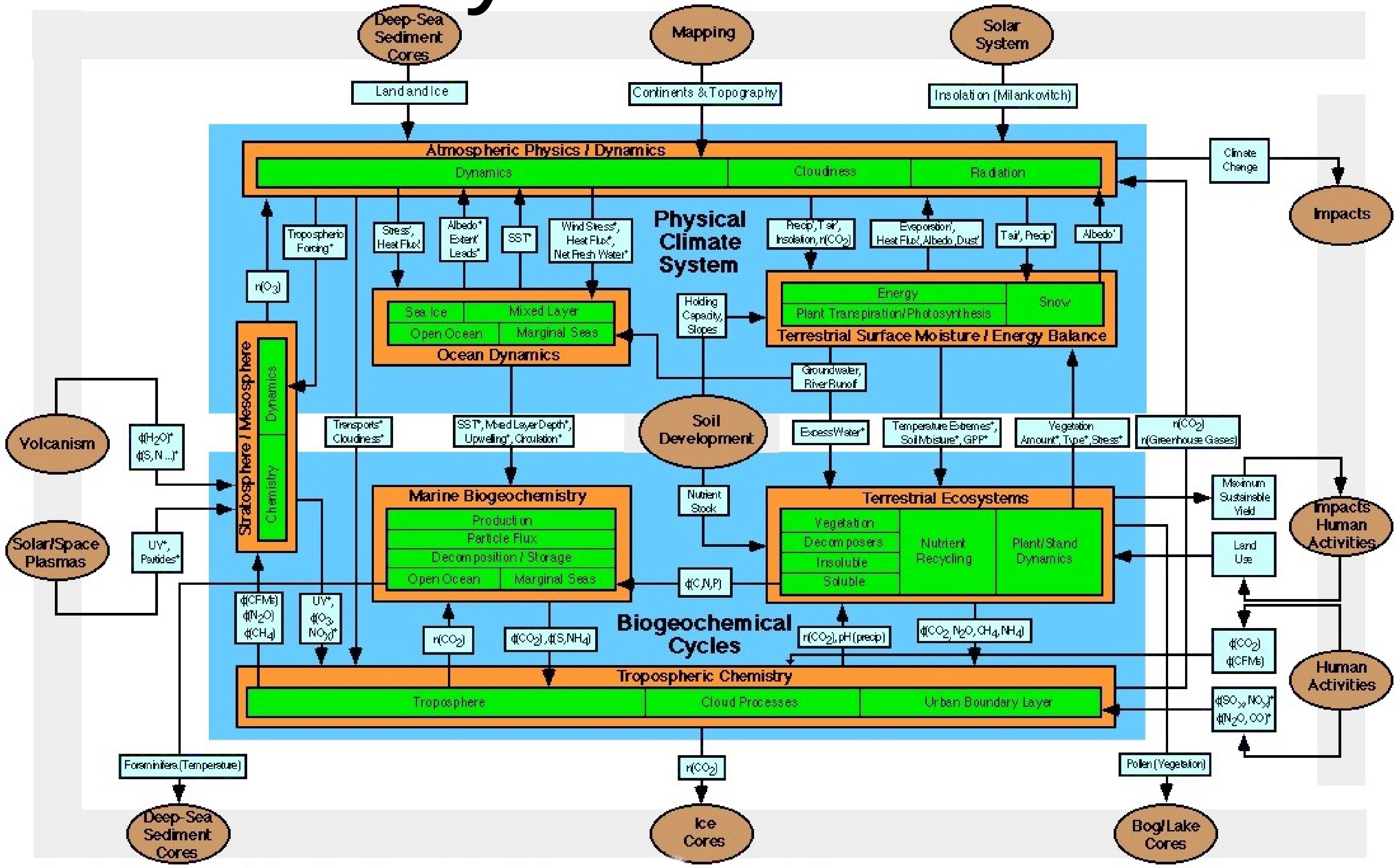
The HPC FTW codes
OR
Climate Models



Graziano Giuliani
ggiulian@ictp.it

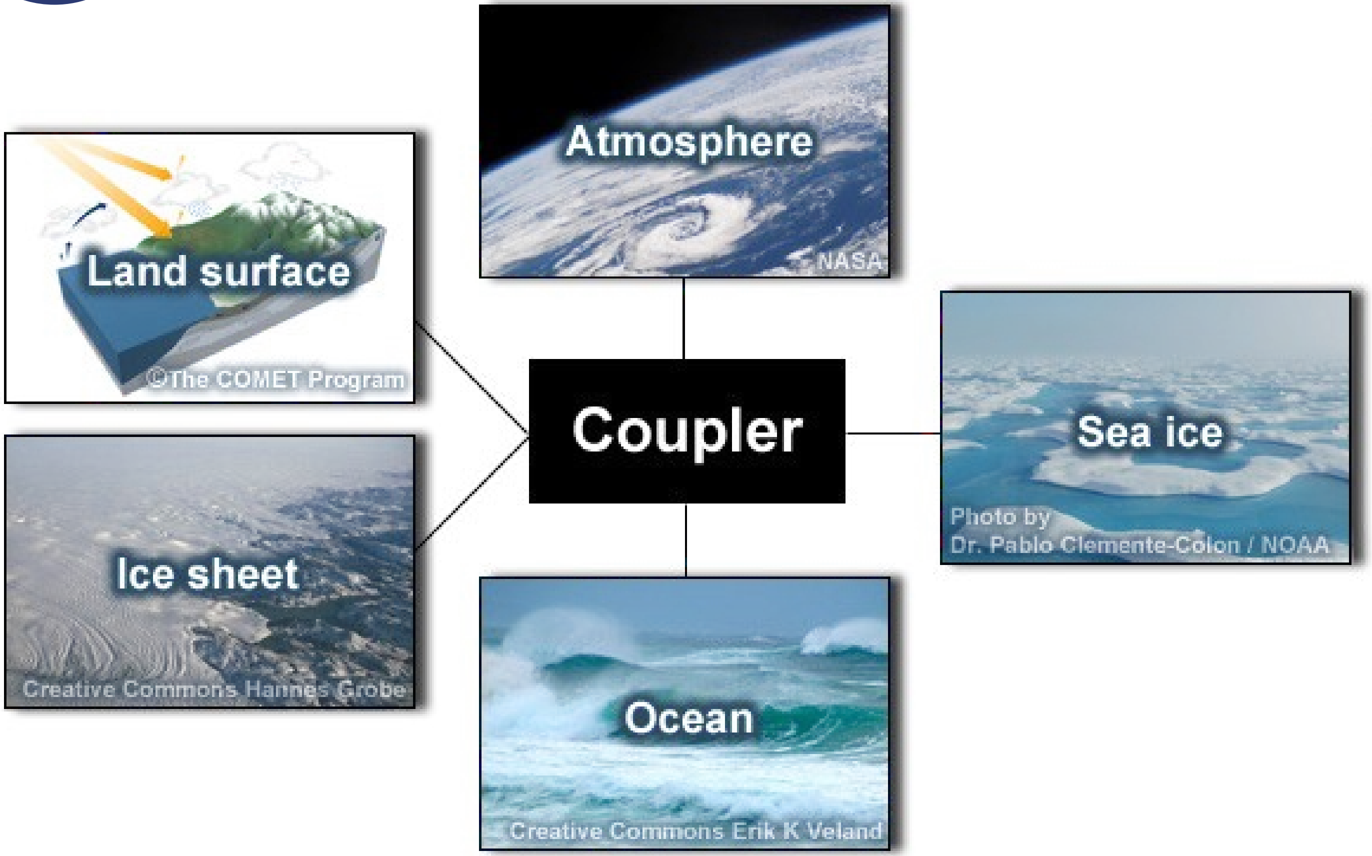
STIMULATE – Ferrara 2019

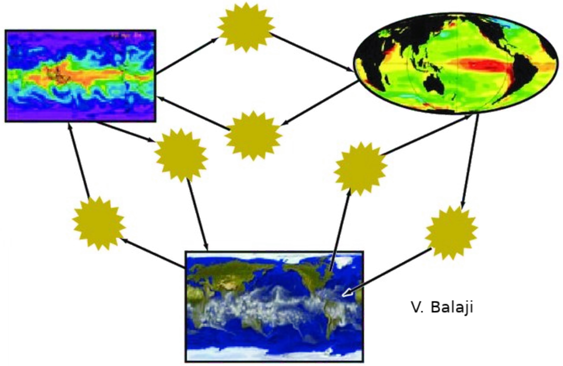
Earth System Processor



NASA

Model Coupling





V. Balaji

Earth fluid modeling

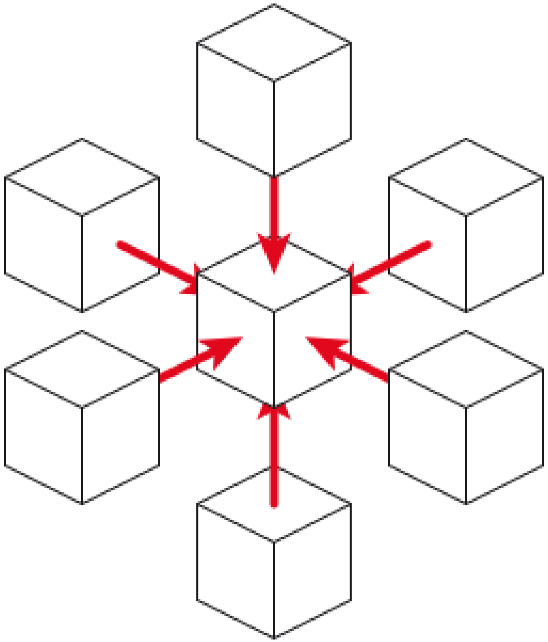
- Based on Fundamental Laws of Physics
  - Sir Isaac Newton’s laws of motion
  - Rudolf Clausius’ 1st law of thermodynamics
  - Arthur Schuster’s equations of radiative transfer.
- Vilhelm Bjerknes, wrote the equations that we use to forecast the wind in weather and climate models
- Lewis Richardson, is the father of numerical weather forecasting
- John von Neumann successfully ran a numerical forecast model on a computer.

Equations

- Complex system of coupled non linear partial differential equations
- No analytical solution is known, no exact initial condition is measurable methods such as finite differences, finite volumes or elements, spectral or Galerkin methods
- Only way to compute time evolution is by step time integration using a CFL limited time integration interval

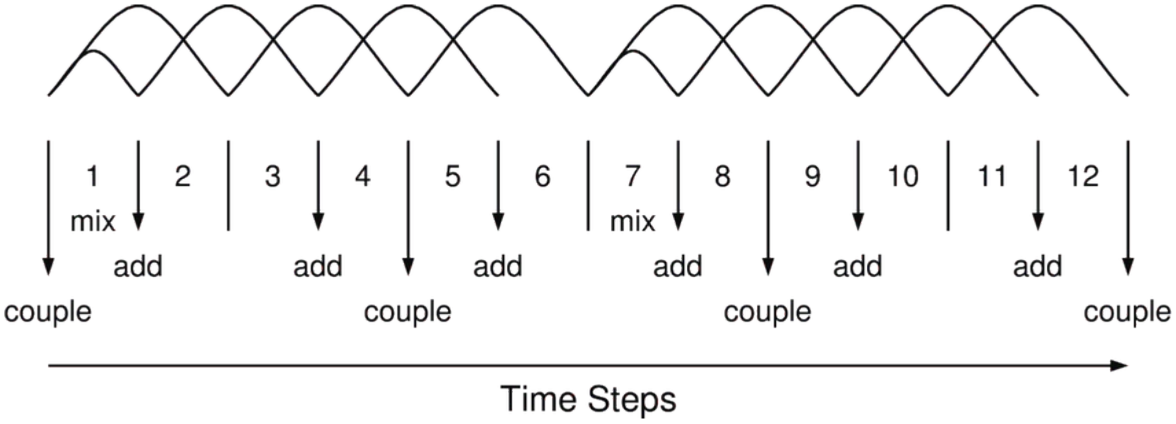
The Stencil Problem

- Stencil codes are a class of iterative kernels which update array elements according to some fixed pattern, called a stencil.
- Most finite difference codes which operate on regular grids can be formulated as stencil codes.



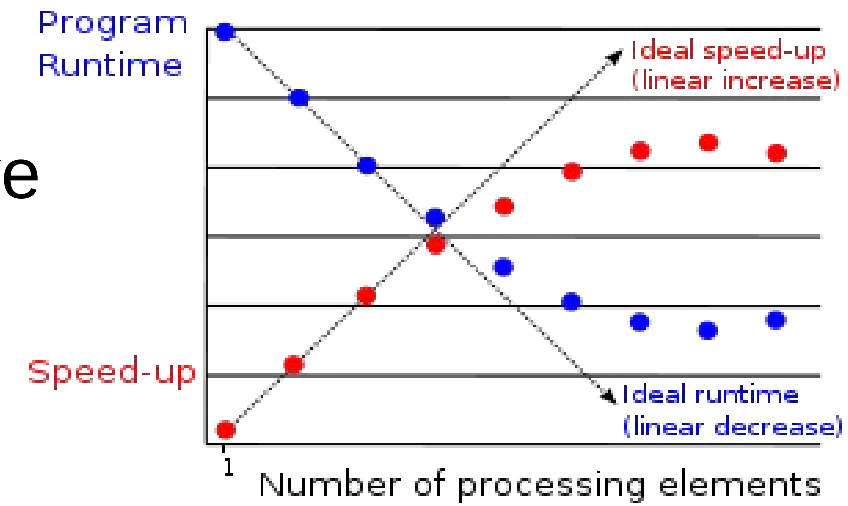
Ghost point communication

- Every timestep, every processor must communicate halo points to fill computational stencil for the numerical solution of the model equations.
- At fixed point in time each model must communicate exchange status variables with other models
- At fixed point in time status prognostic and diagnostic variables must be saved on disk



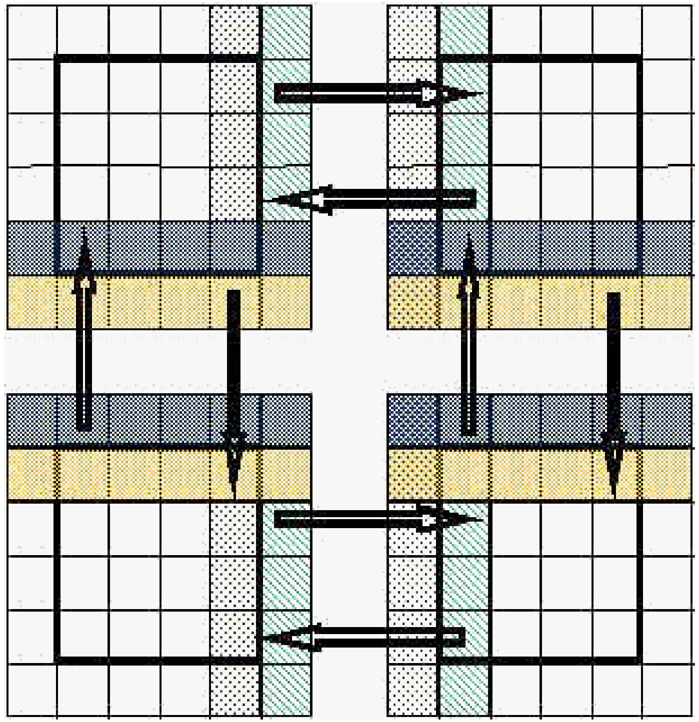
Scalability limit

- Increasing the number of processors:
  - Decrease computational burden per processor
  - Increase communication overhead per processor
- Parallel slowdown for communication bottleneck
- With more processors we can solve a bigger problem, not solve faster a given problem

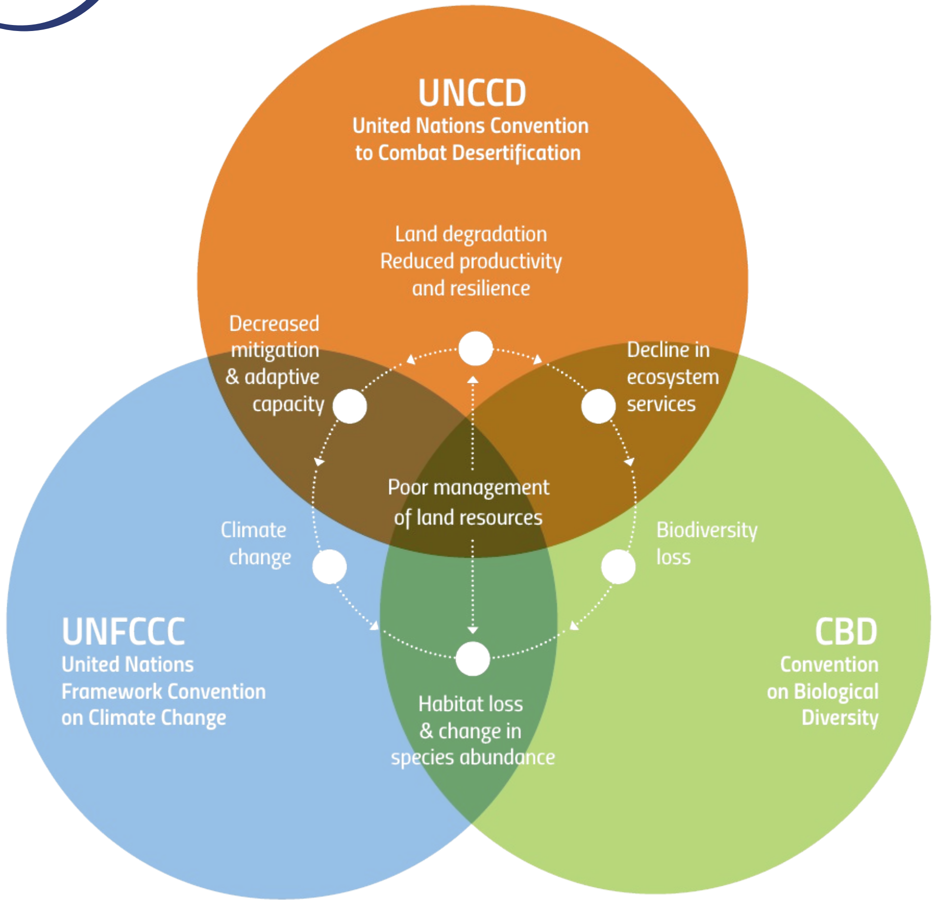


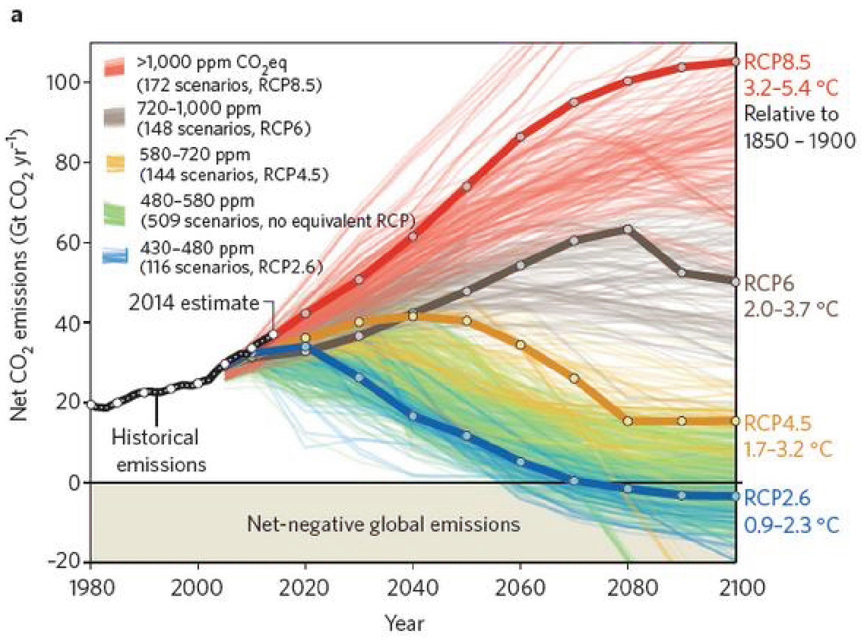
Domain decomposition

- Usual domain decomposition is on a Cartesian 2D mesh



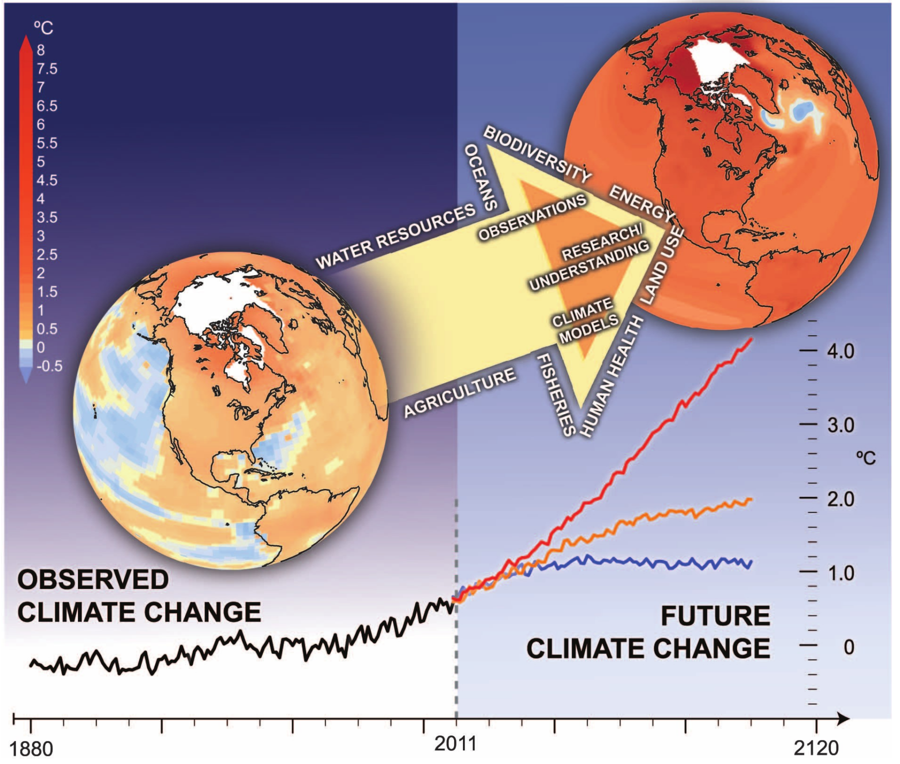
IPCC mission



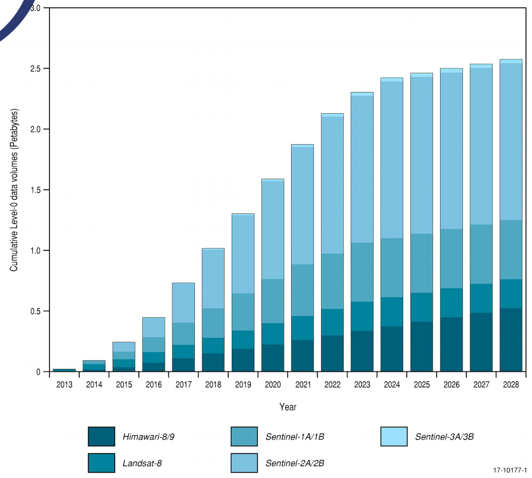


Climate Research

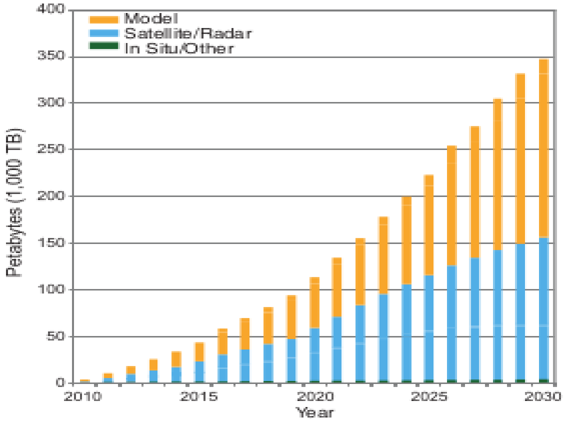
- Documenting the past, historical and paleo earth climates
- Observing actual system status
- Modeling future status
- Ecosystem, health and economic drivers and impacts



Climate Data

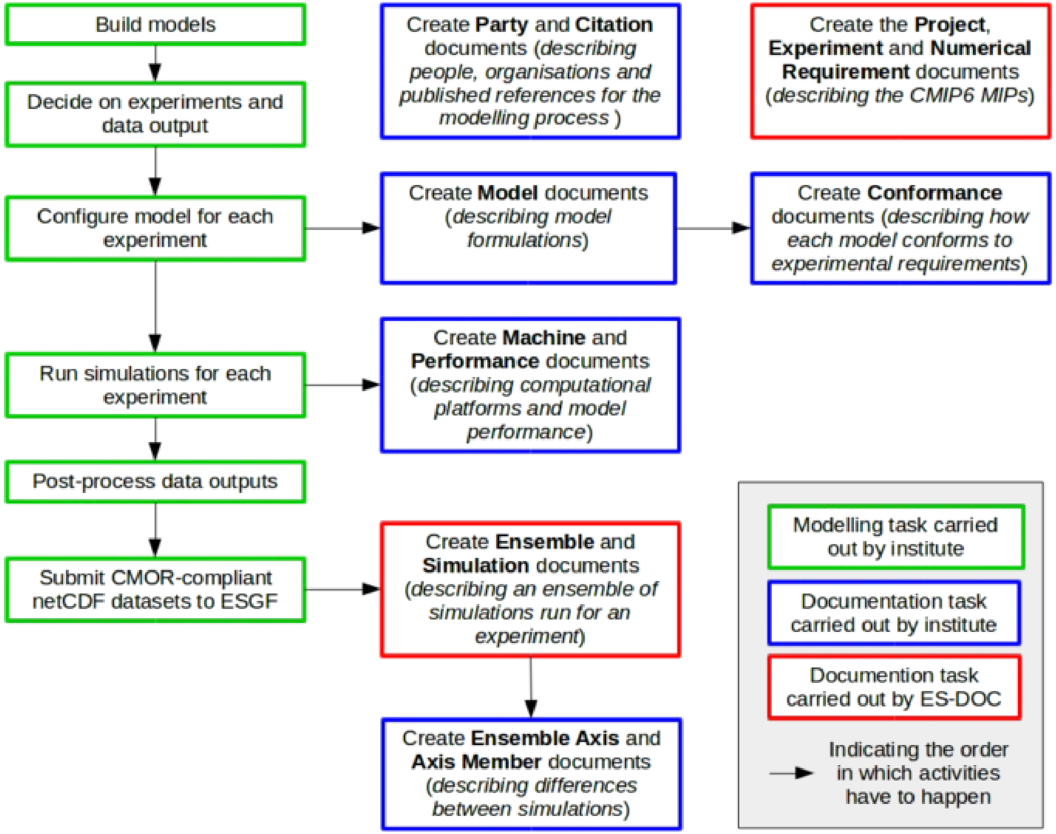


- By the end of 2017, the operational Sentinel-1, 2 and 3 satellites alone will continuously collect a volume of 20 Terabytes per day.



- The CMIP data archives have grown from the 50TB of the the CMIP3 project to the 2.5PB of the CMIP5 project. The same trend is expected for CMIP6 to reach ~100PB of disk storage space.

IPCC GCM



Build models
Decide on experiments and data output
Configure model for each experiment
Run simulations for each experiment
Post-process data outputs
Submit CMOR-compliant netCDF datasets to ESGF
Create **Party** and **Citation** documents (*describing people, organisations and published references for the modelling process*)
Create **Model** documents (*describing model formulations*)
Create **Machine** and **Performance** documents (*describing computational platforms and model performance*)
Create **Ensemble** and **Simulation** documents (*describing an ensemble of simulations run for an experiment*)
Create **Ensemble Axis** and **Axis Member** documents (*describing differences between simulations*)
Create the **Project**, **Experiment** and **Numerical Requirement** documents (*describing the CMIP6 MIPs*)
Create **Conformance** documents (*describing how each model conforms to experimental requirements*)
Modelling task carried out by institute
Documentation task carried out by institute
Documention task carried out by ES-DOC
Indicating the order in which activities have to happen

Acronyms

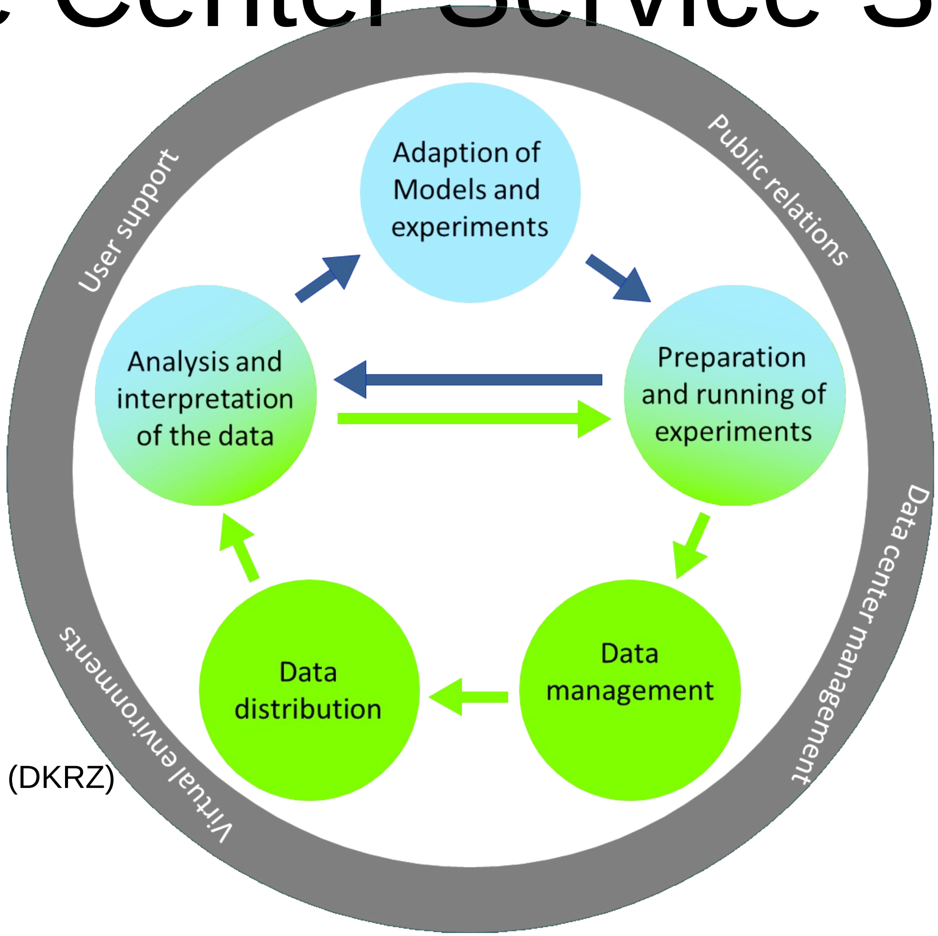
- The World Climate Research Program : WCRP
- Working Group on Climate Modeling : WGCM
- WGCM Infrastructure Panel : WIP
- The Program for Climate Model Diagnostics and Intercomparison : PCMDI
- Coupled Model Intercomparison Projects : CMIP

- **Requirements for a global data infrastructure in support of CMIP6**, *Geosci. Model Dev. Discuss.* https://doi.org/10.5194/gmd-2018-52

WIP CMIP6 guidelines

- The global computational and data infrastructure needs to be formally examined as an integrated element.
- Scientific reproducibility and durability and provenance of data
- Systematic and routine evaluation of Earth System Models (ESMs)
- Mechanisms to identify costs and benefits in developing new models, performing CMIP simulations, and disseminating the model output
- Experimental specifications as machine-readable experiment design on all of the controlled vocabularies
- Review the management of information about users to simplify communications with them

Climate Center Service Structure



Michael Lautenschlager
Deutsches Klimarechenzentrum (DKRZ)

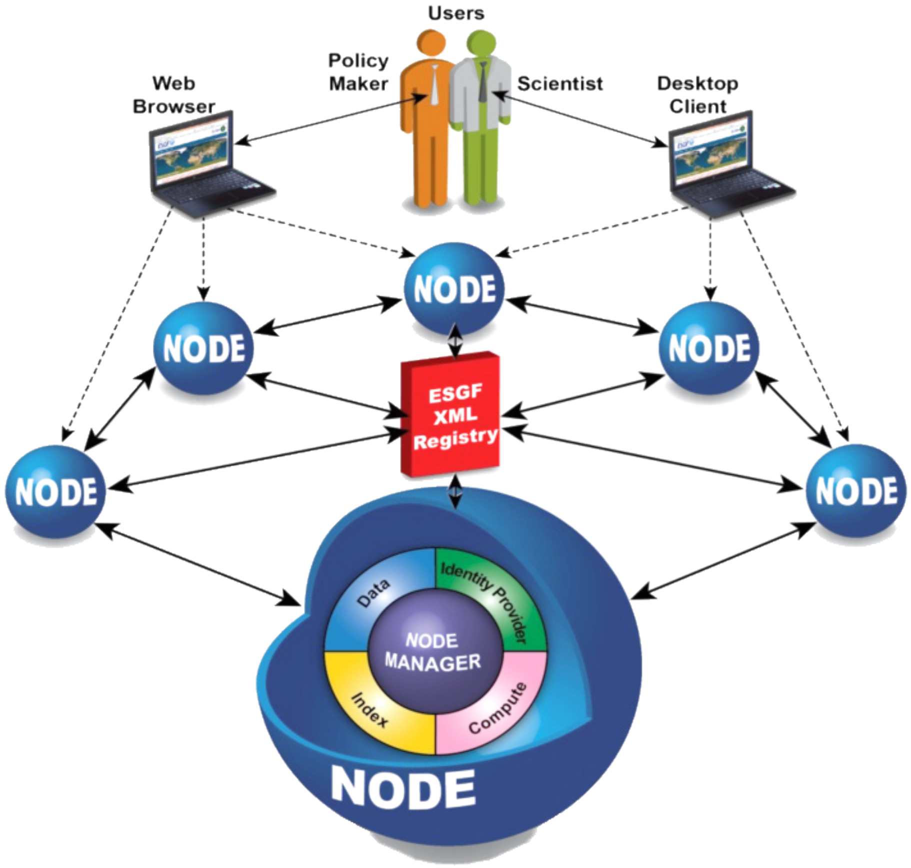
IPCC Model data repositories

- Earth System Grid Federation

- National Sites
- Impact Portals

- Climate Service Companies

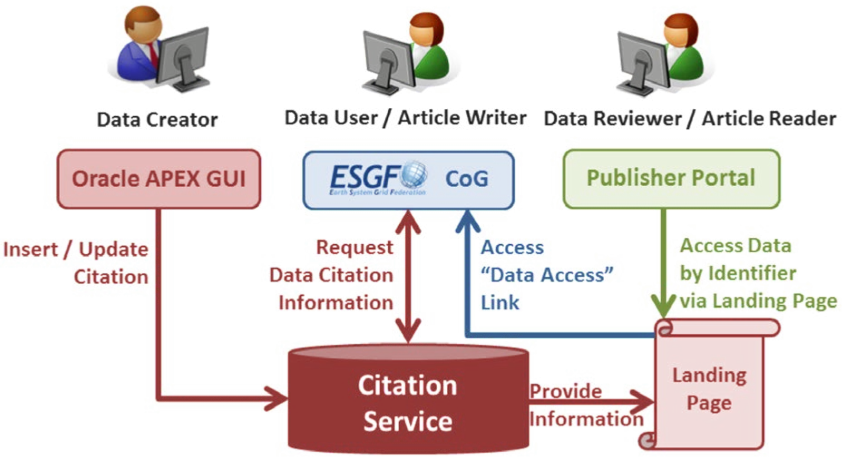
  PAY SERVICES



Data Management

https://www.earthsystemcog.org/projects/wip/position_papers

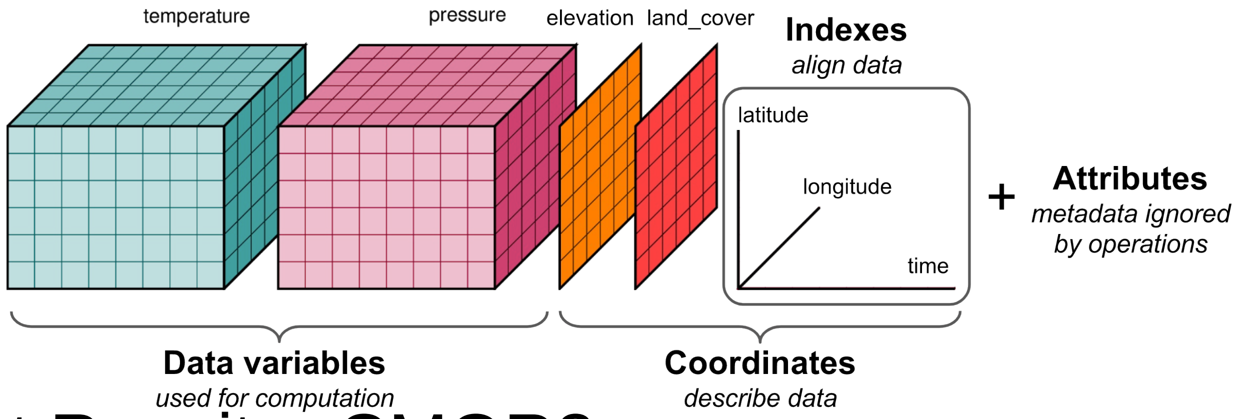
- Replication and Versioning
- Use of Persistent Identifiers
- Data Reference Vocabularies
- Data Request Structure and Process
- Data Quality Assurance
- Data Citation and Long-term Archiving
- File Names and Global Attributes
- Licensing and Access Control
- Errata service



Stockhause, M and Lautenschlager, M 2017 CMIP6 Data Citation of Evolving Data. Data Science Journal, DOI: https://doi.org/10.5334/dsj-2017-030

Data Format

- NetCDF format



- Climate Model Output Rewriter CMOR3
  - Each file contains a single primary output variable (along with coordinate/grid variables, attributes and other metadata) from a single model and a single simulation
  - Variable number of time slices (samples) can be stored in a single file
  - Metadata written are defined MIP-specific tables of information
  - Unit of measure checking through UDUNITS library

Data Analysis Workflow

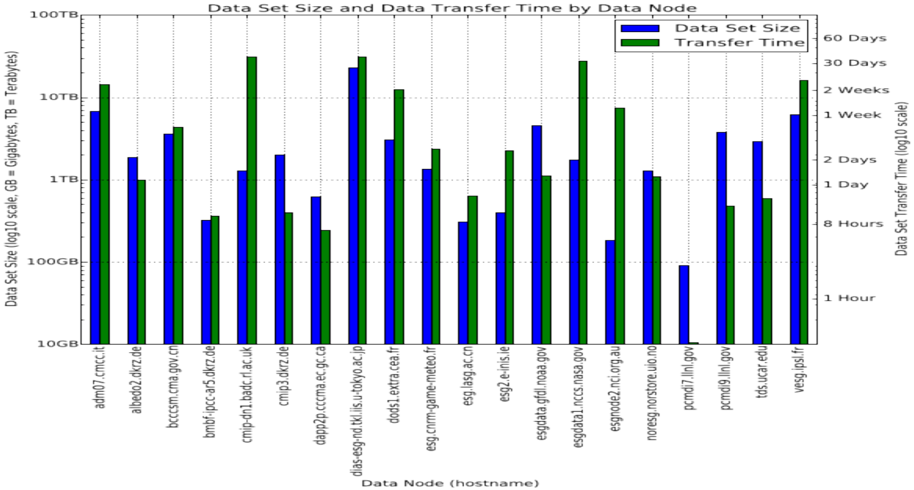
- Data Collection (STAGING)
- Data Pre-Processing (ADAPTATION)
- Scientific work (PROCESSING)
- Result check (VERIFICATION)

Publication and peer review process

Timings

- An Assessment of Data Transfer Performance for Large-Scale Climate Data Analysis and Recommendations for the Data Infrastructure for CMIP6 - Dart, Wehner, Prabhat

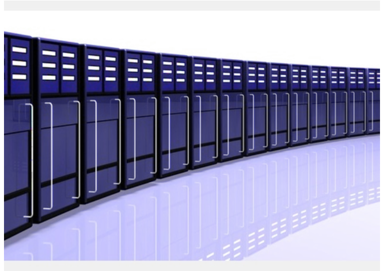
- STAGING – 3 months
- ADAPTATION – 3 weeks
- PROCESSING – 2 days
- VERIFICATION – 10 minutes



STAGING (Data Transfer) is the bottleneck for data analysis

Data Analytic Storage Systems

- Traditional :
  - Move data from Storage to Compute
  - Computation
  - Move results to Storage
- Emerging :
  - DASS
    - Move Analytics to storage/compute nodes
    - Results kept on storage/compute nodes
- ESGF OGC WPS Interfaces
  - Climate analytics through Web
  - Processing Services



Reinvent the wheel?

- A data cube (or datacube) is a multi-dimensional ("n-D") array of values. Typically, the term datacube is applied in contexts where these arrays are massively larger than the hosting computer's main memory; examples include multi-Terabyte/Petabyte data warehouses and time series of image data.
- Google Earth Engine combines a multi-petabyte catalog of satellite imagery and geospatial datasets with planetary-scale analysis capabilities and makes it available for scientists, researchers, and developers to detect changes, map trends, and quantify differences on the Earth's surface.

WIP remark

- “In the future, datasets and software with provenance information will be first-class entities of scientific publication, alongside the traditional peer-reviewed article […] Data analytics at large scale is increasingly moving toward machine learning and other directly data-driven methods of analysis, which will also be dependent on data with provenance tracking.”