Climate Modelling: What lies beneath?

Data, Hardware, Software, People

(Large-Scale European)
Climate Model Infrastructure
in "2024 and beyond"

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is-enes
INFRASTRUCTURE FOR THE EUROPEAN NETWORK FOR EARTH SYSTEM MODELLING

Context

- In 2012 our community produced a ten-year “foresight/strategy” document for the infrastructure we need(ed), and it was updated in 2017.
- These previous foresight documents were written on the back of large science meetings with significant community involvement, both in delivering content, and in shaping the drafts which eventuated.
- IS-ENES3 is funded to do develop a new ten-year plan.
- We had planned to do something similar this time, but given the times we live in, we have had to come up with another plan.
- This presentation is intended both to summarise some current thinking and get input.

What is infrastructure?

"The systems, services, and resources that the community needs to progress large-scale climate modelling"

Which in practice encompasses:

- the **services and software** necessary to sustain scientific workflows,
- the **physical computing systems** (such as data repositories, networks, supercomputers and their underlying hardware), and
- the necessary **personnel and community networks**.

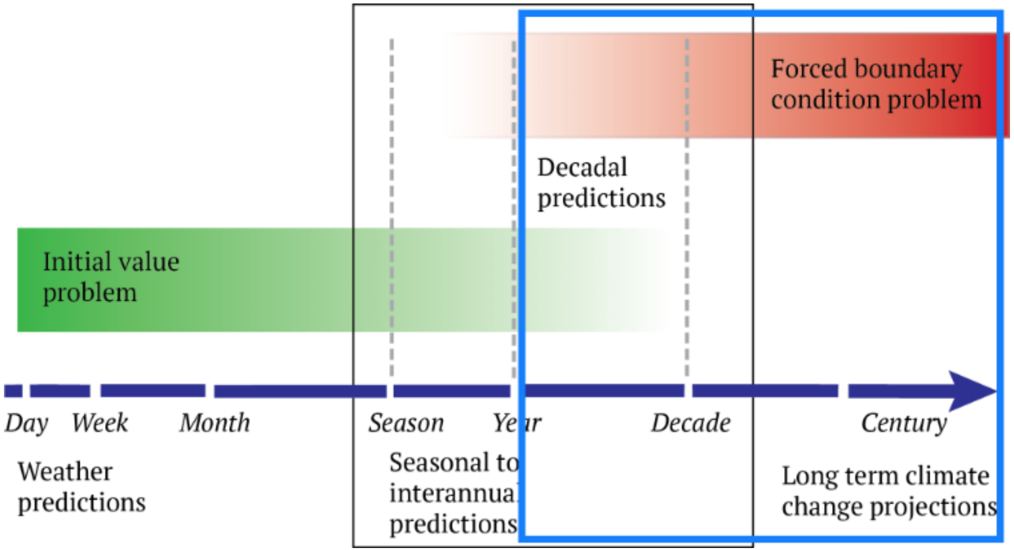
(The focus here is European and large scale, but many of the concepts, issues, and concerns have wider applicability.)

Outline

- Scope
- (Where we begin)
- (Where we end)
- Requirements
  - The Spectrum of Climate Science
- Simulation
  - Computing Context
  - Science Code and Model Complexity
  - Technical Code
- Analysis Workflows
  - Patterns
- (Discussion: Whither shared tools, XIOS, ESMValTool etc?)
- Strategic Statements
  - (towards recommendations)

Scope

Scope – Science Timescales



Scope - Definitions

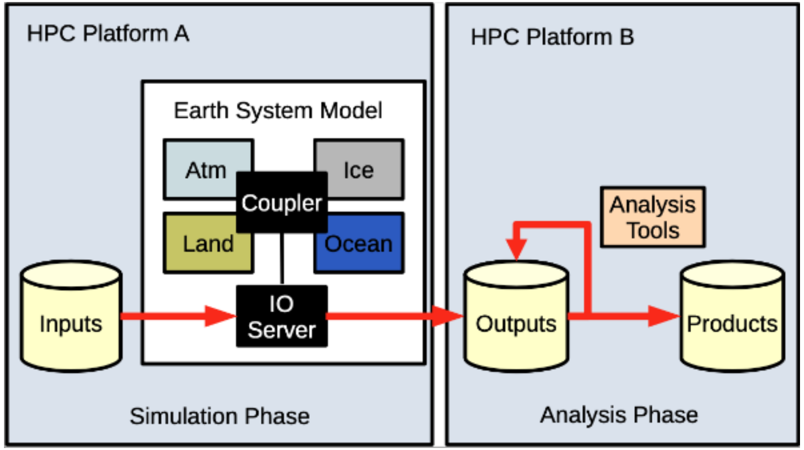
Context (WCRP definitions)

- **Climate system**:
  - The part of the Earth system that is relevant to climate; that is, the atmosphere, ocean, land surface, and cryosphere, their coupling processes and feedback mechanisms.
- **Earth system**:
  - Earth's interacting physical, biogeochemical, biological, and human systems, including the land, the atmosphere, the hydrosphere, and the cryosphere.

Two kinds of model (WCRP definitions):

- **Climate Models**, of regional or global extent (RCM or GCM):
  - Represent the coupled physical climate system components and considers biogeochemical and human systems as either time-varying external forcing on the climate (scenarios) or as downstream systems impacted (forced) by the climate.
- **Earth System Model (ESM)**:
  - Represents both the physical climate and the biogeochemical systems and their interactions as a single coupled system, but the human systems are still generally modelled as resulting in a force on the ESM or as forced systems. Natural phenomena such as volcanoes and solar variations are included as forcings.

Two phases to consider (our definitions)



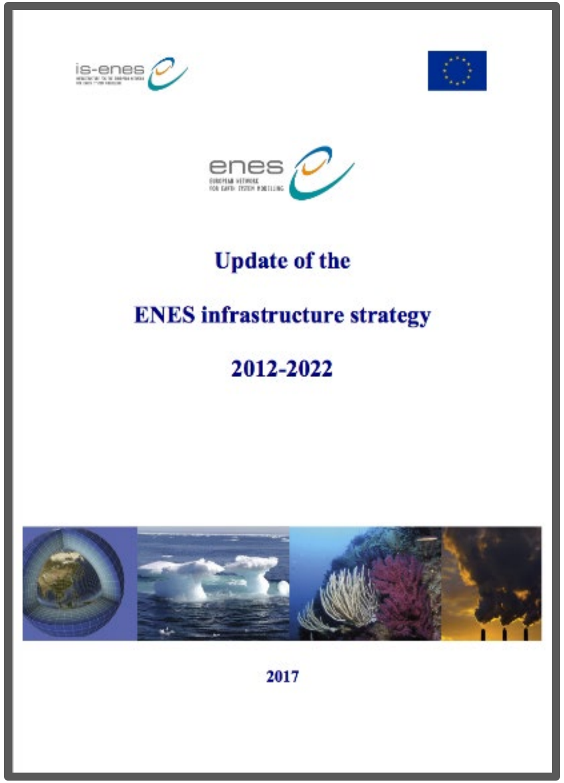
HPC platform A and B may be the same, may be in the same place, but differ, or may be in different places.

Where we have been

Building on the past

Mitchell, J., Budich, R., Jousssame, S., Lawrence, B., & Marotzke, J. **(2012).** *Infrastructure strategy for the European Earth system modelling community 2012–2022*. ENES. https://doi.org/10.5285/ca90b281d6ff4cffb9a9bbdeb5fa63f3

Joussaume, Sylvie, Bryan Lawrence, & Francesca Guglielmo. **(2017).** *Update of the ENES infrastructure strategy—2012-2022* (No. 2; ENES Report Series). ENES. https://portal.enes.org/community/about-enes/the-future-of-enes/ENES_strategy_update_2017.pdf



Target Audiences? Then and Now

1. European bodies trying to understand the infrastructure requirements of our community (e.g. the commission itself, and other infrastructures funded by the commission such as EuroHPC, EOSC etc).
2. National funding bodies, to understand the linkages between nations, and the need for them to "step up to the plate and contribute their part".
3. Our community: To make the link between science aspirations and the infrastructure they need.
    - So we can understand the scientific requirements and deliver the necessary infrastructure.
    - So the "purer" scientists can understand the link between their aspirations and the resources needed to deliver that infrastructure.
4. Those delivering the infrastructure so they can understand how their contributions deliver on environmental goals
    - In some cases this is a very important part of their "remuneration", without which they might be working for Google and friends …

Recommendations - 2012 and 2017

1. Provide a blend of high-performance **computing facilities** ranging from national machines to a world- class computing facility suitable for climate applications, which, given the workload anticipated, may well have to be dedicated to climate simulations.

2. Accelerate the **preparation for exascale computing**, e.g. by establishing closer links to PRACE and by developing new algorithms for massively parallel many-core computing.

3. Ensure **data from climate simulations are easily available** and well documented, especially for the climate impacts community.

4. Build a **physical network connecting national archives** with transfer capacities exceeding Tbits/sec.

5. Strengthen the European expertise in climate science and computing to enable the long term vision to be realized.

1) **On models**: Support common development and sharing of software and accelerate the preparation for exascale computing by exploiting next generation hardware and developing appropriate algorithms, software infrastructures, and workflows.

2) **On HPC**: Exploit a blend of national and European high-performance facilities to support current and next generation science and work toward obtaining sustained access to world-class resources and next generation architectures.

3) **On model data:** Evolve towards a sustained data infrastructure providing data that are easily available, well-documented and quality assured, and further invest in research into data standards, workflow, high performance data management and analytics.

4) **On physical network:** Work to maximize the bandwidth between the major European climate data and compute facilities and ensure that documentation and guidance on tools and local network setup are available to users.

5) **On people:** Grow the numbers of skilled scientists and software engineers in the ENES community, increase opportunities for training at all levels, and strengthen networking between software engineers.

6) **On model evaluation (new):** Enhance sharing of common open source diagnostics and model evaluation tools, implement governance procedures, and expand data infrastructure to include computational resources needed for more systematic evaluation of model output.

7) **On infrastructure sustainability (new):** Sustain the cooperation necessary to develop future model and data technology and support international reference experiments programmes, and strengthen collaboration with other European actors providing services to, or using services from, ENES.

Where we are going

Simulation

- Huge spectrum of “large-scale” climate science.
- We know we need exascale computing for the “right hand problem” (resolution).
- We suspect we can’t use exascale computing efficiently for the “left hand problem” (low resolution, long-time)
- In the middle we have a problem – we might be able to efficiently use exascale computing, but we don’t know how:
  - It’s not just about porting/rewriting code, will it have the necessary arithmetic intensity?
  - Do we have the bodies to do it?
  - There are a lot components. But it’s hard to argue that there are are too many. Too few shared oceans?
  - What is the right amount of shared infrastructure?
  - Domain Specific Languages may be an important tool, but they are not a panacea.
- Variable resolution will become more prevalent
- Machine Learning
  - Might have a big role to play, and that affects the hardware requirements.,
- Cloud Computing
  - (Is a red herring)
  - New interfaces to data, new workflow requirements.

Analysis

- Lots of different analysis modes to support, all of which generate requirements for standards (or conventions) for data, vocabularies, and interfaces.
  - The clean distinction between the workflow for simulation and analysis is going to break which has implications!
  - Variable resolution grids will introduce new requirements for tools and standards and descriptions.
- Data lives a long time, and analysis communities need to know the provenance of simulation data, which is not the same as the provenance of analysis products.
  - We are still not in the sweet spot for model documentation.
- Data infrastructure is moving much faster than simulation infrastructure and more people are using the data infrastructure: which means we need even more software engineers to keep up.
  - The advent of cloud and pangeo don't change the pain points as much as some might think. At scale *managing* data is the *foundational* problem.
- Shared analysis tools are important.
  - ESMValTool will continue to evolve as will lower level tools like CDO and CF-Python.

People

- Hiring smart people remains hard. Keeping smart people remains hard, especially when they can get paid much more elsewhere.
  - In some countries this is more problematic than others. Issue in include salaries, precarity and responsibility (is there a career structure to keep software engineers? Can individuals chop an change between “science” and “infrastructure”?)
  - Luckily we have interesting problems.
- More?

Services

- What are the shared large-scale services?
  - (Yes, this is overlaps with our sustainability, but what do we want to summarise here?)

Timescales and reality (the myth of co-design?)

Activity	Timescale
Science/Engineering Career	o(40) years
Mitigation Target (e.g. 2030s)	o(20) years
Develop, deploy, maintain a “major” model component.	o(10-20) years
Major data products (CMIP scenarios)	o(10) years
CMIP/IPCC phase	o(7) years
Supercomputer	o(5) years
Major science project	o(2+4+4) years
Political Cycle (and politicians)	o(4) years
Configured Model	o(2-5) years
Human infrastructure design	o(2-5) years
Apprentice Climate Modelers (science, engineering, both)	o(1-3) years
Minor data products	o(1-2) years
Financial Year	1 year (!)

There is a lot of hysteresis in the development, deployment, and usage of climate models and their data.

It takes decades to develop a modelling system, during which there will be many hardware cycles.

More years to develop a CMIP class model, and then we use it for years, creating data with lifetime from years to a decade.

The hardware on which a configured model is deployed will likely change during its lifetime.

But applications need decisions on much shorter timescales, sometimes within financial years, or planning or electoral cycles.

New modelling requirements generated now may be delivered years after those who requested them have moved on.

These timescales do not align, overlaps can be very short! To get any benefit, everyone needs to be thinking long-term about what they want, and preserving those wants in “institutional memory”.

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Collaboration depends on aligned timescales

(for various definitions of aligned)

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Requirements

Requirements and Landscape

(Not enough time to cover all these in detail, but effectively six categories in a word salad for today:)

WCRP Lighthouses:

- **Explaining and predicting climate change** (EPESC) (annual to decadal)
- **Safe Landing Climates** (pathways to the future)
- **My Climate Risk** (local perspective, storylines)
- **Digital Earth** (integrated systems, km-scale)

Global Science

- **CMIP5, CMIP6, CMIP7** (MIPS past and future)
- **SM(I)LEs** (More data sharing)

Technical Collab

- **ESGF** (R&D, delivery)
- **Standards & Software: ESMValTool, Workflow, OASIS, XIOS, CF etc**

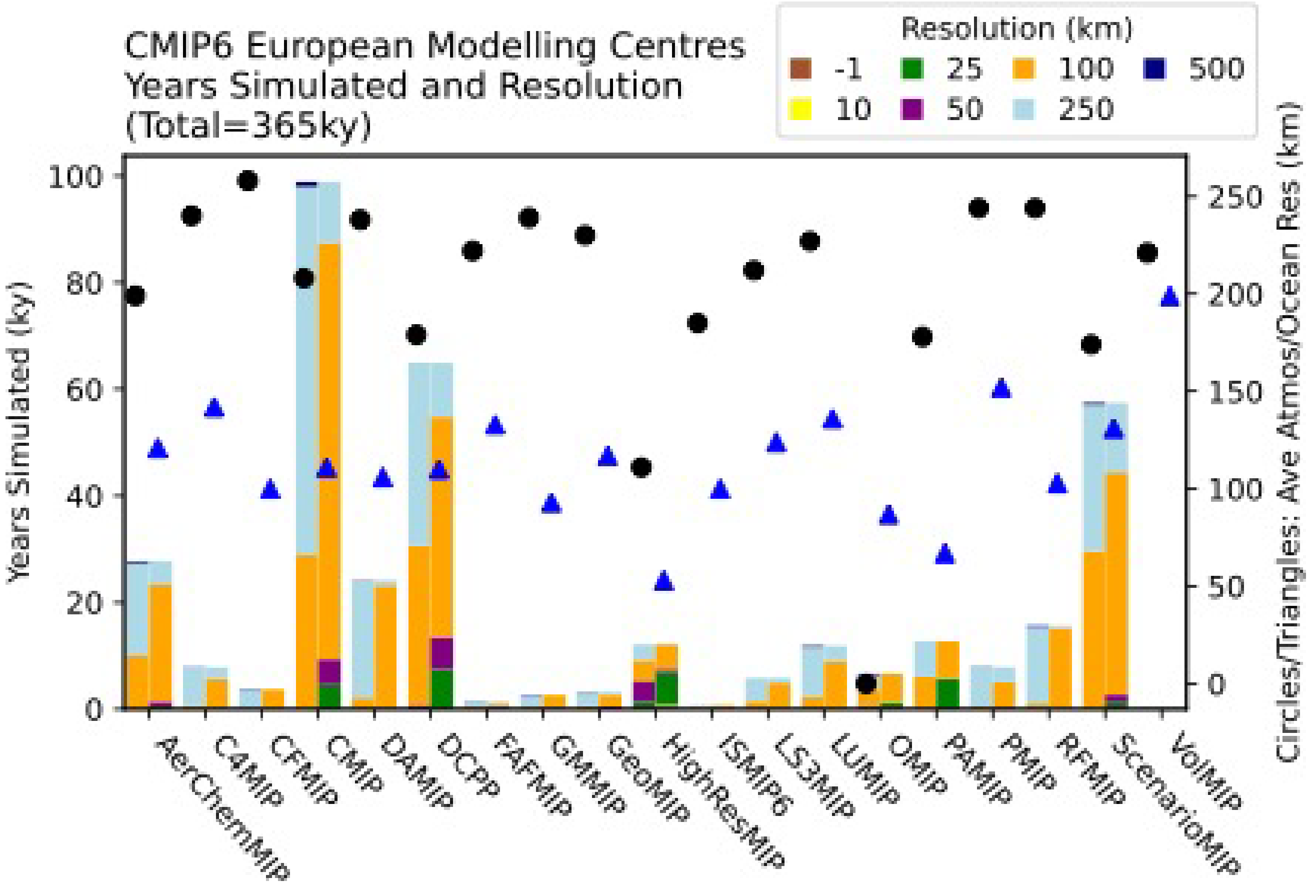
European Science

- **ESM2025, NextGEMS** (ESM & GCMs *varying* resolution) **EERIE, OptimESM** (Oceans and *variable* resolution)
- **DESTINE** (high resolution, EO etc)
- **Others:** NEMO, **SI3,** EPOC, OCEAN:ICE (*collab., obs, & duration*)

European Technical Integration: EuroHPC, Copernicus, ESA, EOSC etc

Climate Services: Portals, data products, projects (feeding operational projections?)

European contribution to CMIP6: Simulated Years

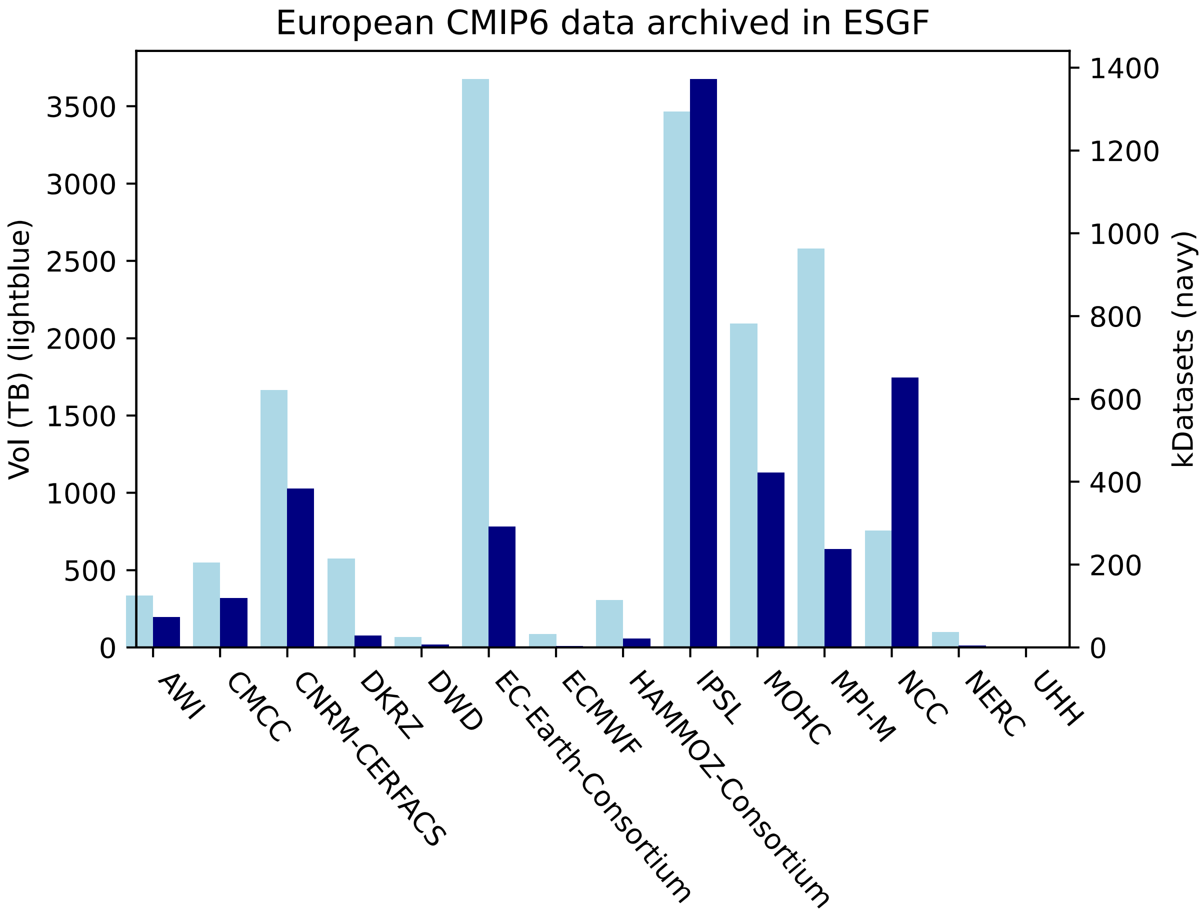


Important to realise where most of the effort has gone.

(858 kYears in all of CMIP, so Europe = 42% of CMIP simulated years. Implications for diversity!)

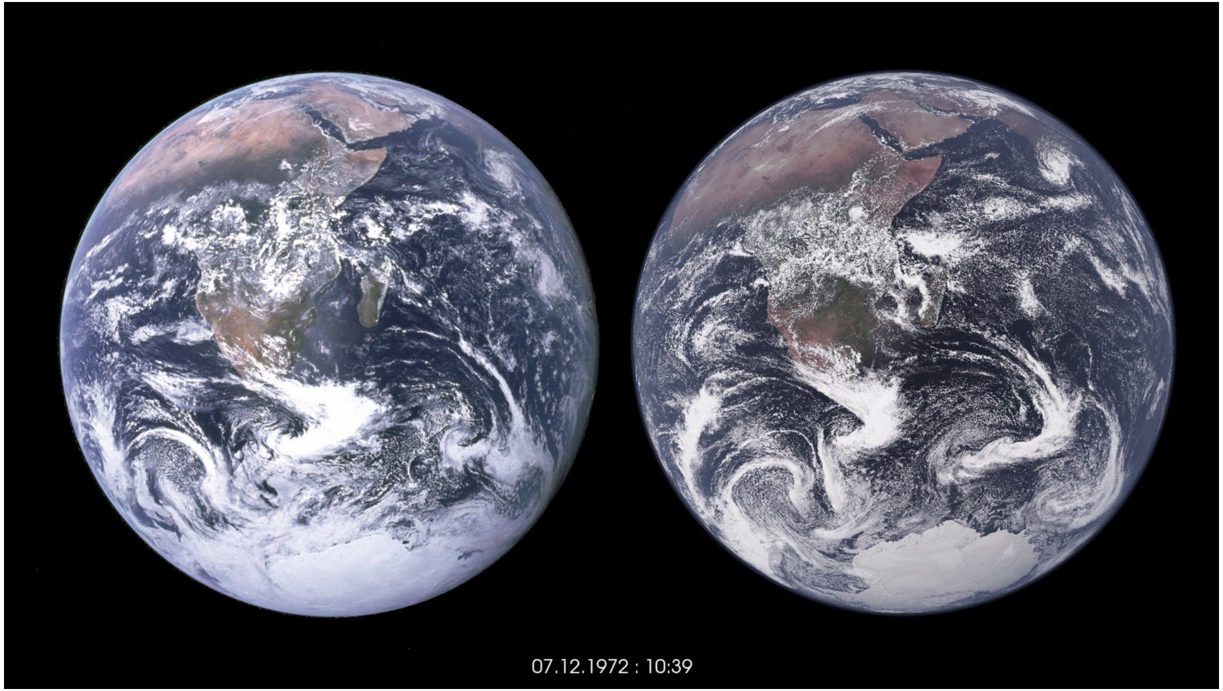
European Contribution to CMIP6: Data

Divide by two, ESGF dashboard doesn't quite do what I thought it did.



Blue Marble

- Motivation is to demonstrate capability and motivate, not (in this instance) to do science. To immerse people in what we can do!



1km ICON

NASA Apollo 17 photo left, visualization right.

Simulation is a ***forecast*** with a GCM and an ocean initialized two days before,

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The Spectrum of Climate Science

		10K Time	Spinup, Control & Millenium	Scenarios (Past, Future, Sensitivity)	Single Model Large Ensembles (SMLEs)	Decadal Prediction (Hindcasts, Forecasts)	Equilibrium /Transient Timeslices	Process Studies	Storyline Timeslices
Duration		> 1000y	o(1000)y	o(100)y		o(10)y		o(10-100)d	
Domain	ESM	x	x	x	x				
	GCM		x	x	x	x	x	x	x
	RCM			x			x	x	x
Speed (SYPD)		> 50	> 4	> 4	> 1	> 1	> 0.5	> 0.1	> 0.1
Ensemble Size		1-1000	o(1)	o(10)	10-100	o(10) x NY	o(1)	o(1)	o(1)
Atmos XY Res (km)		o(500)	100-500	25-500	50-300	25-500	1-100	1-10	1-10
Ocean XY Res (km)		300+	100-250	25-250	25-250	25-250	10+	2.5+	2.5+
Exascale Status		Currently impossible			Not currently usable				Currently some capability

The columns are meant to be indicative, but to span the things we know people are doing.
The rows are meant to show various characteristics which impact on infrastructural requirements (hardware, data production, code scalability and speed etc).

Hardware (and computing trends)

Computing Context

(Not enough time to cover all this in detail, but effectively more categories in a word salad for today)

Hardware: Compute

- **Accelerators**: Data movement, arithmetic intensity.
- **Heterogeneity:** Very different characteristics between CPU and GPU systems. Will we see FPGA in the next 10 years?
- **Memory and Storage:** Tiering, bandwidth and latency (HBM)?
- Big consequences for programmability (portability, performance, productivity).

How do we get parallelism in the absence of strong scaling? New algorithms, parallel in time?

Machine Learning

- **Emulation** of existing components, parameterisations and and resolution.
- **Developing new models** using high frequency data e.g. impact related.
- Big consequences for workflow and data handling.

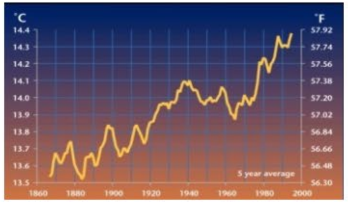
Cost

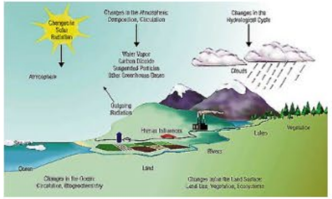
- Hardware drives us to high resolution, high cost, small ensembles. Big user communities.
- Still need CPU systems, procurement issues?
- Consideration of NetZero issues. Power source, power used.

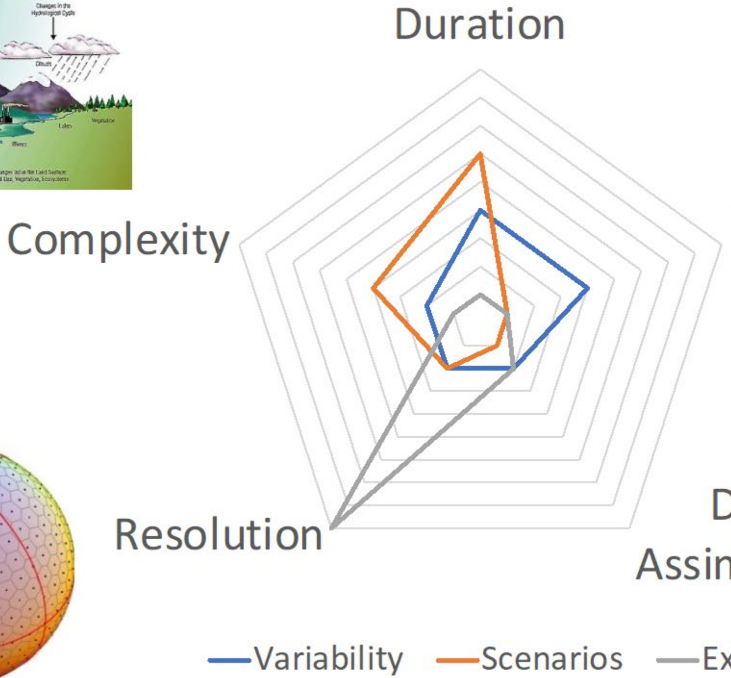
How do-we /can-we use more compute?

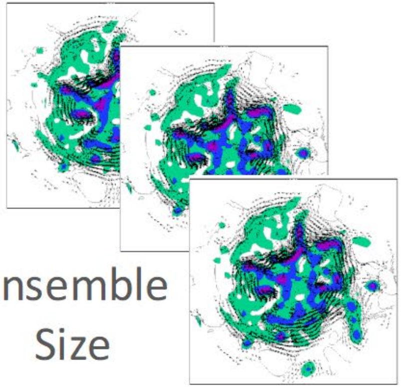
The way we think about this diagram is now wrong (if it was ever right).

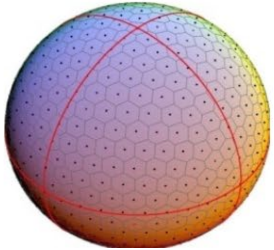
Big machines may only be usable for big ensembles OR high resolution, but not both OR feasibly, only high resolution!

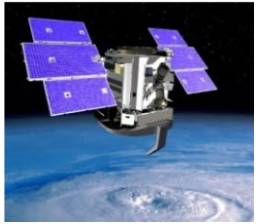






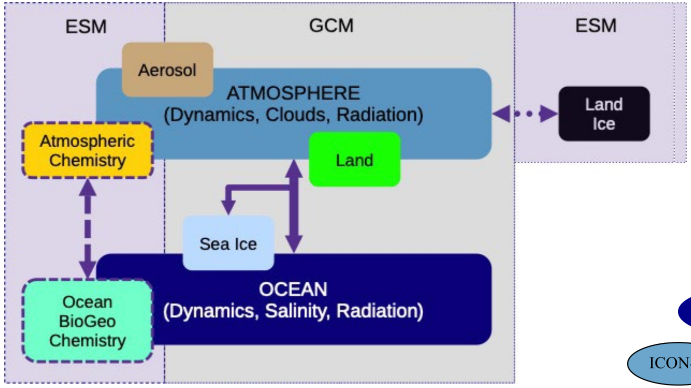




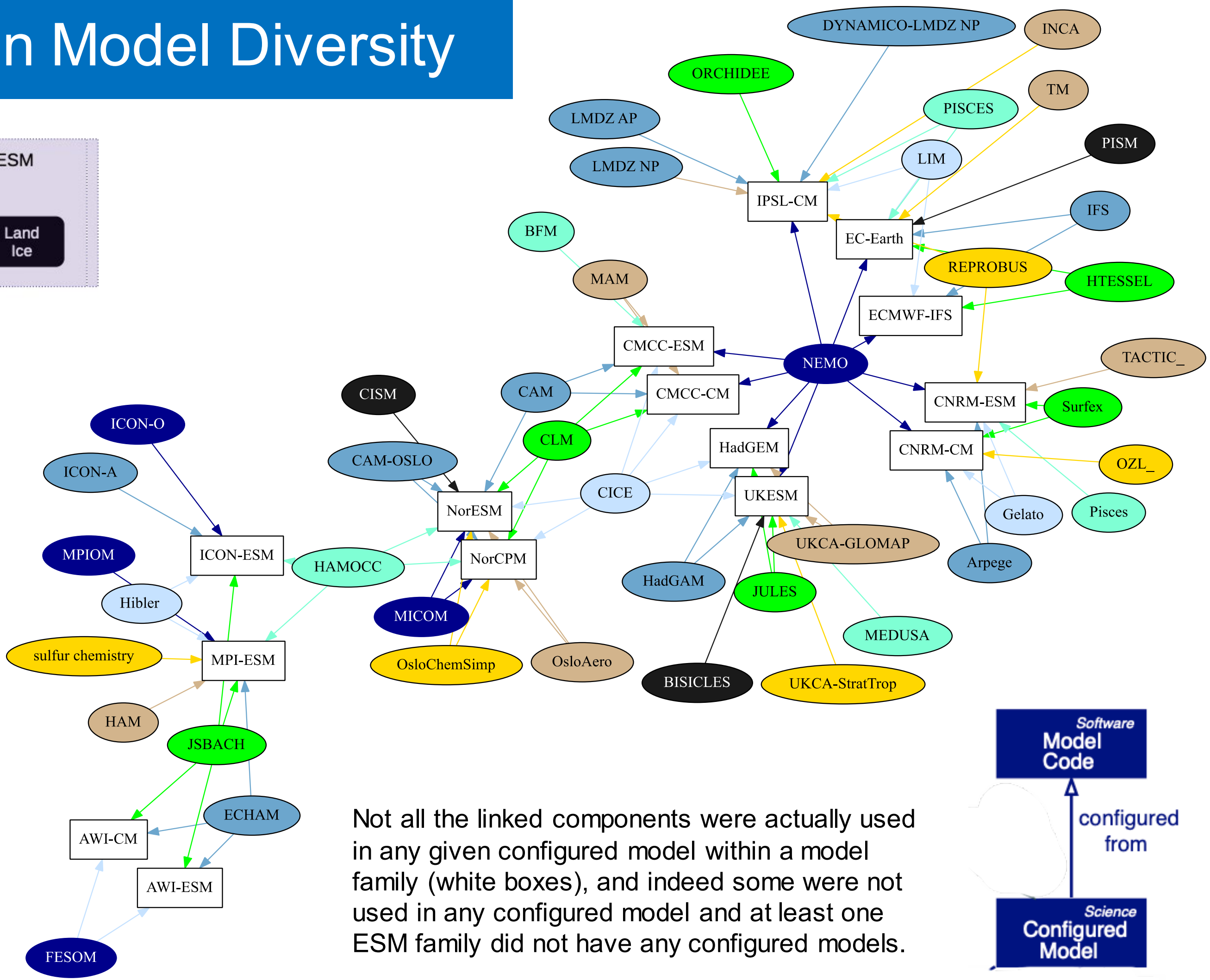


Software

European Model Diversity



The components supporting European model diversity as registered within CMIP6 `source_id` descriptions.



Not all the linked components were actually used in any given configured model within a model family (white boxes), and indeed some were not used in any configured model and at least one ESM family did not have any configured models.

Models are not just dynamical cores!

- We know quite a lot about the scalability of dynamical cores, and most of the DSL effort has been on them. But what about all those "earth system components". Lots of code, lots of short loops and if/then/else, how well will these work on GPUs? What about advection of *many* tracers?
    - Our current approach is to rewrite/port and hope. Is that really the best we can do? (No)
    - Major algorithmic rewrites.
- We already run oceans and atmospheres at different resolution. What about the other components?

- That diversity is important, but do we understand it, can we exploit it?
- How do these components differ?
- Can we pull out the physics packages and ask the same question?
- What are we doing about scale-aware physics?
- How about the same exercise for RCMs?
- Are we over-dependent on one ocean?

That was then:

- What about a new sea ice dependency?
- How will this change with next generation models?

Variable Resolution

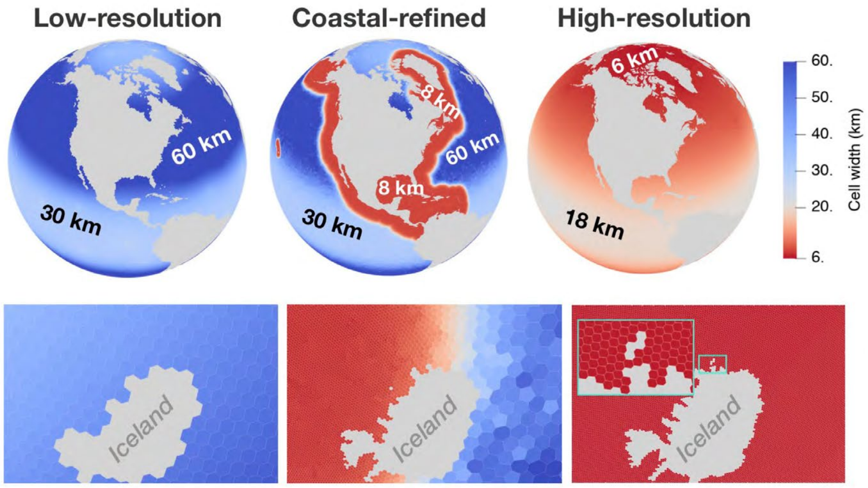
If we put resolution in the right place in the right components, we can have high resolution and ensemble sizes up to ten times larger

We can't afford to run ESM components at high resolution dynamics: so "3D" coupling for e.g. UKCA and PISCES underway in Europe.

We probably can't afford physics at the dynamics resolution (and don't really need it). CESM experimenting with physics at 5/9 atmosphere resolution.

Regional modelling can be done with stretched grids as well as embedded models with more easy two-way coupling.

Ocean models are eddy rich in some areas and not in others, and eddy scales vary with latitude and depth. Variable resolution oceans put resolution where they need it.



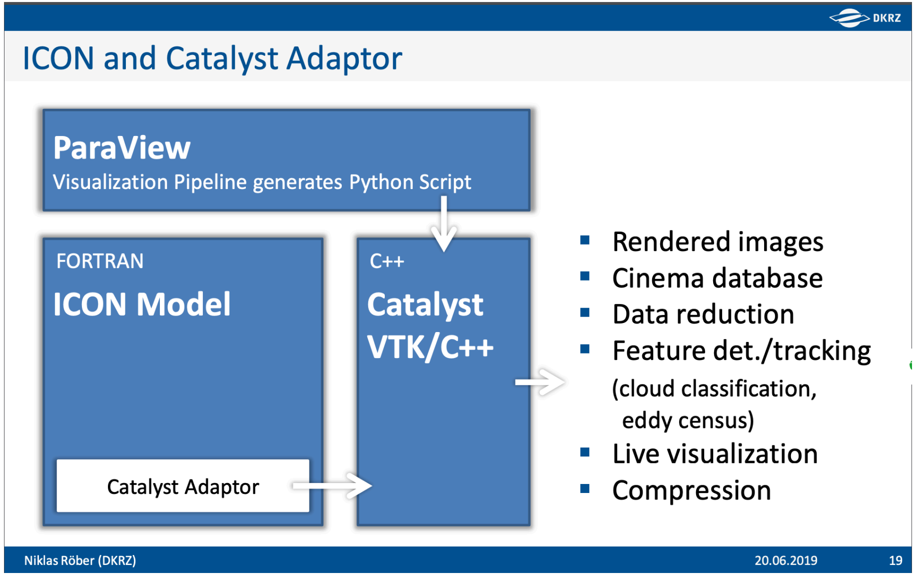
Cost: x1 x7 x66

Consequences for modellers, analysts, and analysis tool builders!

From E3SM https://e3sm.org/variable-resolution-mesh-design/

In flight data analysis and visualisation

- Many analysis tasks require high frequency high resolution data which it will be impossible to store beyond some ephemeral state during the model run.
- Visualisation, Feature Tracking, Forced Models (Hydrology, ML etc)



Röber, N., Böttinger, M., & Stevens, B. (2021). Visualization of Climate Science Simulation Data. *IEEE Computer Graphics and Applications*, *41*(1), 42–48. https://doi.org/10.1109/MCG.2020.3043987

Couplers, IO/Servers and Friends

- What would we want to say about these in terms of the next ten years?
  - Obvious things about performance, support for variable resolution grids, for easier hybrid
  - Diagnostics sub-model servers (a la XIOS roadmap)
  - Merging couplers and IO/Servers (a la XIOS roadmap)
  - Can we do better in NHSY using ESDM like approaches (XIOS is considerable overhead, is simple multi-file output simpler).
  - Role of YAC, YAXT etc?

Downscaling and CORDEX

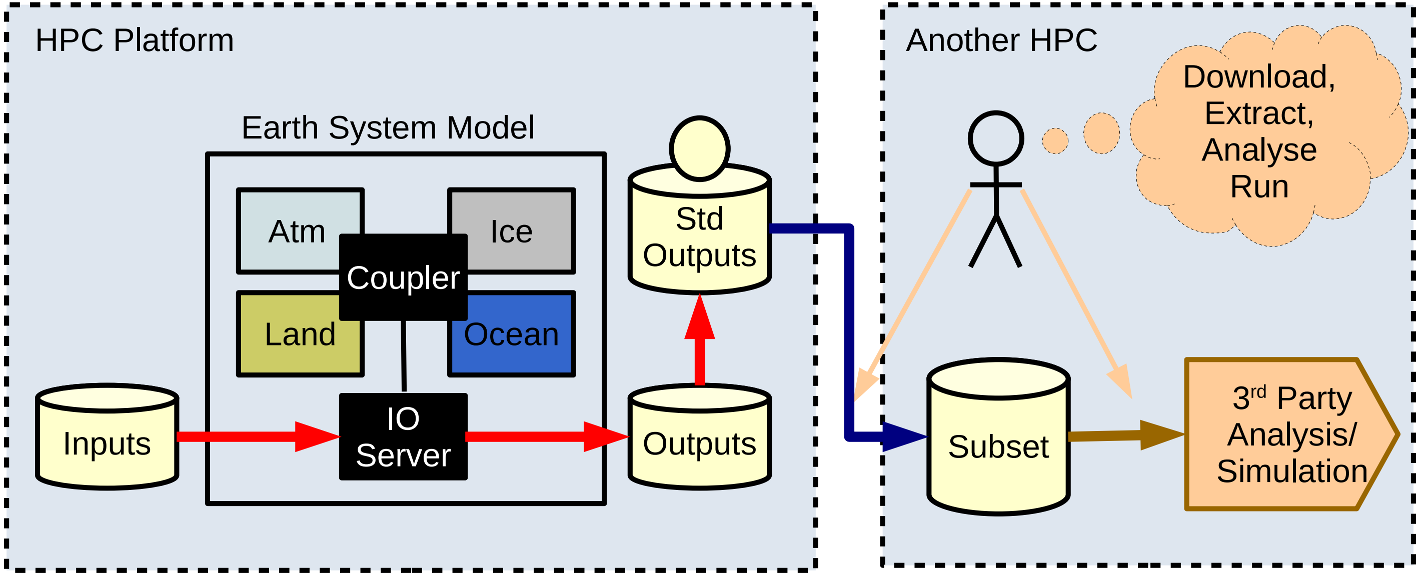
- Nearly everything said about global models applies to regional models, the only substantive difference is that they are cheaper in proportion to the domain size (for a given physics package etc).
- Is there a reason to treat RCM and CORDEX differently (in terms of strategy)?

Evaluation and Analysis

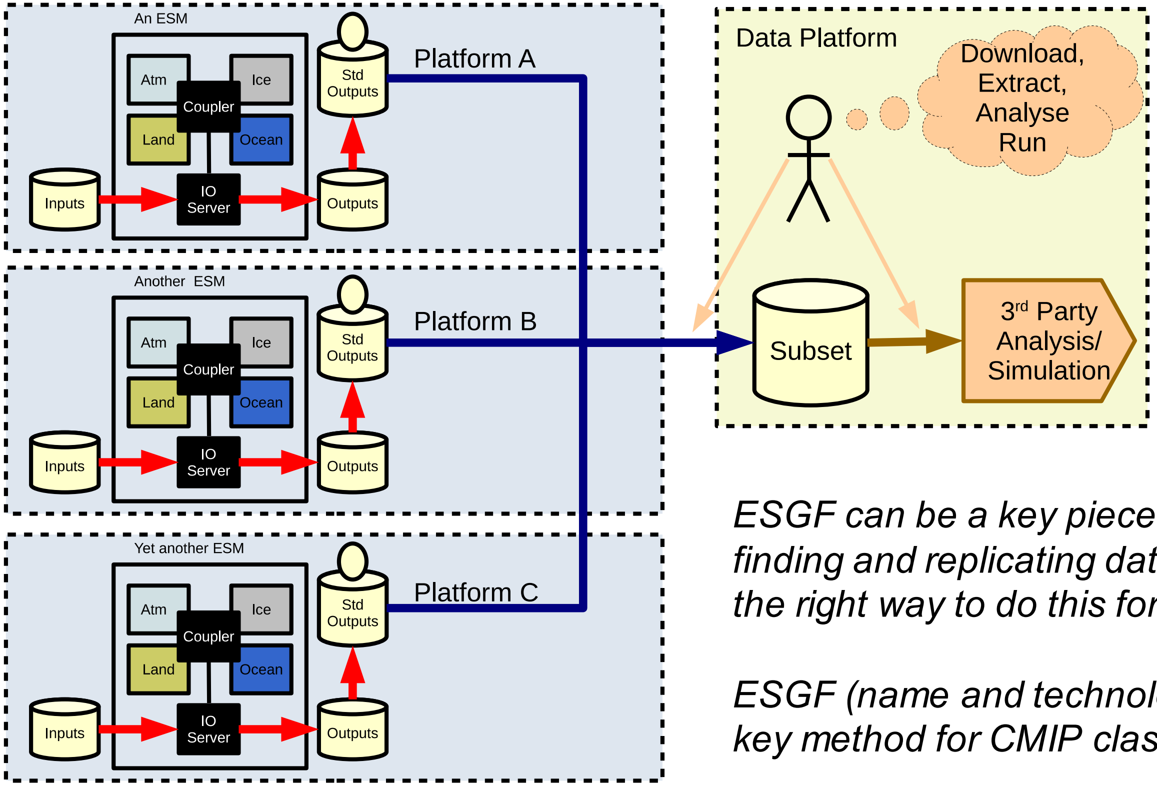
- What do we want to say about the roadmap for ESMValTool and CF Tools (I know a lot about the latter and less about the former).

Data

This mode of activity is nearly obsolete



3. Coordinated Experiment with Centralized Analysis



This is how we do CMIP data analysis, but also the key mode for big European collaborative projects. We can use the ESGF, or something else, or both.

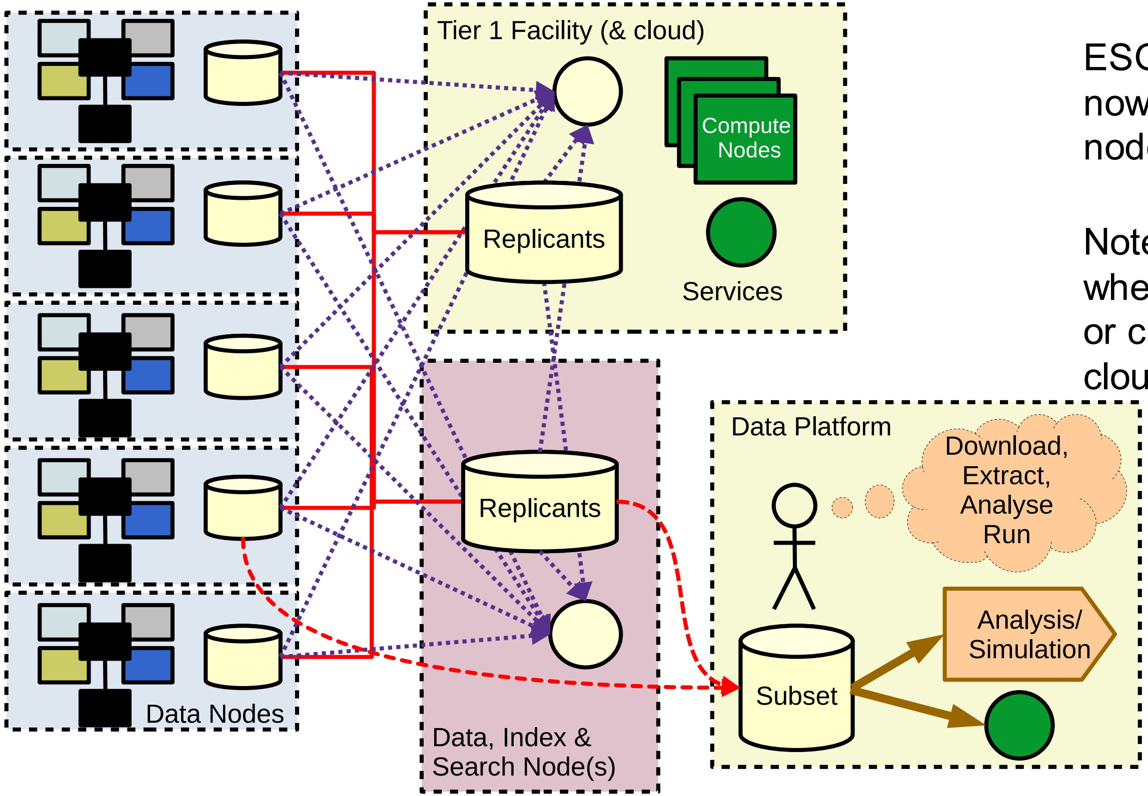
This mode will remain very important over the next decade.

ESGF can be a key piece of the story for publishing and finding and replicating data, but it is not a given that it is the right way to do this for all European activities.

ESGF (name and technology might change) will be the key method for CMIP class activities.

Why do two different things? Well, ESGF can be onerous!

A more complex (ESGF) like view



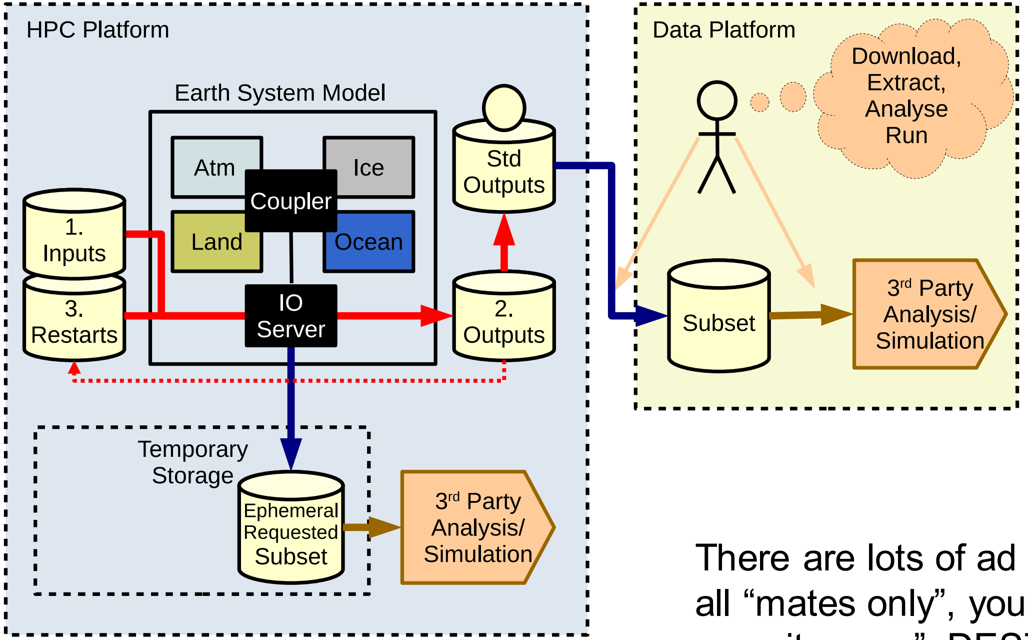
ESGF as "middleware", although we now have the concept of compute nodes and services to consider.

Note that this view is agnostic about whether the Tier 1 facility is traditional or cloudy (or utilizing pangeo on cloud).

Note also that this doesn't necessarily need ESGF to deliver the middleware but something needs to publish data (S3 or webserver) and something needs to deal with index and search.

Why do two different things? Well, ESGF can be onerous!

"In-situ analysis on ephemeral data"



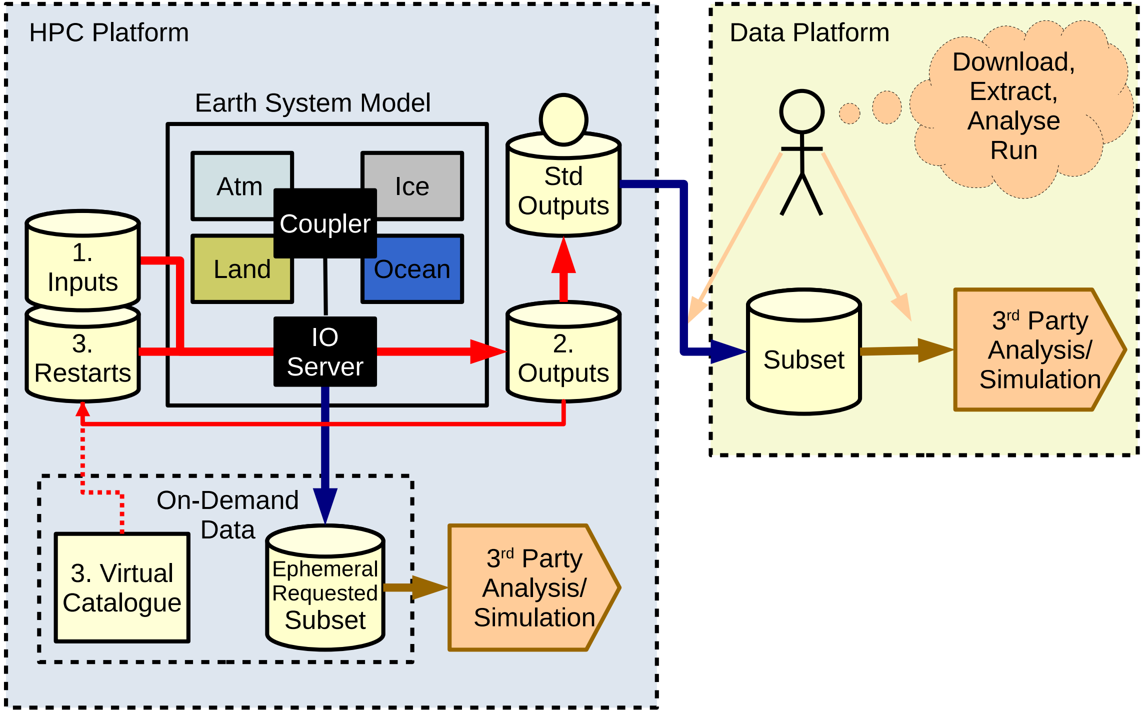
This involves publishing an experiment opportunity, and allowing "preferred" third parties to do "something" during the model execution using "extra" data.

Examples: hydrological model using high frequency data, visualization, tracking cyclones etc.

Could also be an ensemble being analysed "in-flight".

There are lots of ad hoc solutions to this building up, but it's all "mates only", you have to be "in the know" and "in the security zone". DESTINE might change this, but any kind of democratization will depend on standards/conventions for publishing experiments and data requests, for workflow, and for data formats. Sound familiar?

A variant of ephemeral data: virtual data

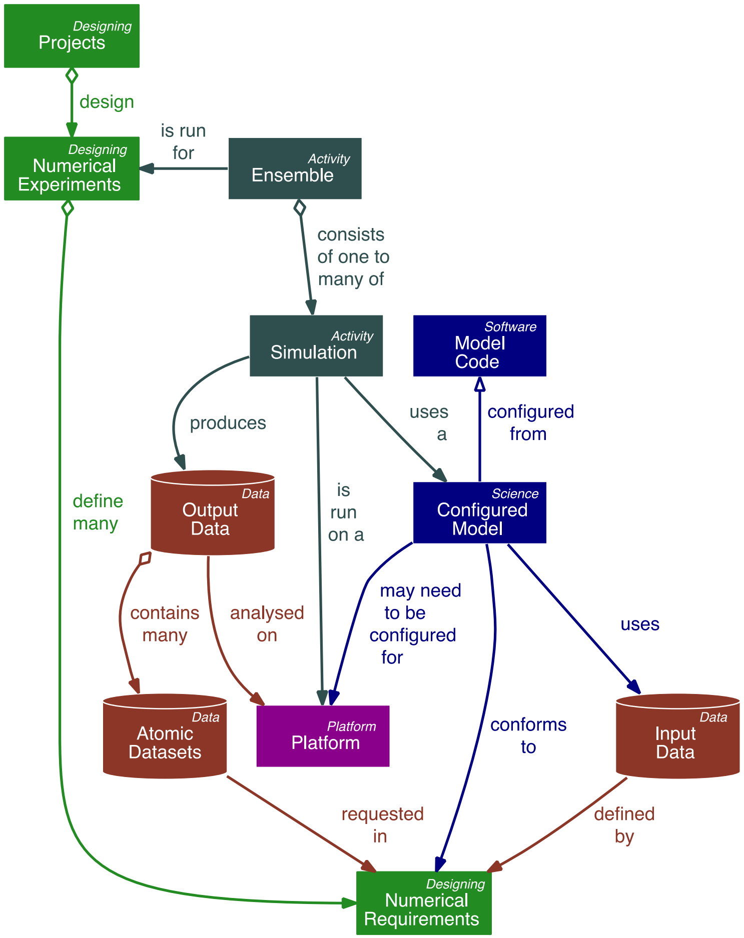


Doesn't need so much a priori knowledge that an experiment will be run, but will have interesting issues for allocating effort and HPC workload management and security.

I think this can only work if we get the previous example working well.

Documentation and Provenance

Simulation



- Experiment documentation concepts working well, tooling needs to take the human out of the loop (Charlotte can't do everything).
- Simulation and Ensemble documentation is not working well. Hard to find out r1i1f1 info, and errata and citation not well linked together.
- Software documentation needs work, both for configured models (where our science specialization may not be fit for purpose) and for the underlying model code.
- The workflow around the data request needs clarity.
- Platform information is hard to get (needs to be part of model runtime workflow)
- Output needs to be fully CF compliant, and CMORisation needs to be less feared.
- Atomic datasets and catalogiing needs to be integrated between the various places it is is done (ESGF, pangeo, data centres, desktops)

Analysis, Errata, and Provenance

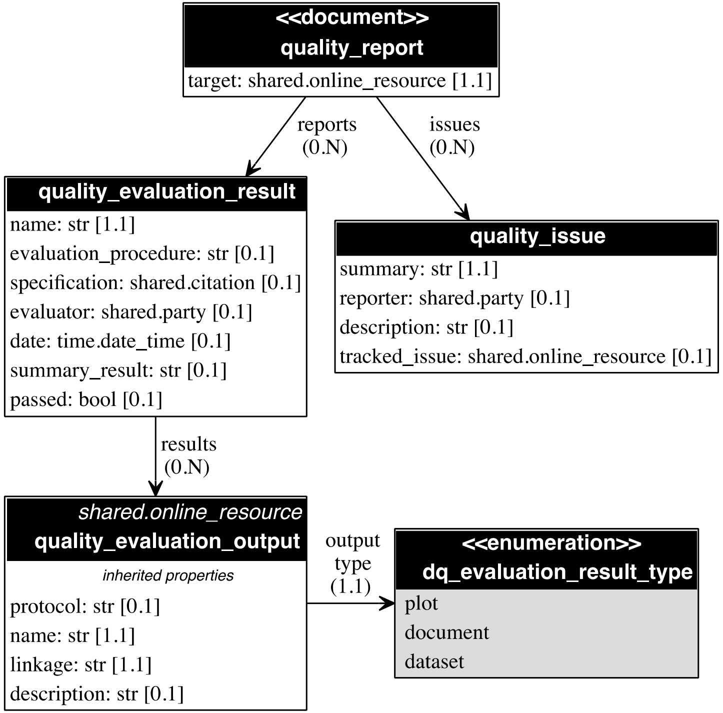
In analysis we are interested in the scientific quality of simulation output which means we need to describe the **inputs**, the analysis **method** itself and **the results**.

This can generate errata and useful information for downstream users, but these ideas implementations and artifacts are not linked between ESGF< ESMValTool, Errata, and es-doc.

ESMValTool provides methods for provenance capture, but is not linked to the citation service.

We have most of the pieces, but they are not easily usable and discoverable, even by and within the physical modelling community.

Integration rather than new functionality?



Integration depends on semantic content, not just services, and certainly not just formats.

People

People and networking

- I haven't written this, but the input we have from (primarily) science leads is mixed. Some have no problem (they say) with recruitment and retention? Is that true? If so for which subdisciplines?

Recommendations – 2017 and 2023

1) **On models**: Support common development and sharing of software and accelerate the preparation for exascale computing by exploiting next generation hardware and developing appropriate algorithms, software infrastructures, and workflows.

2) **On HPC**: Exploit a blend of national and European high-performance facilities to support current and next generation science and work toward obtaining sustained access to world-class resources and next generation architectures.

3) **On model data:** Evolve towards a sustained data infrastructure providing data that are easily available, well-documented and quality assured, and further invest in research into data standards, workflow, high performance data management and analytics.

4) **On physical network:** Work to maximize the bandwidth between the major European climate data and compute facilities and ensure that documentation and guidance on tools and local network setup are available to users.

5) **On people:** Grow the numbers of skilled scientists and software engineers in the ENES community, increase opportunities for training at all levels, and strengthen networking between software engineers.

6) **On model evaluation (new):** Enhance sharing of common open source diagnostics and model evaluation tools, implement governance procedures, and expand data infrastructure to include computational resources needed for more systematic evaluation of model output.

7) **On infrastructure sustainability (new):** Sustain the cooperation necessary to develop future model and data technology and support international reference experiments programmes, and strengthen collaboration with other European actors providing services to, or using services from, ENES.

Extensions:

- On Models: Model the models. How do we expect these models to work on GPU systems, on CPU systems with HBM? What are the likely constraints? Let's not just port and hope!
- On Models: Investigate and deploy variable resolution and invest even more in parallel in time techniques.
- On HPC: Define blend as a need for both CPU and GPU systems and HBM.
- On Machine Learning: There are opportunities we need to investigate.
- On Documentation: Lift our game!
- On People: Examine assumptions around requirements and careers.
- On Evaluation: ?
- On internal infrastructure: ?
- On Sustainability: Seek further opportunities for relationships that do not depend on altruism.

Simulation

- Huge spectrum of “large-scale” climate science.
- We know we need exascale computing for the “right hand problem” (resolution).
- We suspect we can’t use exascale computing efficiently for the “left hand problem” (low resolution, long-time)
- In the middle we have a problem – we might be able to efficiently use exascale computing, but we don’t know how:
    - It’s not just about porting/rewriting code, will it have the necessary arithmetic intensity?
    - Do we have the bodies to do it?
    - There are a lot components. But it’s hard to argue that there are are too many. Too few shared oceans?
    - What is the right amount of shared infrastructure?
    - Domain Specific Languages may be an important tool, but they are not a panacea.
- Variable resolution will become more prevalent
- Machine Learning
    - Might have a big role to play, and that affects the hardware requirements.,
- Cloud Computing
    - (Is a red herring)
    - New interfaces to data, new workflow requirements.

Analysis

- Lots of different analysis modes to support, all of which generate requirements for standards (or conventions) for data, vocabularies, and interfaces.
  - The clean distinction between the workflow for simulation and analysis is going to break which has implications!
  - Variable resolution grids will introduce new requirements for tools and standards and descriptions.
- Data lives a long time, and analysis communities need to know the provenance of simulation data, which is not the same as the provenance of analysis products.
  - We are still not in the sweet spot for model documentation.
- Data infrastructure is moving much faster than simulation infrastructure and more people are using the data infrastructure: which means we need even more software engineers to keep up.
  - The advent of cloud and pangeo don't change the pain points as much as some might think. At scale *managing* data is the *foundational* problem.
- Shared analysis tools are important.
  - ESMValTool will continue to evolve as will lower level tools like CDO and CF-Python.

People

- Hiring smart people remains hard. Keeping smart people remains hard, especially when they can get paid much more elsewhere.
  - In some countries this is more problematic than others. Issue in include salaries, precarity and responsibility (is there a career structure to keep software engineers? Can individuals chop an change between “science” and “infrastructure”?)
  - Luckily we have interesting problems.
- More?

Services

- What are the shared large-scale services?
  - (Yes, this is overlaps with our sustainability, but what do we want to summarise here?)

Recommendations

- We really don’t know how we are going to exploit accelerated computing for ESM models, its’ not enough to say “rewrite your code” the code itself does not necessarily provide the necessary arithmetic intensity. We need to do some “performance modelling” before we do wholesale rewriting (with or without DSLs). Work done thus far is bespoke and/or not shared.
- We will need CPU systems for the foreseeable future.
- We need to work harder on parallel in time and on exploiting variable resolution.
- We need to invest in all the systems around “exploiting ephemeral data”.
- Whatever happens with the CMIP/not-CMIP arguments, the data handling problems are very similar, and don’t change as much as some would say, unless the simulations are “for small communities”.
    - It would be good to maintain a separation of concerns between analysis tools, catalog tools and the infrastructure services (e.g. put it the cloud not a recommendation).

… next steps