

# Digital Twin Thinking for HPC in Weather and Climate

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## Outline

### Digital Twins

Definitions

Interventions

### Promises

Weather and Climate

Choices

### Existing Practice

Increasing Collaboration

### A new world?

ESM-Twins

### Summary

## Digital Twins

### What is a digital twin? Google says”

- ▶ “A digital twin is a digital representation of a physical object, process or service. ... A digital twin is, in essence, a computer program that uses real world data to create simulations that can predict how a product or process will perform.”

You would be forgiven for thinking that sounds rather like what we call a model!

**Destination Earth** defines a digital twins as

- ▶ “mirrors of reality, simulators that replicate reality constrained by **real time data.**”

You would be forgiven for thinking that sounds like data assimilation.

We have been doing digital twins for a long  
time!

## Information Intervention?

Some<sup>1</sup> have postulated a “leap in information intervention” as part of delivering weather and climate digital twins. What could this mean?

- ▶ *“the challenge will be to design a digital twin that allows users to intervene, extract information and influence the system trajectory across time and space, as done — albeit often unwittingly — in the real world.”*
- ▶ *“tasks like simulations, ..., post-processing ...are ...executed on federated computing infrastructures, feed data into virtual data repositories with **standardized metadata**, and from which a heavily ML-based toolkit extracts information that can be manipulated in any possible way.”*
- ▶ *“We can literally grab the earth, anyone, and see what the consequences of their actions mean for how things will evolve, what if ...”*
  - ▶ (We have to put “their actions” into our model, whether that is an a representation of agricultural policy (a model) or some other process or action.)

<sup>1</sup> Quotes from Bjorn Stevens SC20 talk and Bauer et al “A digital twin of Earth for the green transition”.

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- ▶ *“the challenge will be to design a digital twin that can intervene, extract information and influence the system in real time and space, as done — albeit often unwittingly — in the real world”*
- ▶ *“tasks like simulations, ..., post-processing ... a federated computing infrastructures, feed data into data repositories with **standardized metadata**, and for ML-based toolkit extracts information that can be used in a possible way.”*
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**Computational Steering**

**Data mgmnt. & workflow engines**  
to allow (arbitrary?) post-processing.

**Embedding and/or coupling**  
(arbitrary?) models in workflow.

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## Weather and Climate Digital Twins?

“predict how a product or process will perform”  
maybe

“project a set ( $Y$ ) of possible futures and how they interact with  $X$ ”  
( $X$  = a **set** of possible societally relevant systems/actions etc)

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Leads to Two Key Promises:

### Scenario Evaluation

If we do this, then what?  
Typically being expressed in terms of climate, even if the interest is in high impact weather.

### Democratising Access

Going beyond data access, so that those interested in  $X$  can exploit the twin in some new ways.

## Implementation?

Leads to some questions:

1. What do we mean by scenarios? (Who decides and defines the  $Y$  scenarios? How does the  $X$  community interact with the decision and definition?)
2. What do we mean by “going beyond” and “data access” to deliver  $X$  (and for whom, “democracy” is a very inclusive word?)
3. How is this different from existing practice?



## Abstract Practicalities

### Assumptions:

1. At scale, scenarios will be hierarchical: from a small set of expensive simulations  $Y$  we can investigate  $X$  different application scenarios. We might think of  $X$  as applications.
2. To be meaningfully different from existing practice the implementation of “going beyond data access” for  $X$  must be real.
3.  $X$  involves running additional code and or changing parameters/inputs for the code running  $Y$ .
4. True computational steering of  $Y$  can only be done by a very small number of “users” (possibly as few as one).
5. Recomputation of  $Y$  scenarios is not generally affordable to support arbitrary  $X$  (next slide)

## To compute or re-compute?

- ▶ The IPSL contribution to CMIP6 simulated  $\mathcal{O}(50\text{K})$  “useful” years (and  $\mathcal{O}(150\text{K})$  years overall), and in doing so consumed  $\mathcal{O}(6)$  TJ, and stored  $\mathcal{O}(1)$  PB of data for ongoing analysis.<sup>1</sup>
  - ▶  $\Rightarrow$  making 1 PB of useful data cost 2TJ
- ▶ JASMIN currently has  $\mathcal{O}(50)$  PB of spinning disk and consumes under  $250\text{kW}^2$ 
  - ▶  $\Rightarrow$  storing 1 PB of useful data for a year costs 0.16TJ

But

- ▶ We might argue that costs for compute will fall faster than for (spinning disk) storage.
- ▶ We might then argue that will only happen until we make more use of SSD, then compute and storage will fall in tandem?
- ▶ ...and then there is tape. Near zero energy cost when at rest!

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<sup>1</sup>Rounded from figures compiled by IS-ENES3 and reported by M. ACosta at the IS-ENES3 General Assembly, March 2020

<sup>2</sup>Not including cooling, but including a 10K core CPU batch cluster.

## To compute or re-compute?

- ▶ The IPSL contribution to CMIP6 simulated  $\approx 50K$  “useful” years (and  $\approx 150K$  in doing so consumed  $\approx 6$  TJ, and stored  $\approx 100$  PB of data for ongoing analysis.<sup>1</sup>

▶ =>

- ▶ JASMIN under 2000 cores spinning disk and consumes

▶ =>

for a year costs  $0.16TJ$

But

- ▶ We might think compute will fall faster than for (spinning disk)

- ▶ We might think that will happen until we make more use of SSD, then compute and storage will fall in tandem?

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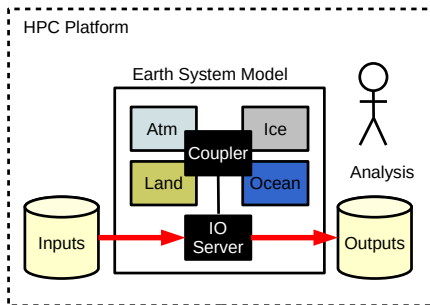
More caveats: We can do better by looking at specific runs not big bulk averages. We need to understand usage patterns.

**Currently vastly cheaper to store for re-use than re-compute and likely to remain so.**

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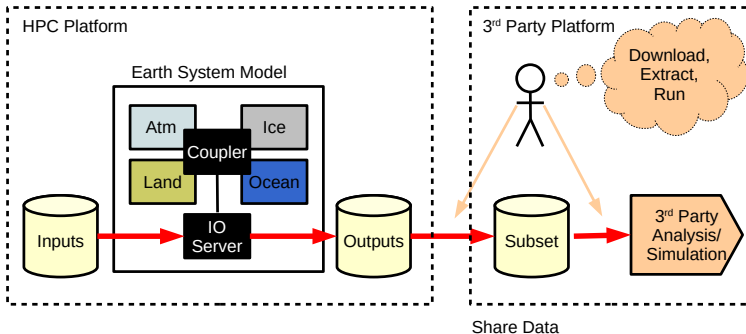
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## Phase 1: Individuals and Groups.



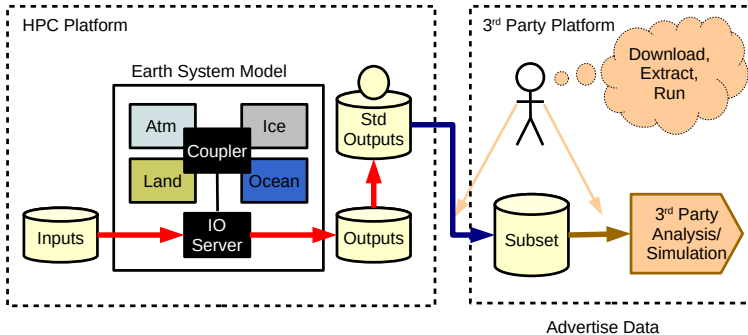
- ▶ All parties are well known to each other and communicate using personal contact.
- ▶ Often relatively inexpensive. Much re-running of simulations.
- ▶ Experiment definitions may or may not be well understood by all parties. Simulator are authors.

## Phase 2: Collaborating with your mates. Multiple groups running same simulations



- ▶ Sharing files “as is”, with ad-hoc information systems (e.g wikis)
- ▶ Considerable overheads for data consumers (unfamiliar formats, documentation etc).
- ▶ Experiment definitions may or may not be well understood by all parties. Simulators are authors.

## Phase 3: Collaboration at a distance (in time and space). Multiple groups ...

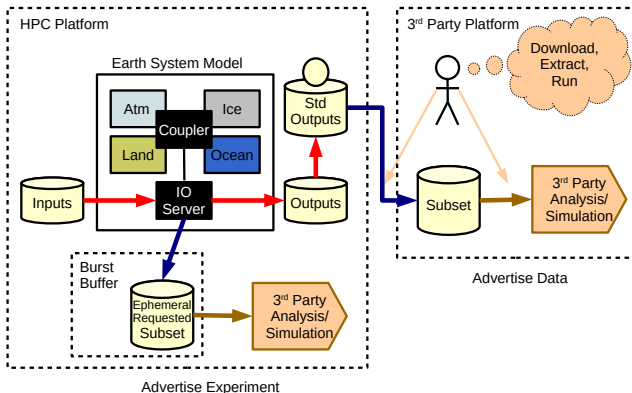


- ▶ Data producers and data consumers groups are not (well) known to each other.
- ▶ Standardised data files are described using machine readable catalogs and shared using standard protocols. Significant overheads in production to reduce friction in consumption.
- ▶ Experiment definitions may or may not be well understood by all parties, but simulators generally not authors.

# From an ESM to a Digital Twin - A simple vision

## A vision for Digital Twin Model Systems

- ▶ Important distinction between **coupled** components and **forced** components.
- ▶ Coupled components exchange data in memory.
- ▶ Forced components change data via (fast) disk.
- ▶ Forced components run in parallel via scheduler using **ephemeral** data.



- ▶ Note importance of Data Standards for both routes!

- ▶ Community have to agree on the experiment that is run so that not only those running the ESM itself, but those exploiting **both** the ephemeral and standard data have what they need and understand the simulation context.
- ▶ Standard data goes to data lakes.

## Implications - Part 1

- ▶ There is a technical route to split notions of  $X$  and  $Y$  around  $X$  being forced by  $Y$ .
- ▶ Definitions of  $Y$  need to be well promulgated (“Advertise Experiments”).
  - ▶ But  $X$  community may still want to interact around definitions of  $Y$ .
- ▶ Coupling models is “business as usual”, we worry about performance, portability, productivity as we always have.
- ▶ Higher frequency and/or higher resolution data can be available for a shorter time than standard outputs on high performance storage.
  - ▶ The group of users will likely still need standardised data interfaces, but are more likely to be like the phase 1/2 community.
  - ▶ The more democratic this is, the more they may need their own analysis environments.
  - ▶ Community of third party simulators using forcing data; will need HPC access and resources.

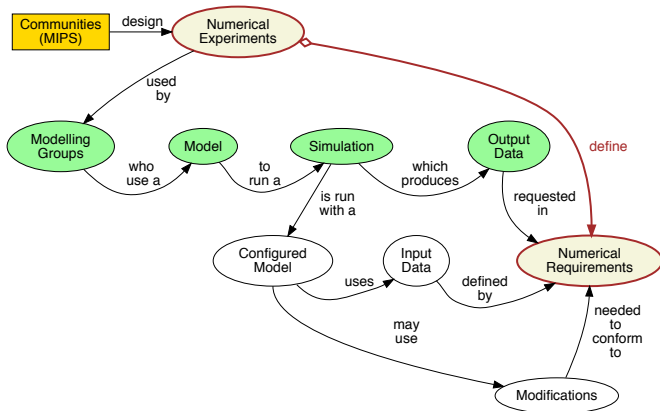


## Implications - Part 2

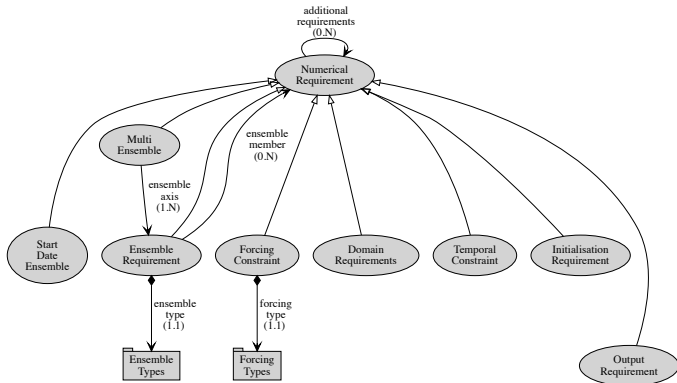
- ▶ Interaction between scheduler, burst buffer and third party simulations needs thinking about.
  - ▶ Existing HPC concepts all about “job control”, but we might need to think a bit more about pub/sub (both interfaces and “opportunity advertisement”).
  - ▶ Those running  $Y$  may not be in a position to consider resourcing all  $X$  (or even desire to do so, nor in a position to evaluate the cost or value of  $X$  ...if  $X$  is related to human behaviour it might involve very large numbers of small simulations.)
- ▶ Increasing role for virtualisation on HPC platform, to support third party computational environments. Containers not a luxury, a core service!
- ▶ Third party analysis environments can be very different technically than core simulation environments (a la <https://jasmin.ac.uk>).

## On Advertising Experiments

Simulations are complex:



## Communities need to agree on requirements



Some of these requirements will be generated by “privileged”  $X$  communities, but all  $X$  communities need to understand what has been done and why.

See Pascoe et.al (2020):<https://doi.org/10.5194/gmd-13-2149-2020>.

## Summary

- ▶ Weather and Climate has a lot of experience with Digital Twinning.
- ▶ ...but we have made promises about increased potential for “user intervention”.
- ▶ We cannot afford to recompute or save everything.
- ▶ A practical route to increasing user intervention involves providing access to ephemeral data as well as more traditional data sharing.
- ▶ Ephemeral data can be used for more detailed analysis and chaining further simulation, but
- ▶ We may need to think quite hard about making that possible for others “beyond your mates”. Implications for scheduling, new ideas (for HPC) about pub/sub job connection etc.