
# Porting OptClim Optimisation system to ARCHER2

## Session will begin at 15:00

archer2 epcc safe THE UNIVERSITY OF EDINBURGH

# Porting OptClim Optimisation system to ARCHER2

ARCHER2-eCSE04-07

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and acknowledging help from ARCHER2 and NCAS support

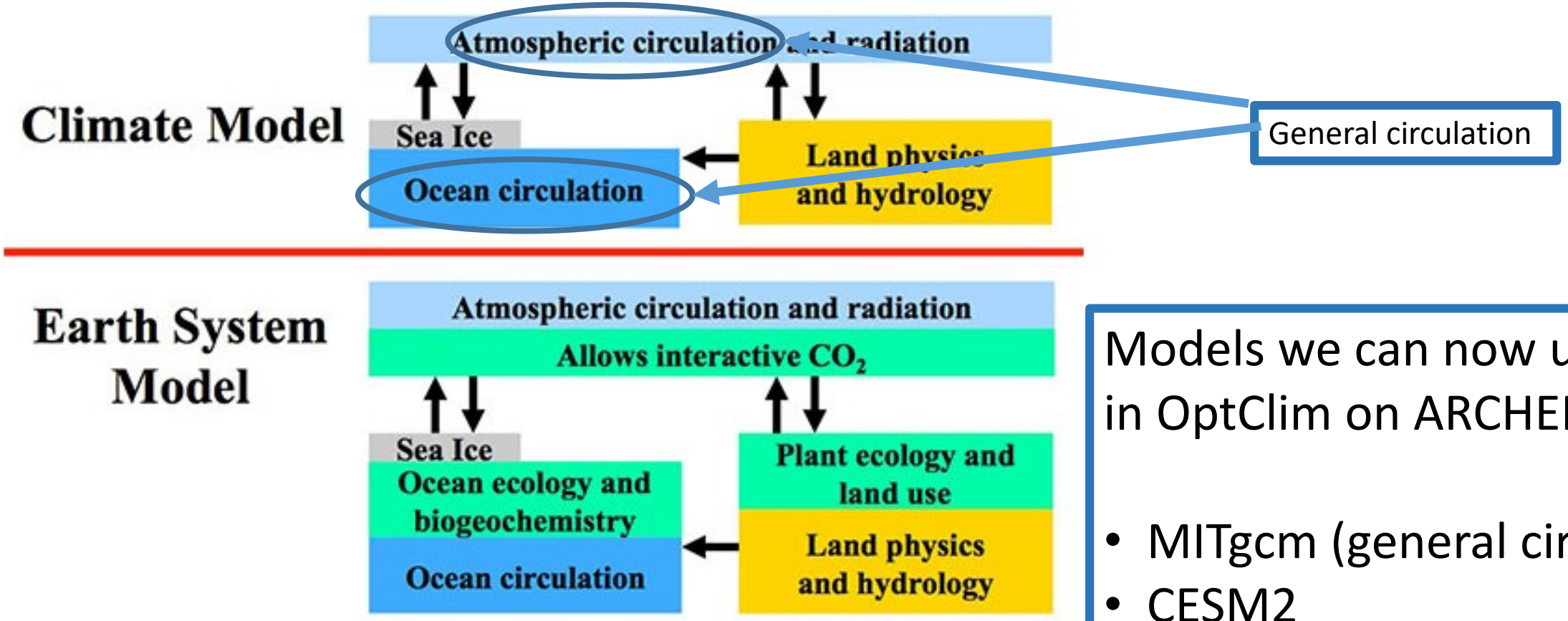
# Porting OptClim Optimisation system to ARCHER2

## Outline of talk

"Optimisation": NOT to go faster – but to better represent reality

- Earth system models
- Concepts of OptClim and of Particle Filtering
- OptClim on ARCHER2 for 3 models
- Particle Filtering on ARCHER2
- Orient potential users.

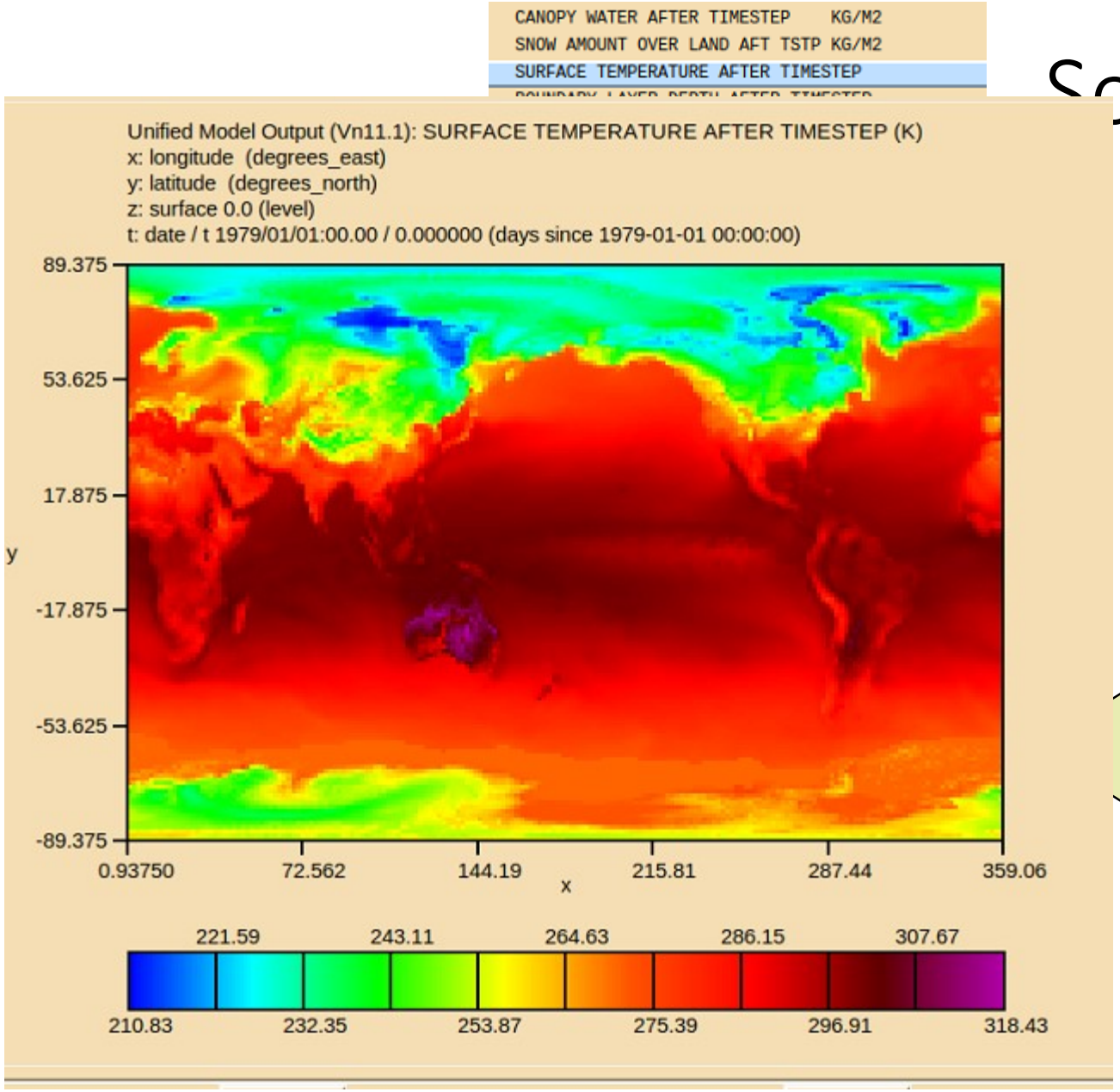
# An Earth System Model (ESM) closes the carbon cycle




Models we can now use in OptClim on ARCHER2:

- MITgcm (general circulation)
- CESM2
- UKESM-1

https://soccom.princeton.edu/content/what-earth-system-model-esm




# Schematic of a model

Initial state

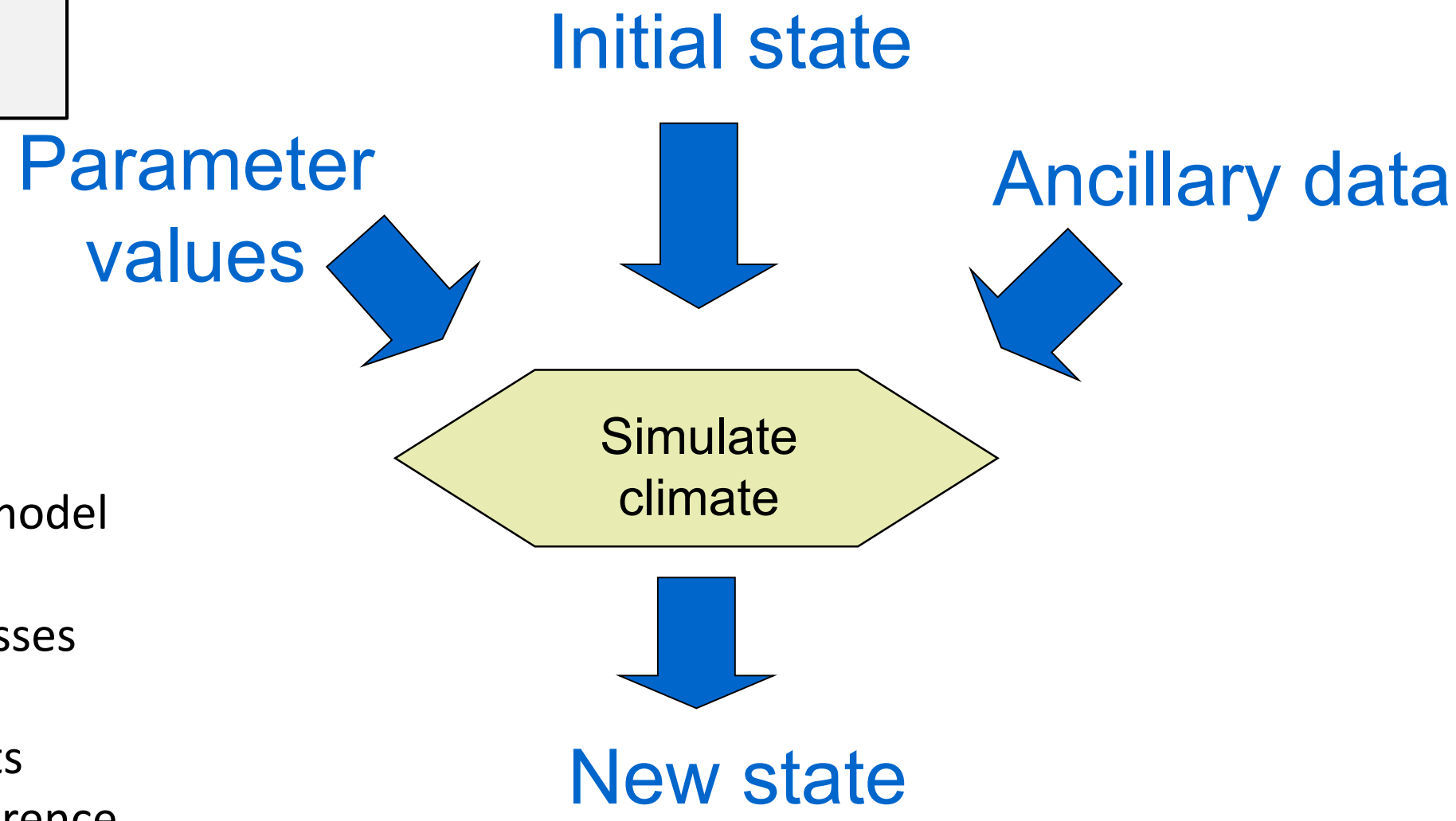
Ancillary data

Simulate climate

New state

# Schematic of a model

```
....
CT=5.0e-05
ENTCOEFF=1.87
.....
```




Typical use:

- Copy a reference model
- Change some parameters/processes
- Run simulation
- Post process results
- Compare with reference

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# Responding to uncertainties in models

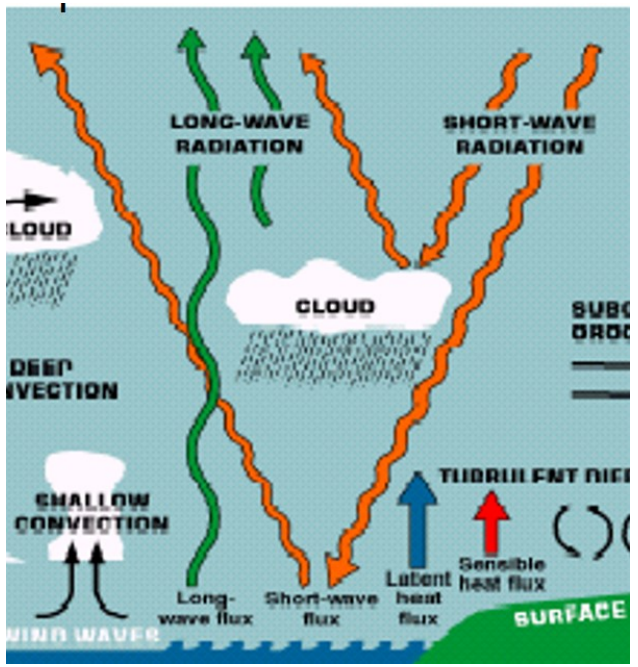
- Parametrised processes

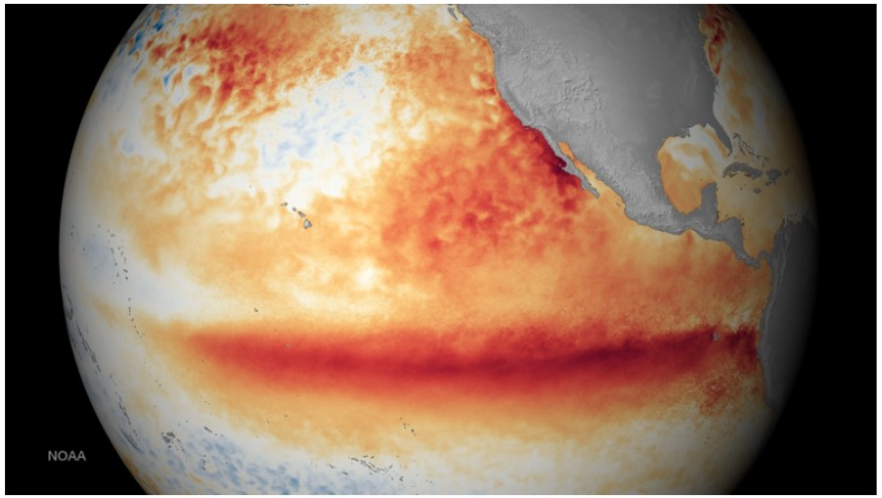
OptClim: find parameter values that best fit observation.

- Imperfect tracking of historical time-series with systematic change

Particle filtering, based on an ensemble of simulations

From Kevin Trenberth, NCAR




Credit: [NOAA National Environmental Satellite, Data, and Information Service (NESDIS)]

# What's different about these models?

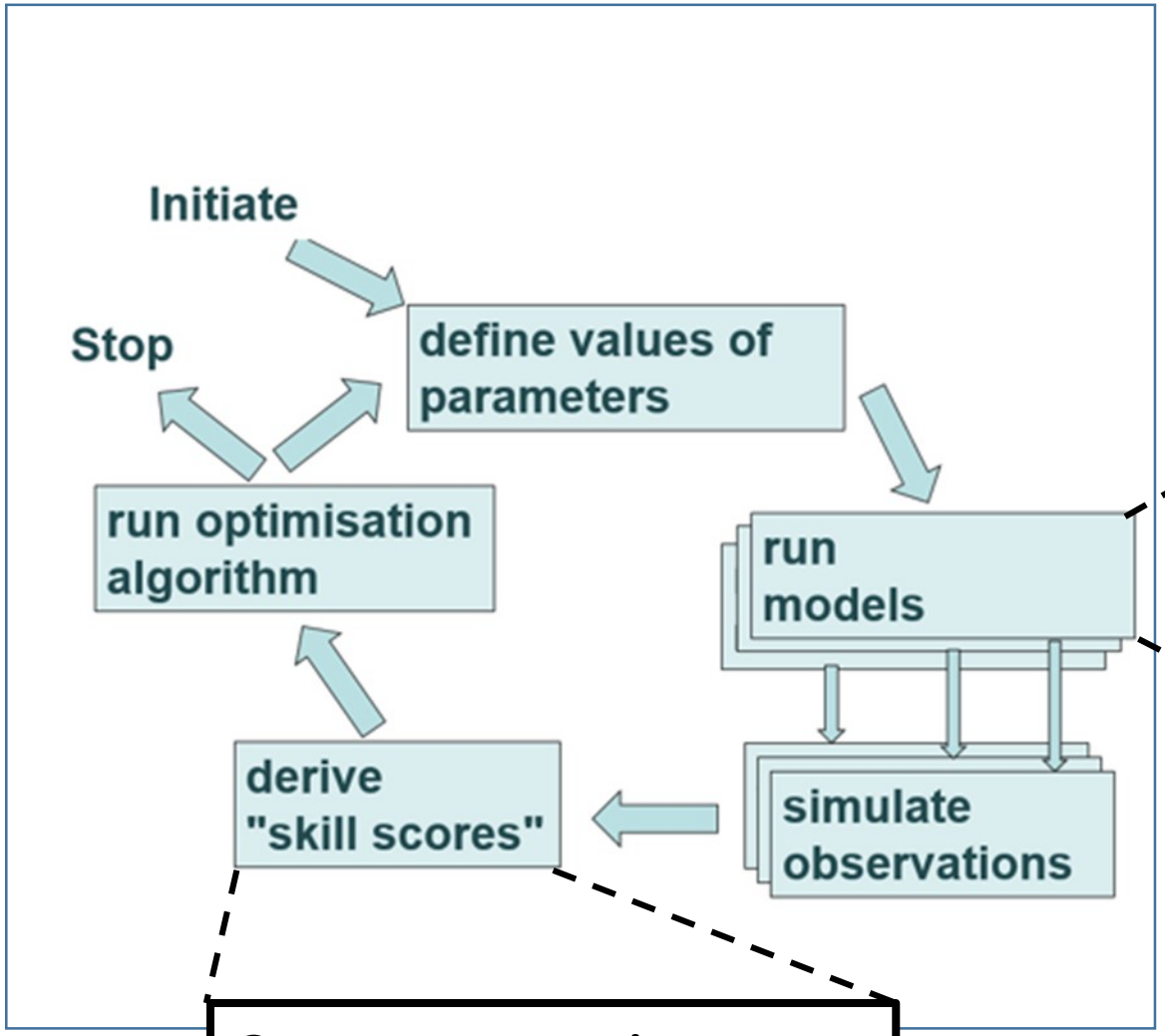
<u>Characteristics</u>

1. Expensive run times
2. These are deterministic models

<u>Consequences</u>

1. Need to minimise number of runs
2. Potential for algorithmic approaches

# OptClim: Schematic and Illustration



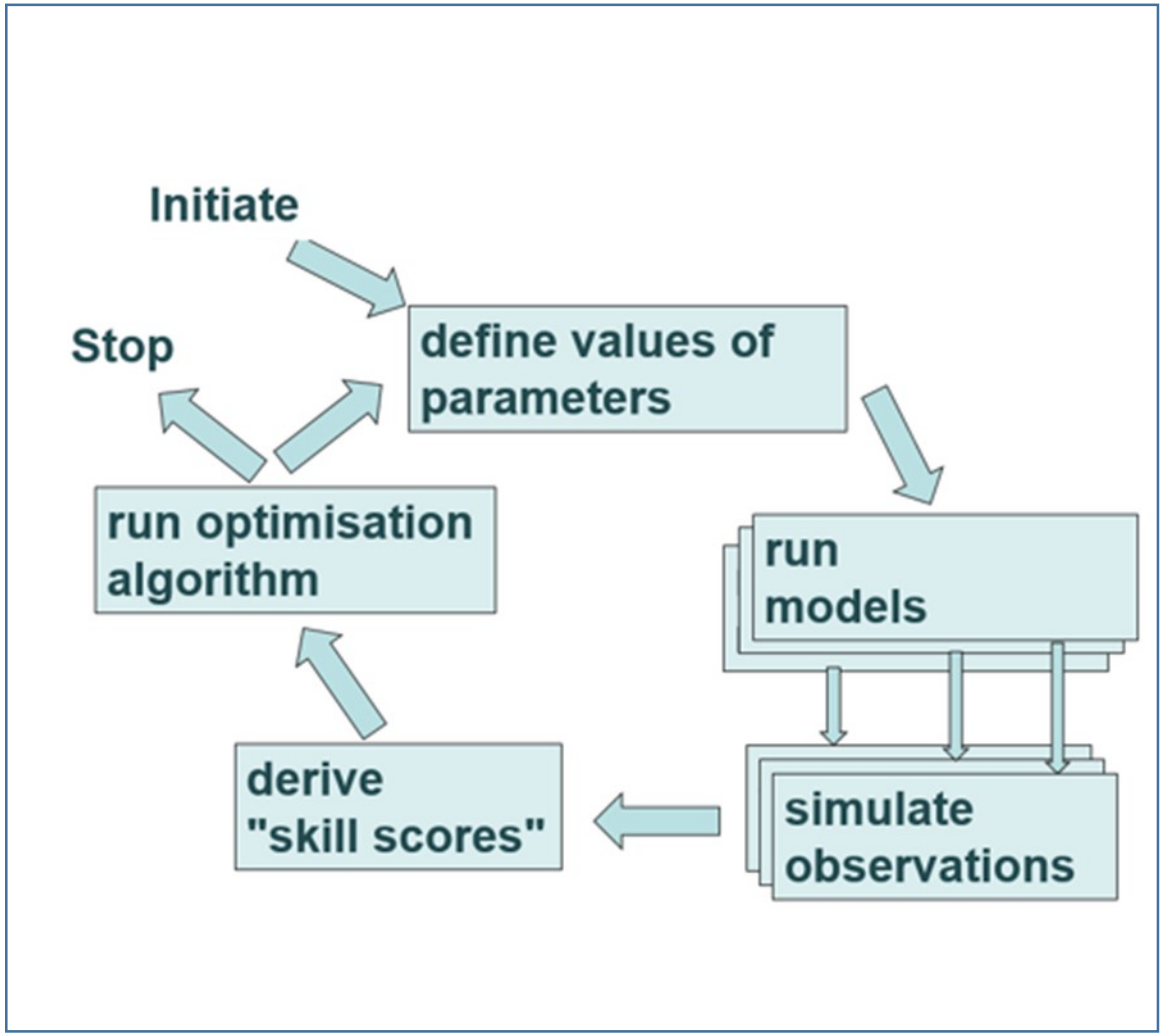

Clone a reference "base model"

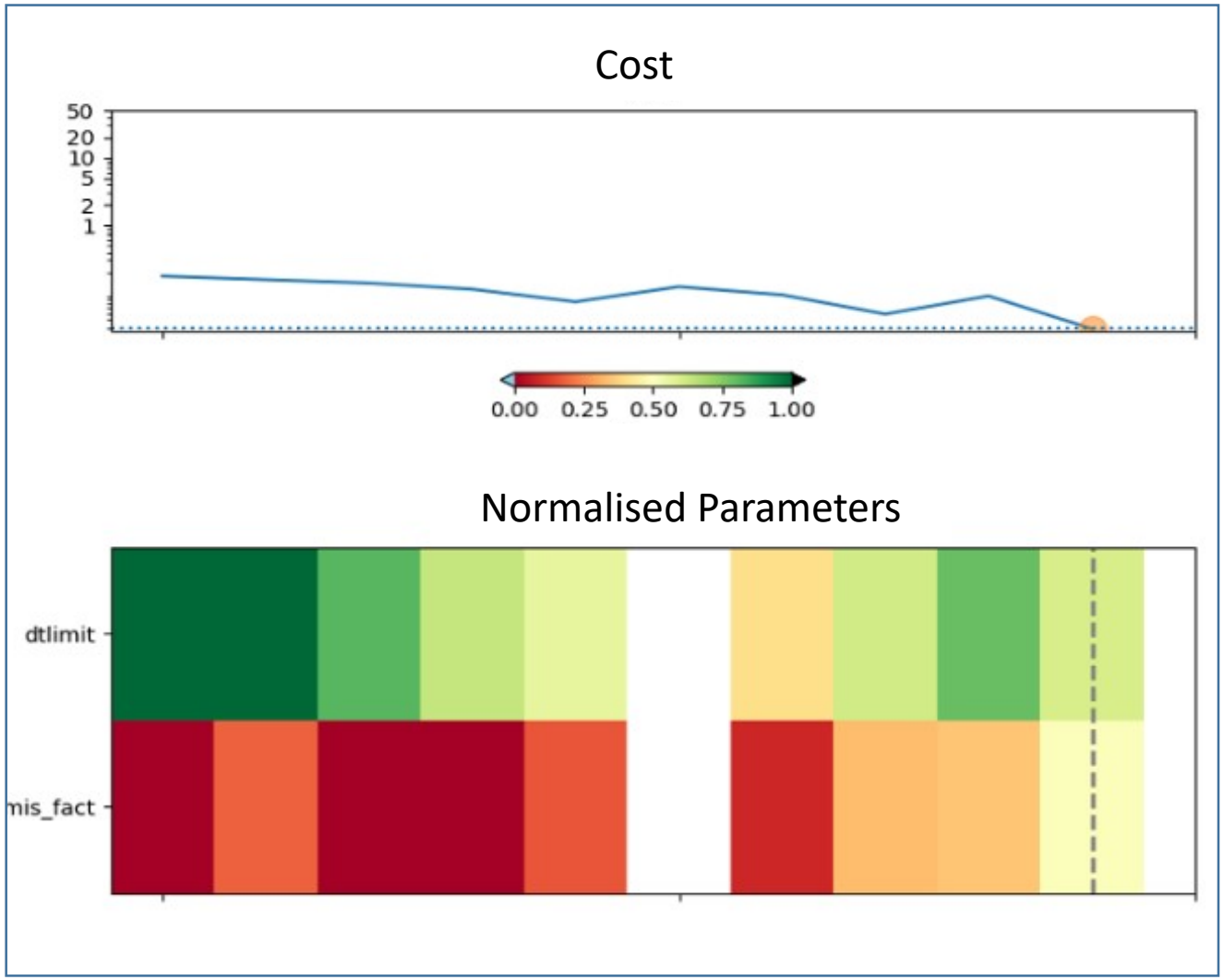
Amend parameters

Run simulation

Compare against observations

# OptClim: Schematic and Illustration

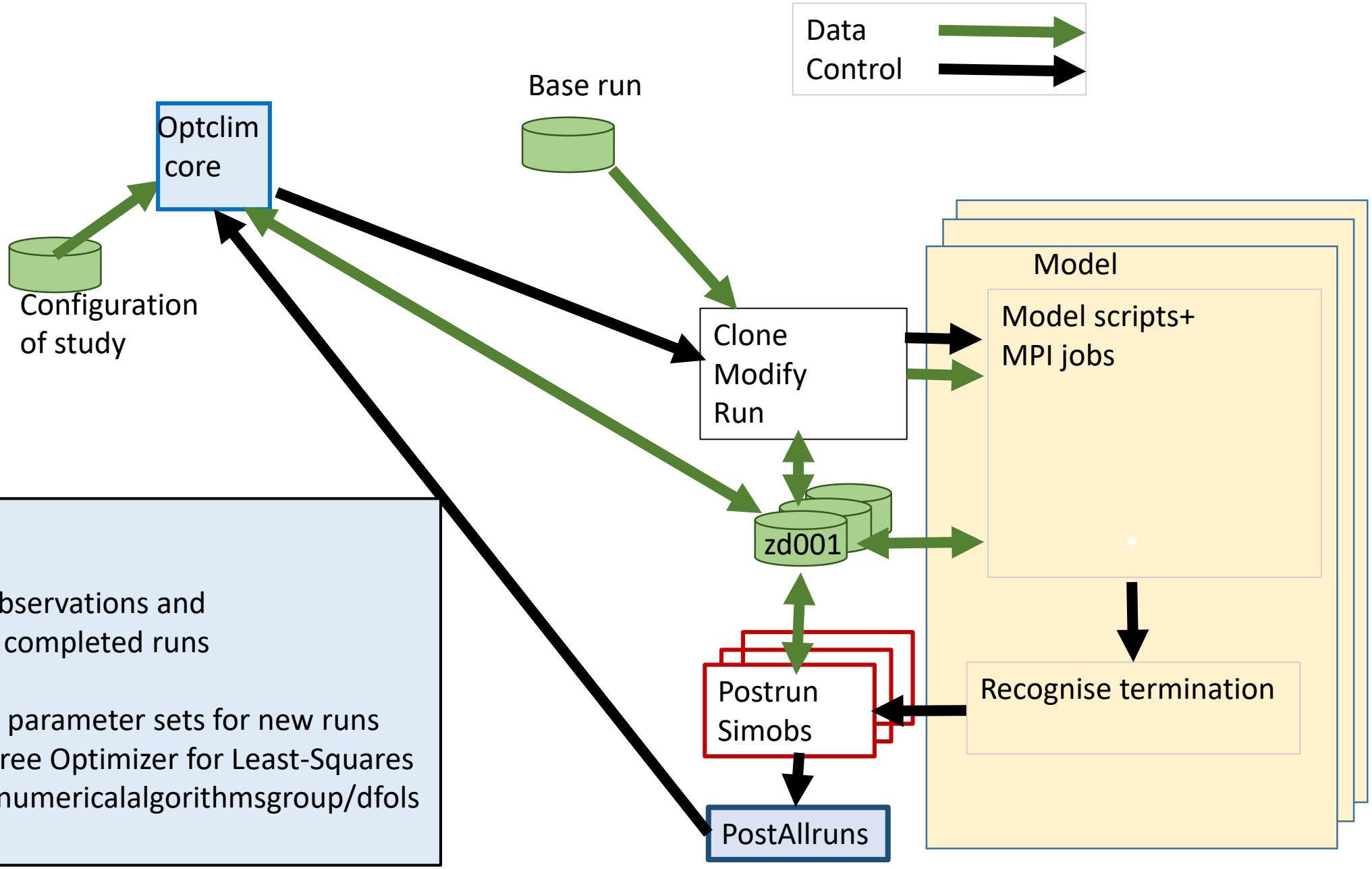



System test with dummy “observations”

# OptClim

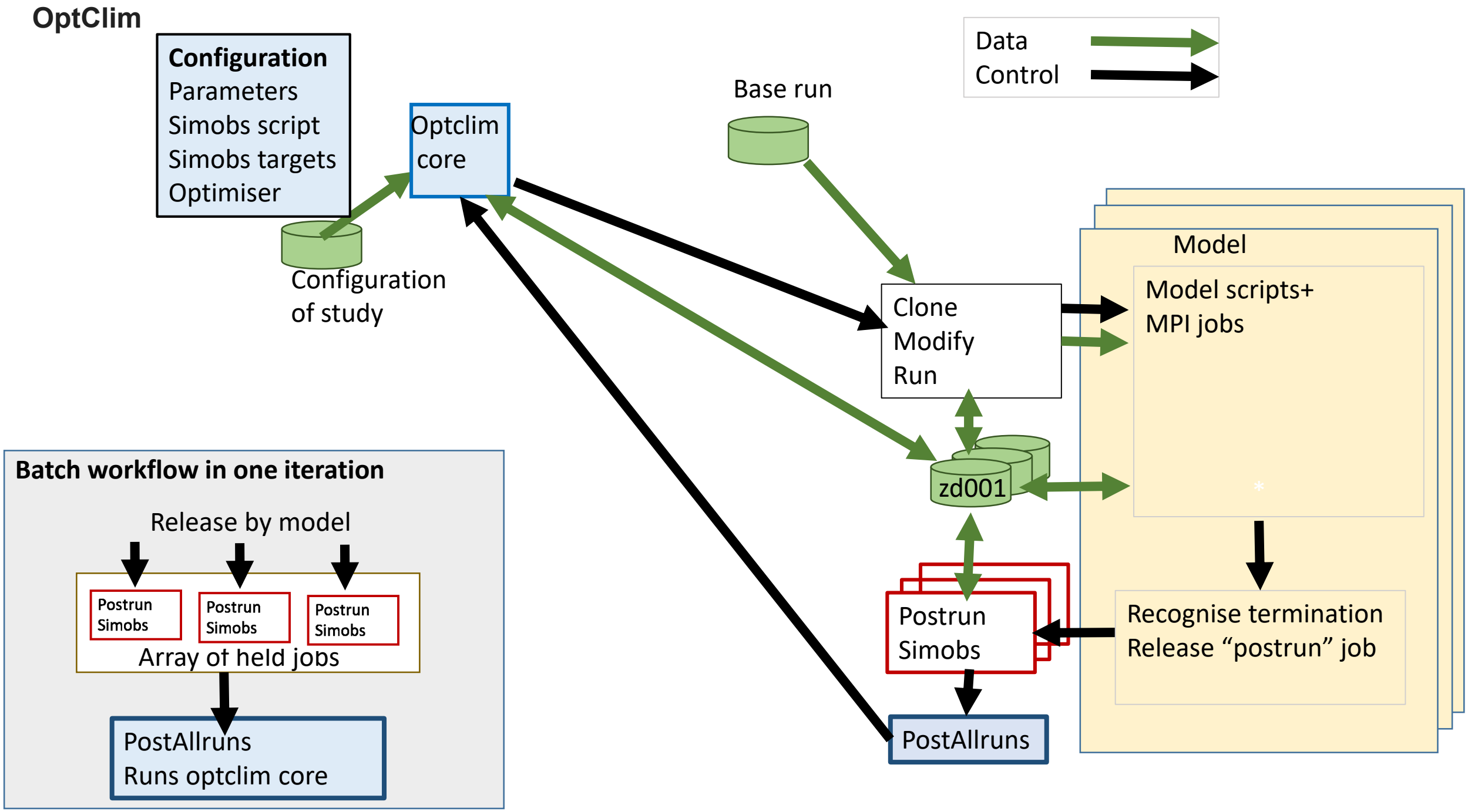
**Interface Directories:**
Studies/zd/…
../zd001
../zd002
../zd003




**OptClim core**

Gathers simulated observations and parameter values of completed runs

Optimiser generates parameter sets for new runs
DFOLS : Derivative-Free Optimizer for Least-Squares
https://github.com/numericalalgorithmsgroup/dfols


OptClim
Configuration
Parameters
Simobs script
Simobs targets
Optimiser
Optclim
core
Configuration
of study
Base run
Data
Control
Clone
Modify
Run
zd001
Model
Model scripts+
MPI jobs
Postrun
Simobs
Recognise termination
Release "postrun" job
PostAllruns
Batch workflow in one iteration
Release by model
Postrun
Simobs
Postrun
Simobs
Postrun
Simobs
Array of held jobs
PostAllruns
Runs optclim core

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# Port of OptClim2 to ARCHER2

- OptClim2 runs on University cluster Eddie (with UM4.5)
- Goals:
  - Minimise code redevelopment – use existing code from Eddie
  - Port to ARCHER2  (Slurm job management)
  - Add support for three exemplar models
    - MITgcm-ECCO
    - CESM2
    - UKESM 1
- Outcome:
  - “Beta release” level: some support probably needed (and offered on best-efforts basis) for new users of OptClim with these models.

# 1st phase: MITgcm-ECCOv4

Has directories for:
src, bld, run; simple scripts.

- Base model
  - Add a command  to  Slurm script
- Clone:
  - Copies  the run directory
- Modify params in namelists:
  - Current OptClim code
    f90nml.py
- Run:
  - Simple Slurm command sbatch

# 2nd phase: CESM models - layer above Slurm

Web service serves models and data.
Uses workflow and commands above Slurm

- Base model:
  - Use modified workflow for OptClim
- Clone
  - Call CESM clone command
- Modify parameters:
  write to simple text file
- Run
  - Call CESM run command

# 3rd phase: UKESM – most complex

- Rose & Cylc run the model suites from server PUMA

  Communication from OptClim to PUMA is the challenge.

# Running UKESM on ARCHER2

**PUMA**

**Rose/cylc server**

Suite defines a model using text files.
(and an optional GUI)

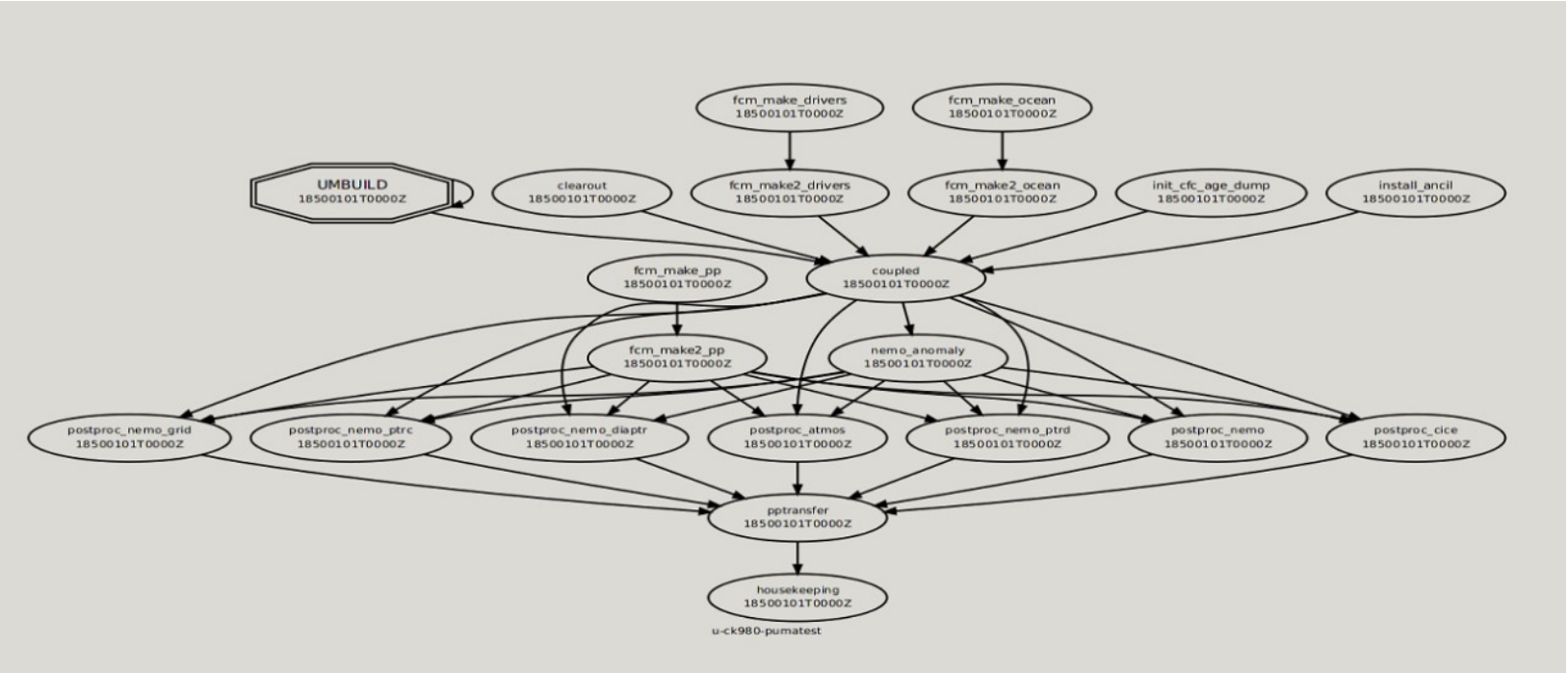
"rose suite-run"

**ARCHER2**

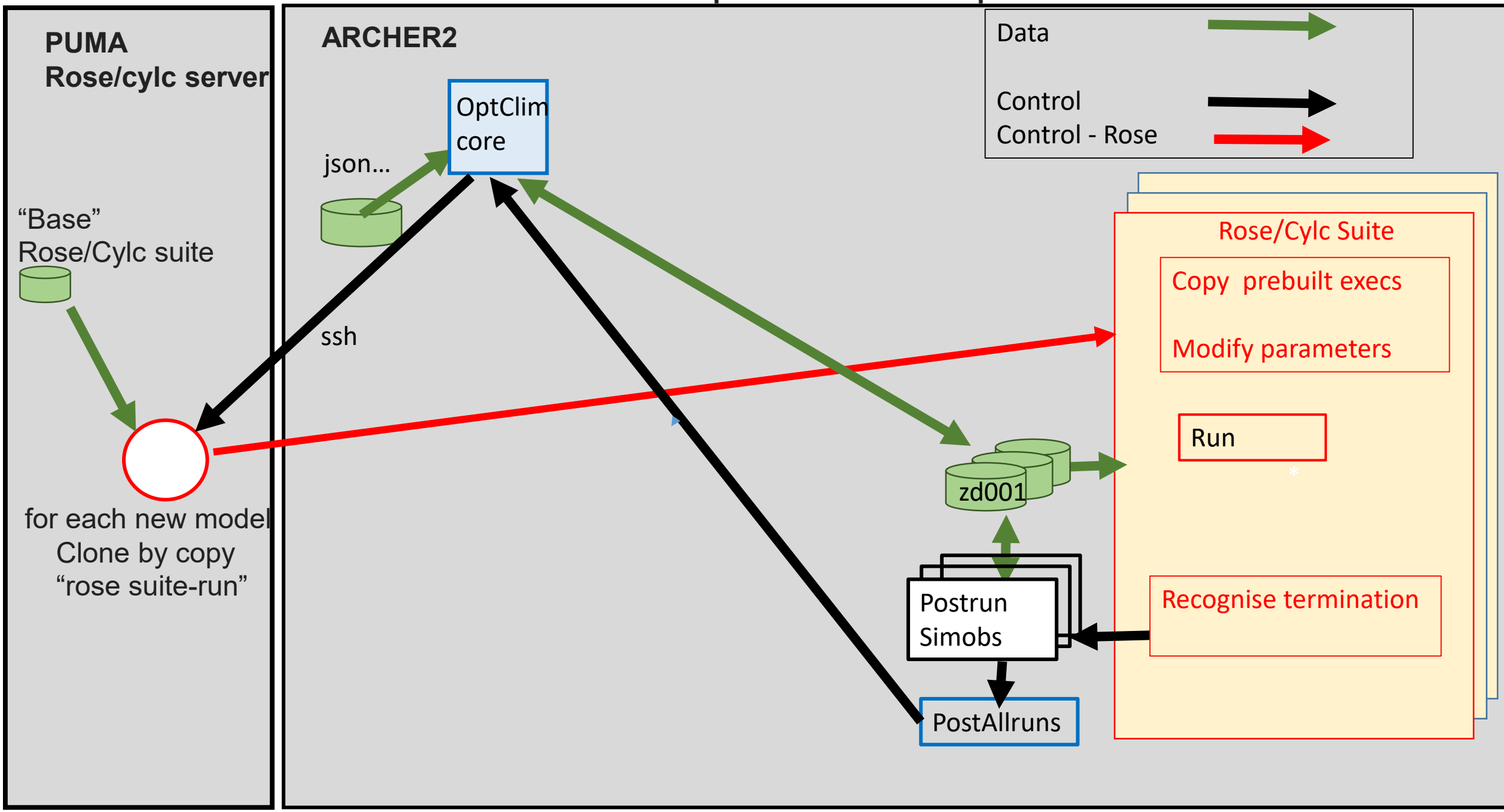
Rose/Cylc tasks

build

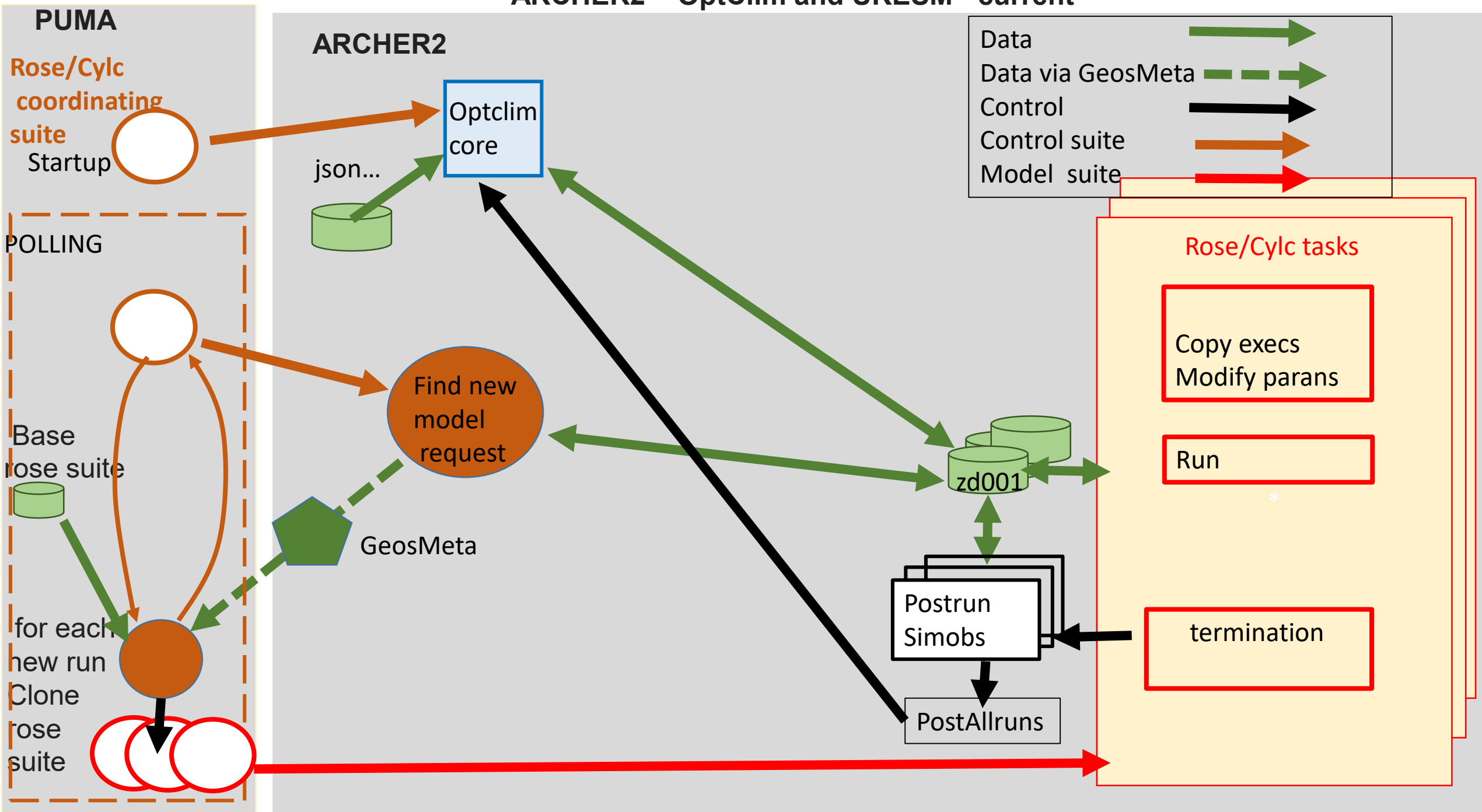
run *



# ARCHER2 – OptClim and UKESM plan

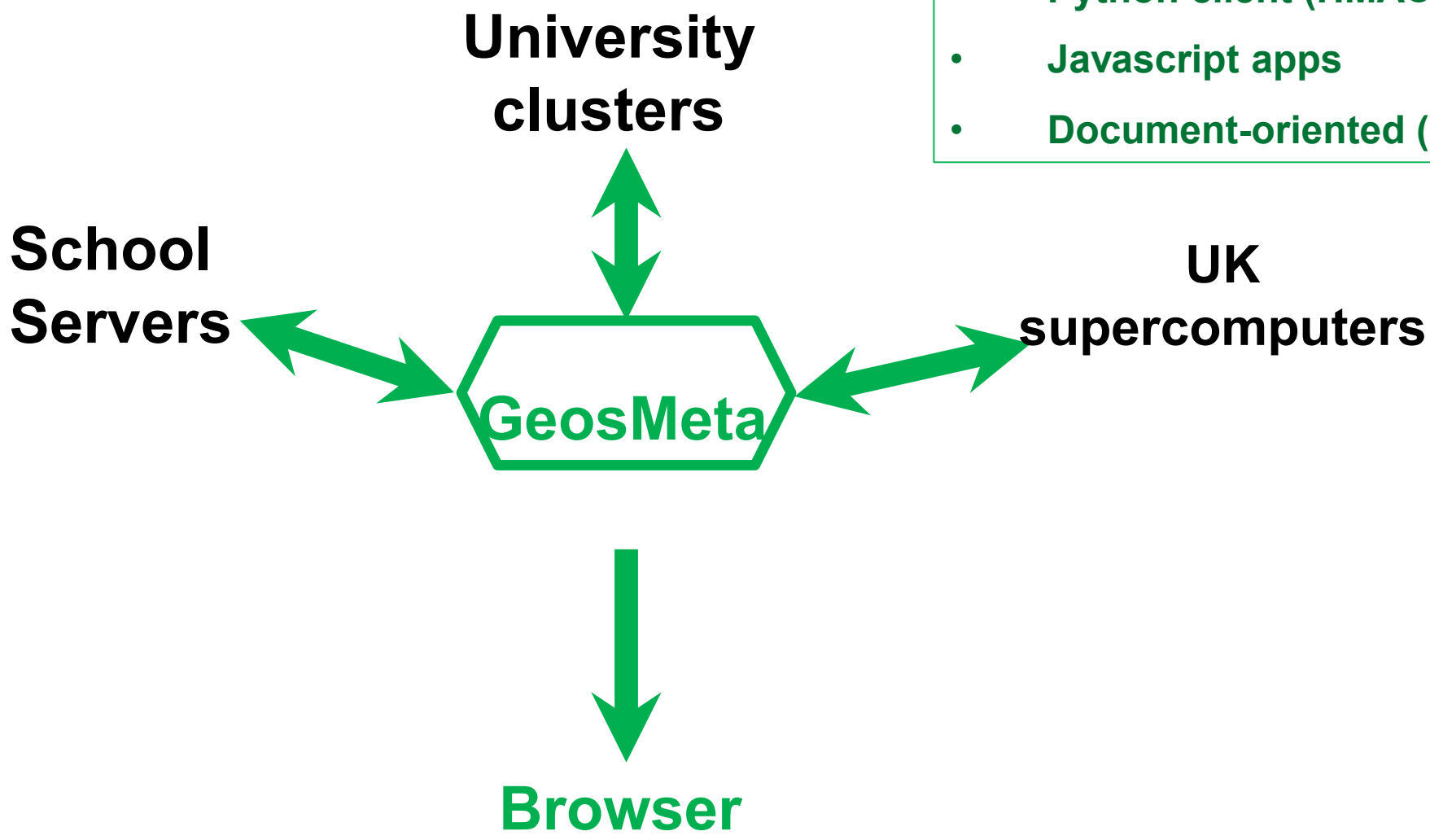


# ARCHER2 – OptClim and UKESM - current



# GeosMeta: flexible service to hold metadata

- Secure RESTful web service
- Python client (HMAC)
- Javascript apps
- Document-oriented (noSQL)



# Using GeosMeta to pass messages

**MESSAGE CONTENTS**

**Document type: “suiteRequest”**

**Base suite name**

**Interface directory path**

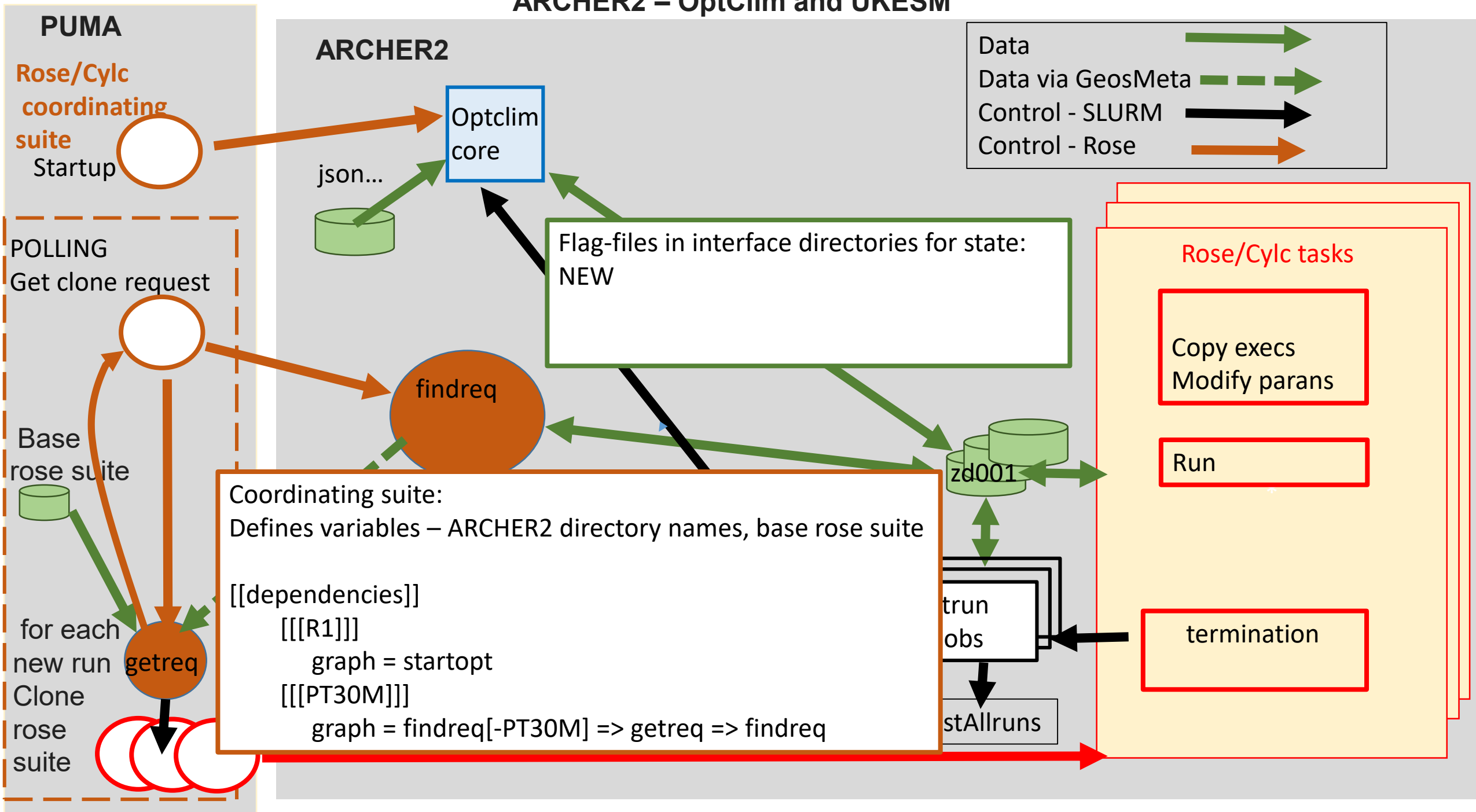
**Status: clone needed / request received.**


Good news:
* Use GeosMeta as message passing layer

Bad news:
Dependency on GeosMeta admin.

Hoped-for news:
* New PUMA in ARCHER2

# ARCHER2 – OptClim and UKESM



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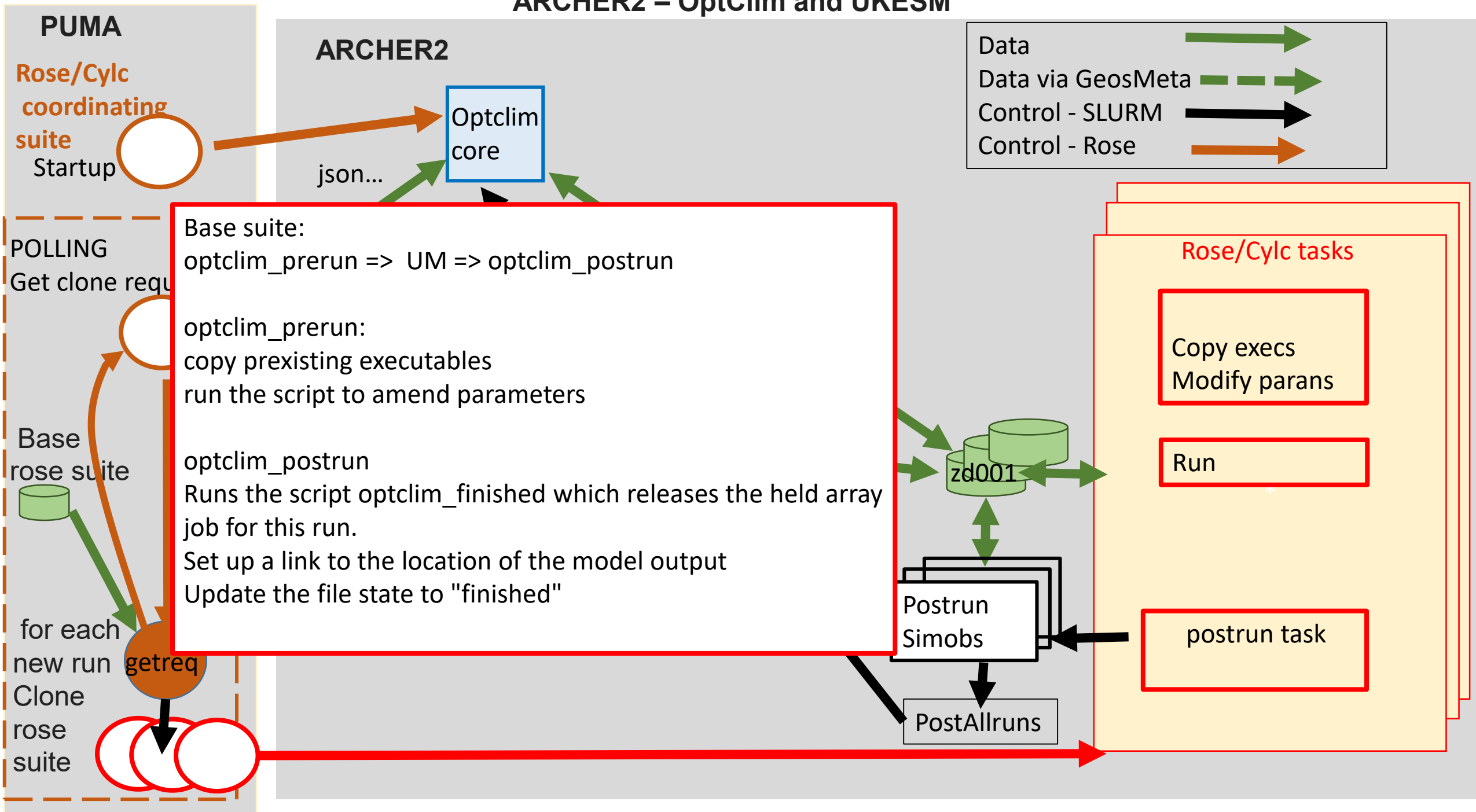
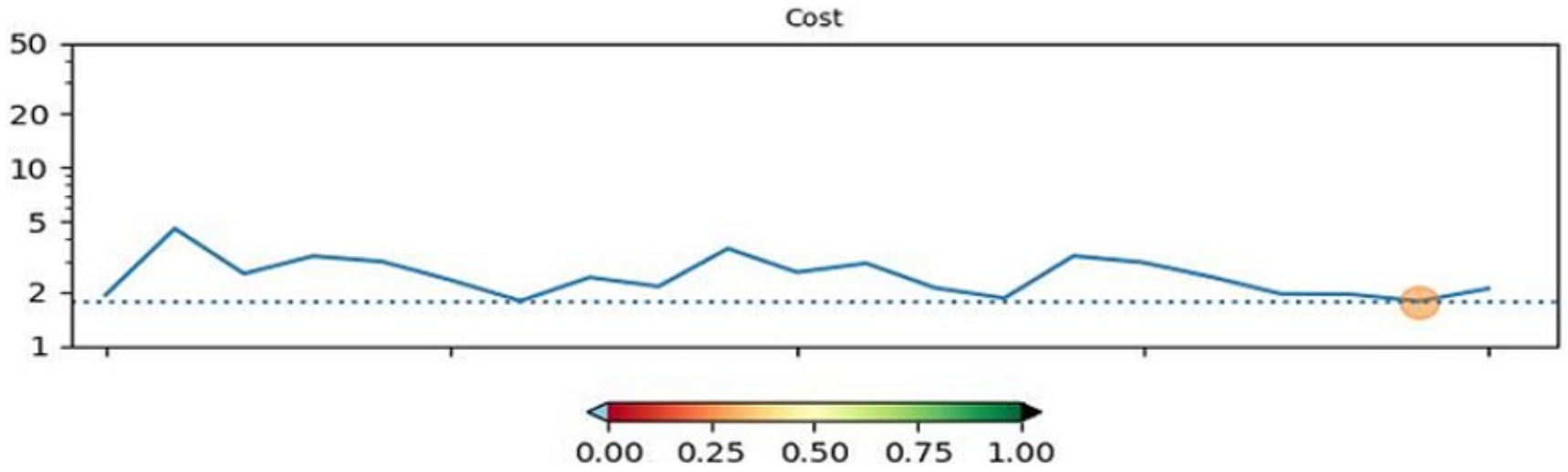
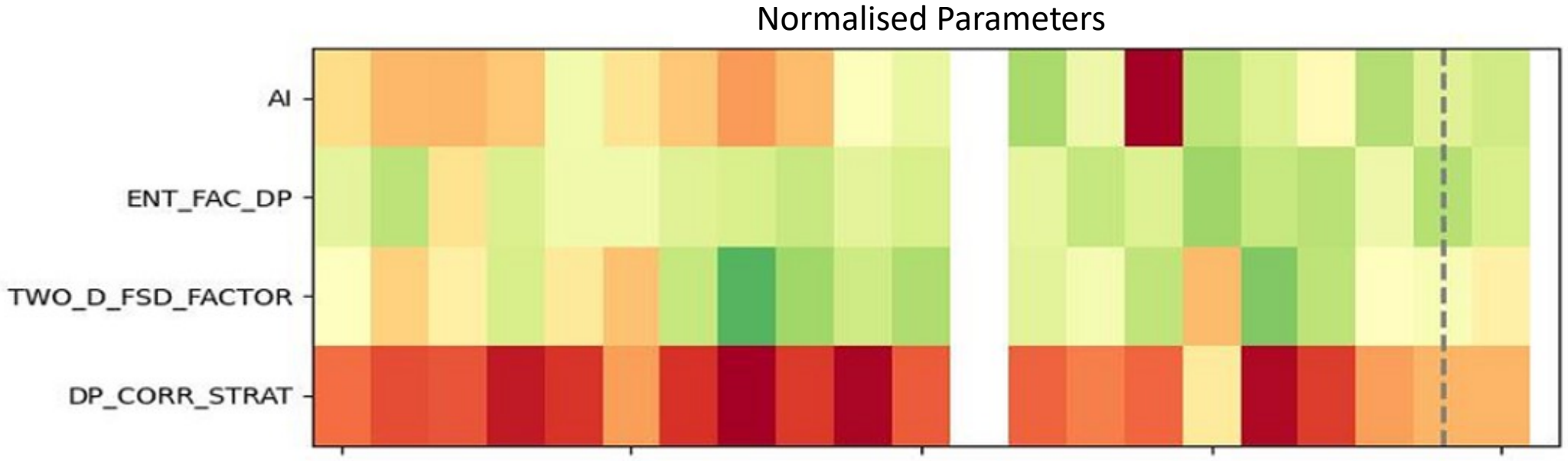


# OptClim: “Real-world” trial: u-be303, Atmosphere only UM11 UKESM1.0



# Guidance for potential users of OptClim

Need to:

- Select parameters,  observations
- Write code to make simulated observations

May need some support

- Installing and configuring OptClim for first time

Initial users with UKESM will need some support:

- Models' suites vary in style: how to add pre/post run tasks
- UKESM requires use of GeosMeta: easy to set up but with admin support from Edinburgh

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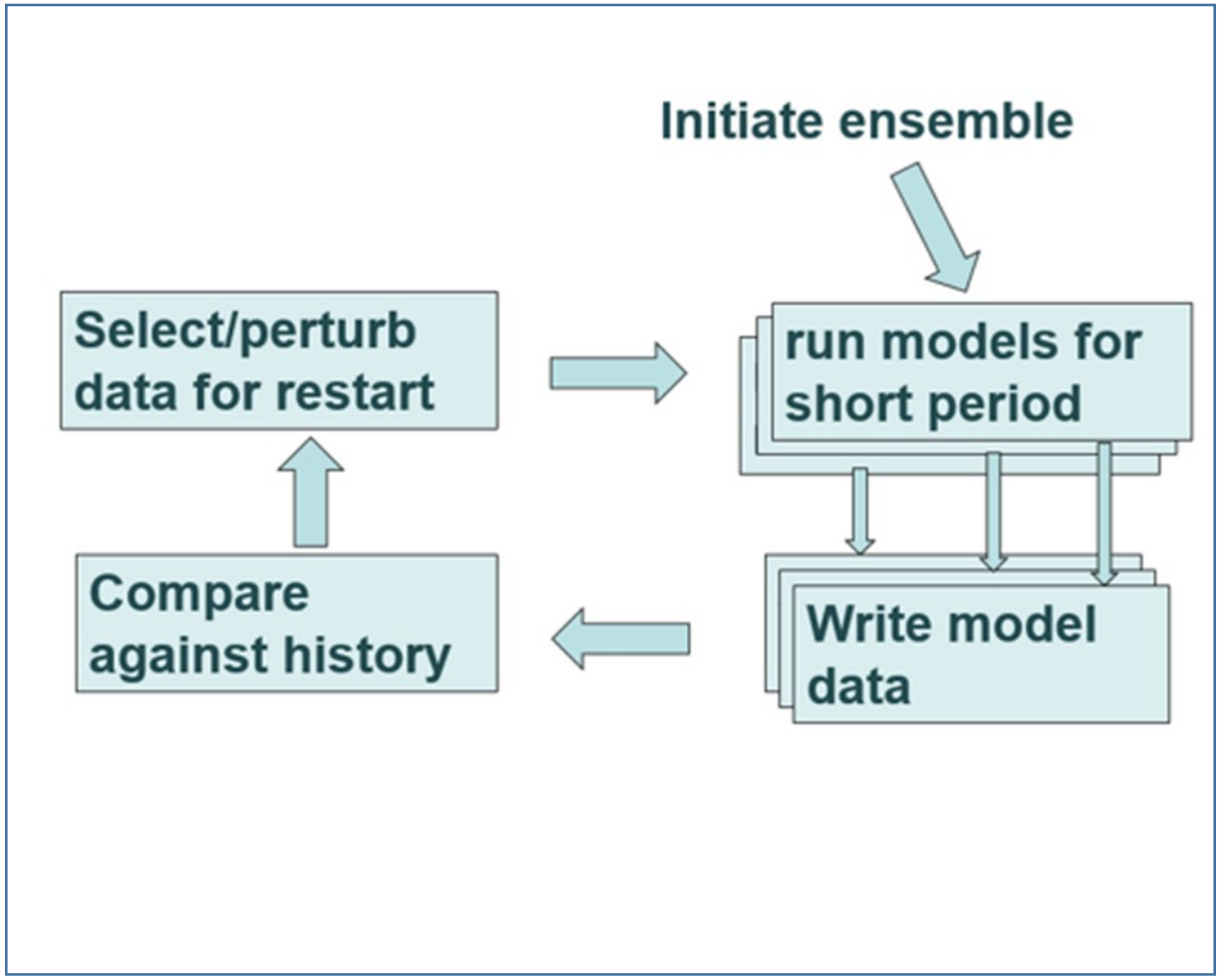
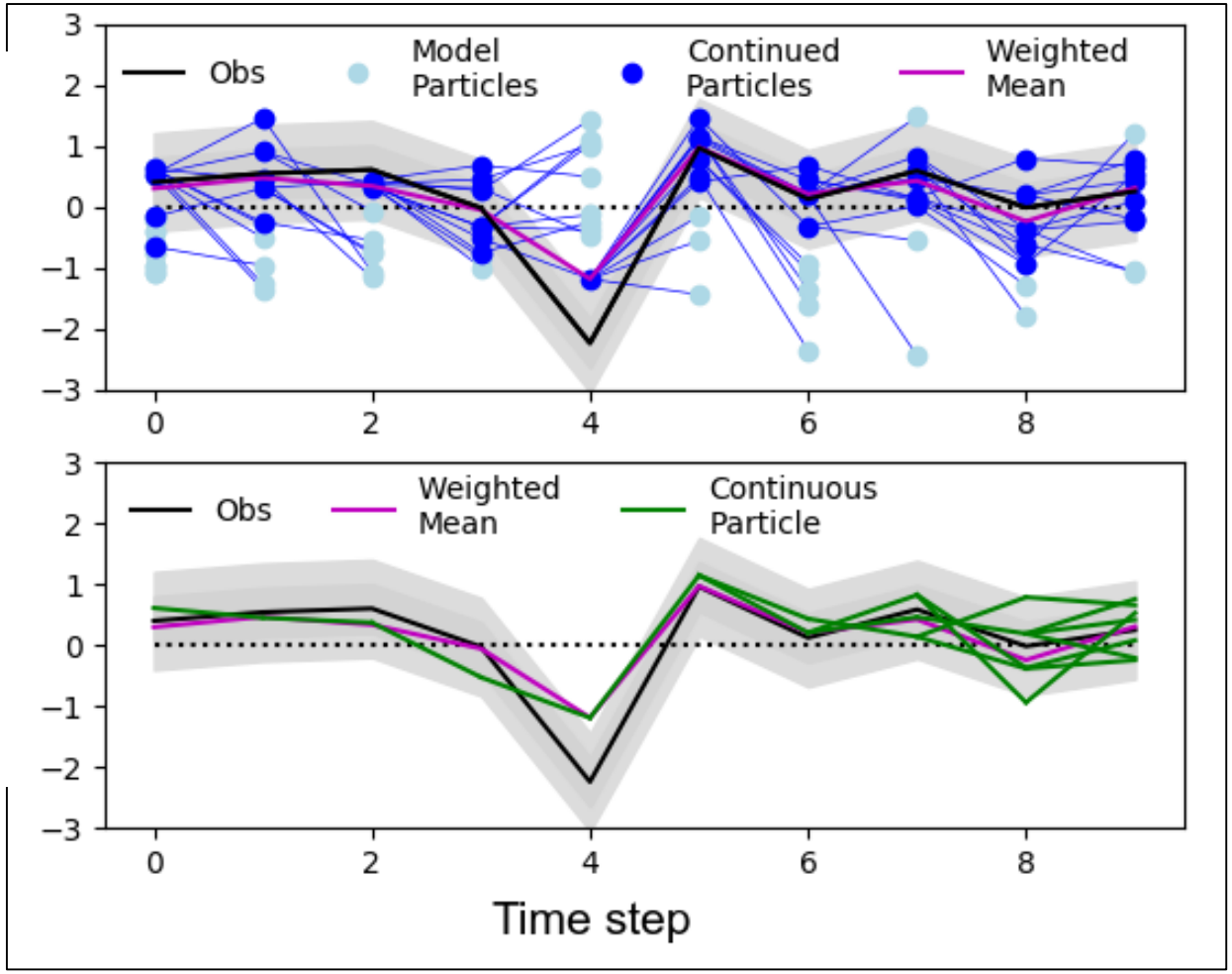
# Particle Filtering: Schematic and Illustration



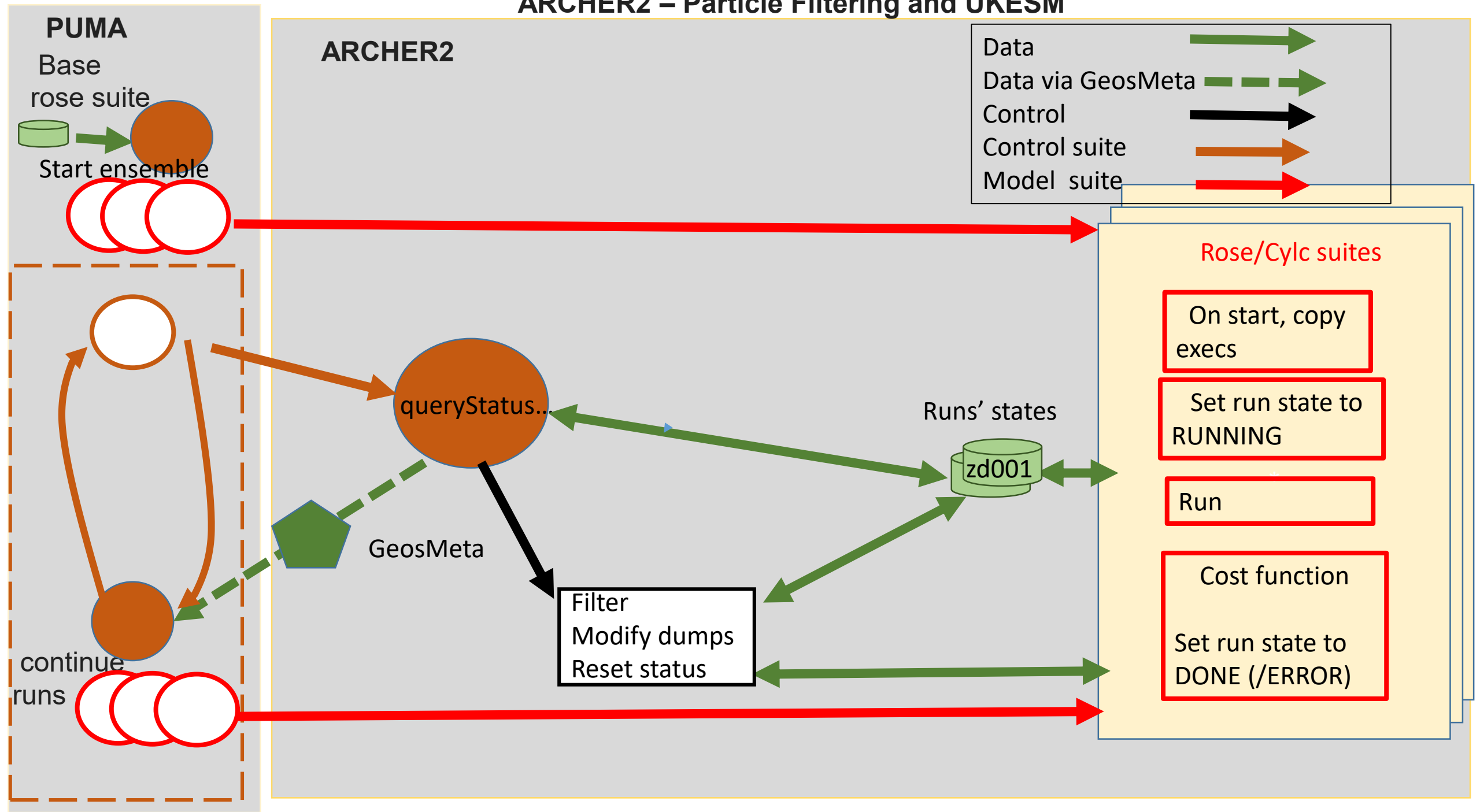




https://doi.org/10.5194/cp-2022-55
A Schurer et al.

# Particle Filtering for UKESM on ARCHER2

- Porting Objectives
  - Minimise code – learning from ARCHER2-OptClim
  - Test with u-cc519: standard N48 suite at UM11.8.
- User provides:
  - Historical data
  - Goodness of fit
  - Perturbation of restart data
- Status
  - Tested the system with dummy filtering
  - Real-world example en-route

# ARCHER2 – Particle Filtering and UKESM



# Summary: in response to models' uncertainties

- Ported OptClim to ARCHER2
  - Uses OptClim workflow in Slurm
  - Supports MITgcm, CESM, UKESM
  - "Beta": some support needed – UKESM especially

- Implemented Particle Filtering with UKESM on ARCHER2
  - Different workflow – polling from the "coordinating" Rose suite
  - Tested the system with dummy filtering
  - Real-world example en-route

# Thanks - and further information

- Thanks to:
  - eCSE grant
  - ARCHER2 support
  - NCAS - Rosalyn Hatcher, David Case, Grenville Lister

- Project report https://www.archer2.ac.uk/ecse/reports/eCSE04-07/

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