# Addressing the calibration bottleneck using machine learning: Application to the CNRM-CM6-1 model

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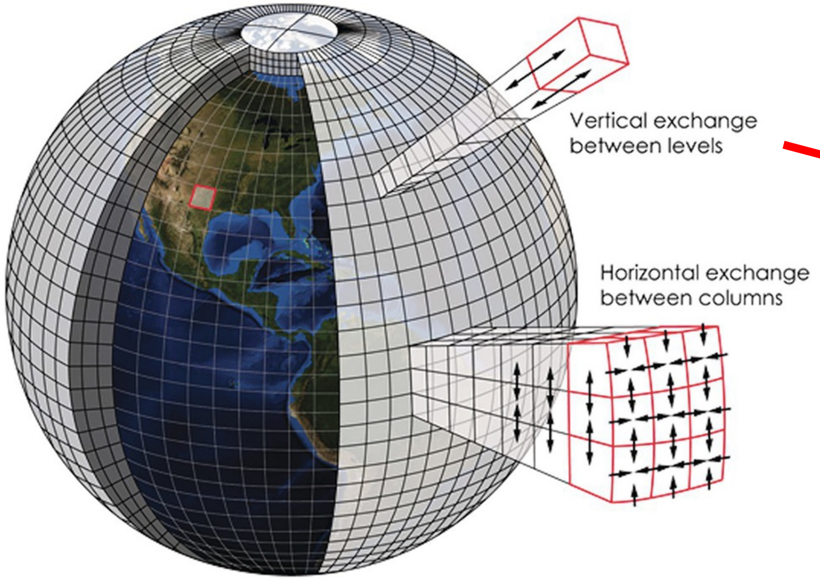
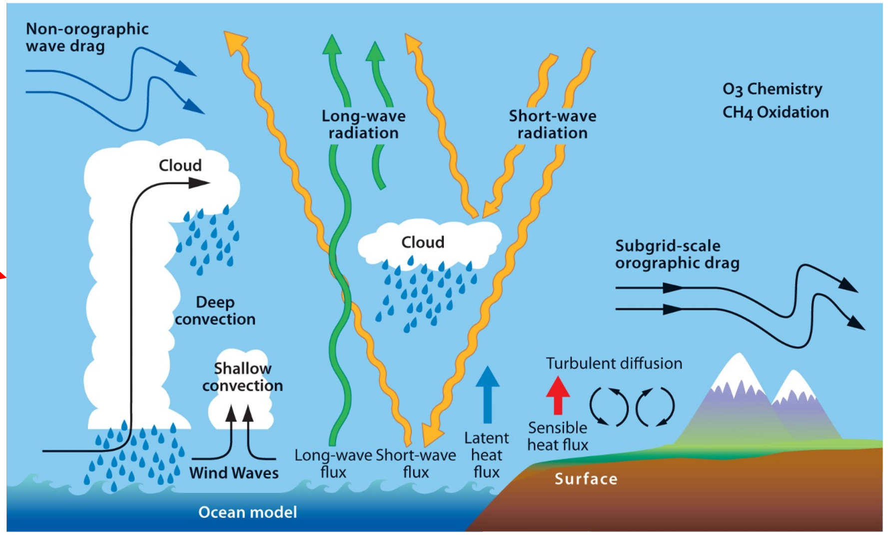
# Climate models - basics




$$\frac{\partial \boldsymbol{x}}{\partial t} = \mathcal{D}(\boldsymbol{x}) + \sum_{p} \mathcal{P}_p(\boldsymbol{x})$$




***Developing a climate model:***

- Choose a set of equations issued from fluid dynamics, thermodynamics, with some approximations.
- Discretise them on the sphere to solve them numerically
- Thereby introduce a model resolution:
  - ➢ some processes are explicitly resolved, some not >> parameterizations
  - ➢ note some processes need to be parameterized whatever the resolution (e.g., radiation, microphysics)
- Do it for each component of the climate system and couple individual models together

# Climate model calibration

***Climate model*** = a software
+ external forcings
+ horizontal/vertical grids
+ a scientific content (i.e., fluid dynamics equations, parameterizations)
+ values for model internal/uncertain parameters >> ***calibration***

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## *Calibration (or tuning)*

- Common to most modelling frameworks
- Can be seen as an optimisation procedure under constraints (or ***metrics***), possibly with priorities/weights.
- Need for high-quality ***references/observations***, with well-quantified uncertainties
- +1 W m$^{-2}$ at TOA ~ +0.5–1.5 K of global mean near-surface temperature (*Hourdin et al. 2017*).
    - ➢ *Given current uncertainties, present-day global-mean temperature in a climate model is mostly a result of tuning.*

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## *A bottleneck for climate model development*

- ***High dimensionality*** of the parameter space ~O(10)
- Climate model numerical simulations are ***computationally expensive***
  - ➢ An exhaustive exploration of the parameter space is not directly possible.
- Large number and variety of metrics O(10-100++), sometimes subjective
- ***Overfitting*** issue, treatment of ***uncertainties***

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## *Calibration of CNRM-CM6-1* (*Voldoire et al. 2019, Roehrig et al. 2020*)

- Manual calibration, 1 or 2 parameters at the same time, mixing well-defined metrics and more subjective considerations
- Calibration of stand-alone components before coupling, priorities among metrics
- Often questioning the model physical content. But difficult to disentangle true model structural limits from “just” a poor calibration?

# A rationale for addressing the calibration bottleneck

***History matching***

- Determine the plausible sets of model parameter values rather than optimize
- Or equivalently rule out the ***implausible*** sets of model parameter values
- For a given set of ***quantitative metrics***
- Considering ***reference/observations uncertainties***
- And introducing priors for ***model structural errors*** (interpreted here as tolerances to error)

***Machine learning***

- ***Emulate*** the model behaviour (i.e. the dependence of metrics to model parameters), to explore at very weak cost the parameter space.
- Consider also the ***emulators' uncertainty***
- ***Gaussian processes*** nicely provide predictions with an uncertainty estimate

***Iterative refocussing***

- Be as ***parsimonious*** as possible in terms of true simulations
- Start with a 'few' simulations and progressively add new ones to improve the emulator quality, but only where it is needed
- Possibly add new metrics along the way, based on more expansive simulations (pre-conditioning with cheaper configurations)

➢ *A **formalized calibration procedure**, transparent and reproducible.*
➢ *A semi-automatic and efficient framework, that allows us to **quantify the true benefit of a new development** more rapidly*
➢ *More **rigorous comparison** between parameterizations or model physics.*
➢ *Possibly not a single acceptable configuration but several: being able to explore the **model parametric uncertainty** of its emergent properties.*

*Bower et al. (2010), Williamson et al. (2015, 2017)*

# The technical framework

1. Define targeted (scalar) ***metrics*** $f$, their ***reference values*** $r_f$ and associated ***uncertainties*** $\sigma_{r,f}$
2. Identify the relevant model ***parameters*** $\boldsymbol{\lambda}$, and their "acceptable" range >> ***input parameter space*** $\Lambda$
3. Define a simulation strategy, build an experimental design, run simulations >> ***learning dataset***
4. ***Emulate*** $f(\boldsymbol{\lambda})$ for each metric (Gaussian Processes)
5. Identify the sub-space of $\Lambda$ which is compatible with references for all metrics

   >> ***Not-Ruled-Out-Yet – NROY – space***

   considering
   - The reference uncertainty
   - The emulator uncertainty
   - The model structural error (tolerance to error) $\sigma_{d,f}$

   >> ***Implausibility*** measure $I_f$, ***cutoff*** $T$

$$I_f(\boldsymbol{\lambda}) = \frac{|r_f - \mathrm{E}[f(\boldsymbol{\lambda})]|}{\sqrt{\sigma_{r,f}^2 + \sigma_{d,f}^2 + \mathrm{Var}[f(\boldsymbol{\lambda})]}}.$$

$$\mathrm{NROY}_f^1 = \{\boldsymbol{\lambda} \mid I_f(\boldsymbol{\lambda}) < T\}$$

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6. Iterate over several waves to reduce the emulators' uncertainty in $\mathrm{NROY}^{N-1}$, until convergence

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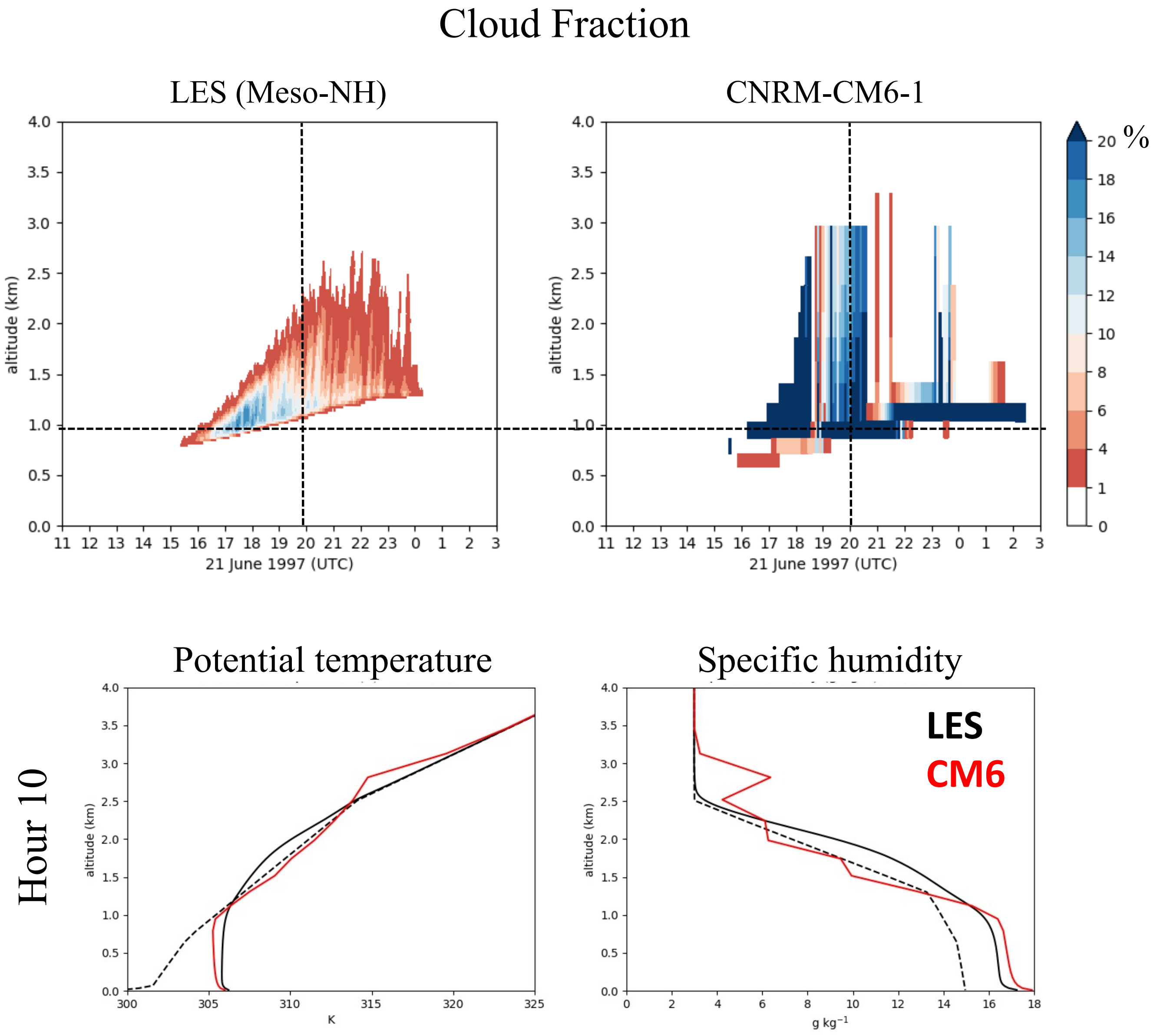
# First application: 1D configurations of CNRM-CM6-1




***1D (Single-column model) vs Large-Eddy Simulation (LES):***

➢ ***inspire the development of atmospheric parameterizations, validate and calibrate them***

ARM-Cumulus: diurnal cycle of continental cumulus

In CNRM-CM6-1:

- Overestimate of cloud fraction
- Cloud base too low
- Boundary layer not deep enough, mixing too weak
- Intermittency and numerical issues

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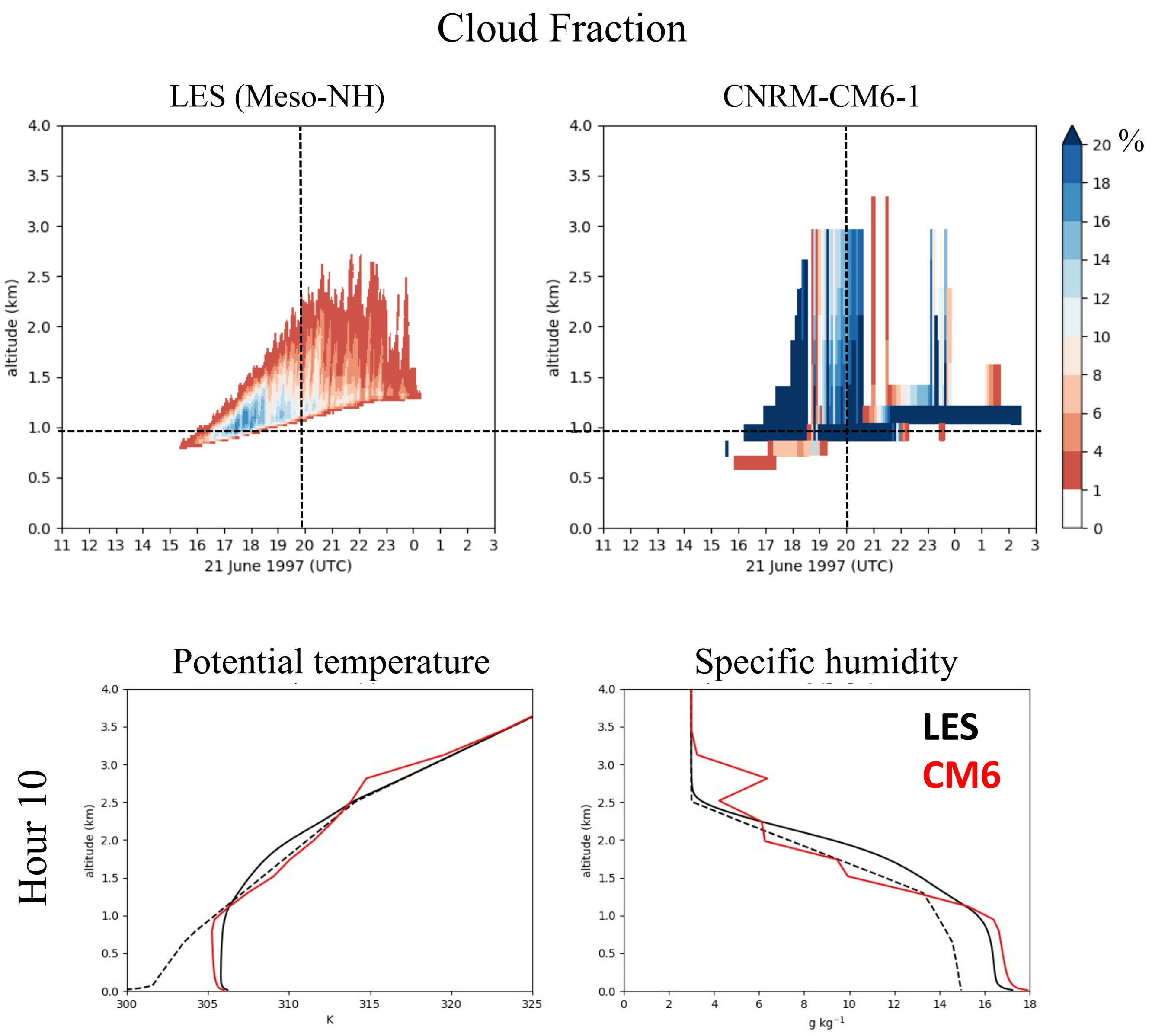


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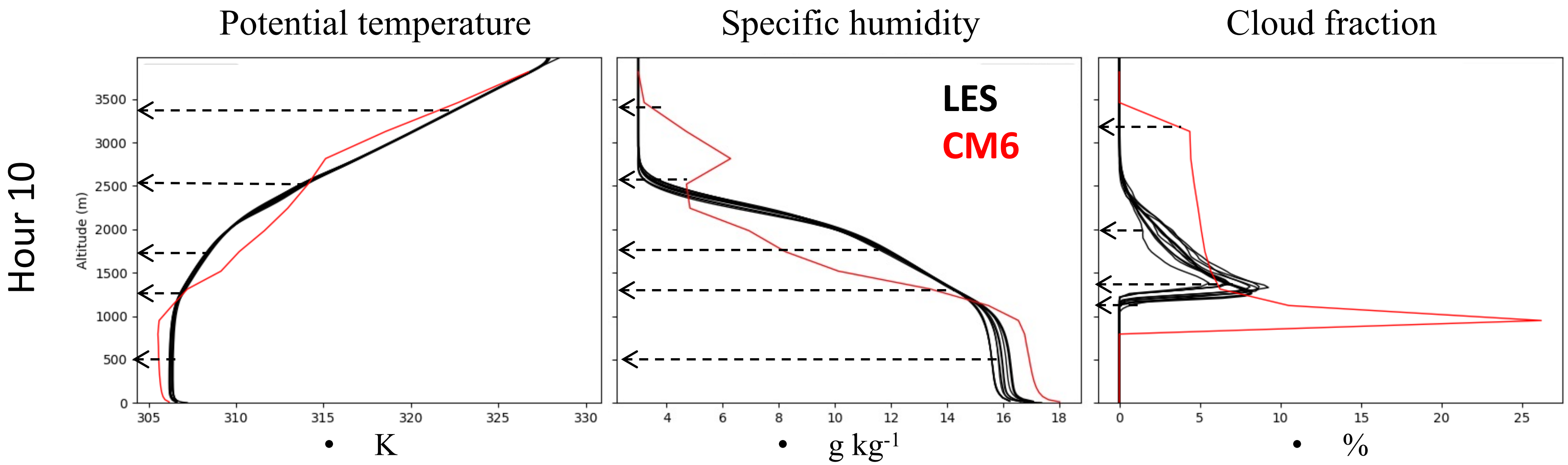
➢ ***Poor calibration, or intrinsic limits?***

# Calibration setup

- **14 metrics**: temperature, specific humidity and cloud fraction at a few levels (Hour 10)
- **Reference**: LES simulation with Meso-NH, uncertainty from an ensemble of LES simulations

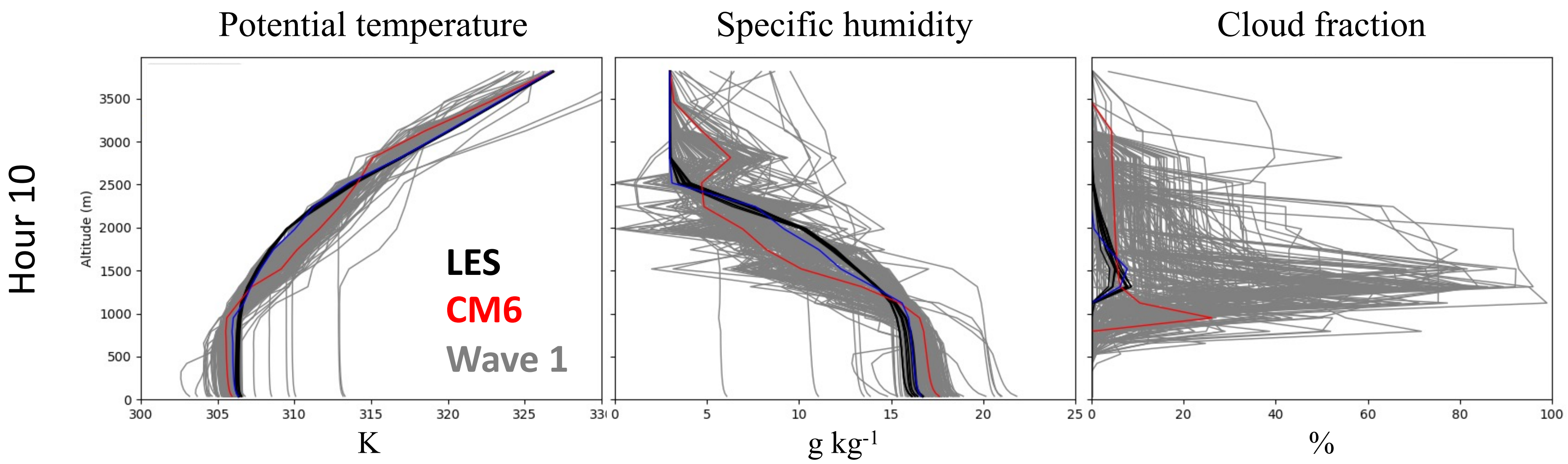



- **26 parameters**:
  - 13 related to convective transport (entrainment/detrainment, drag, buoyancy parameter)
  - 2 related with convective closure
  - 1 related to convective cloudiness
  - 6 related with liquid water microphysics
  - 4 related to turbulence
- Wave 1: 200 simulations, sampling based on a Latin hypercube
- Next waves: 200 simulations (within NROY$^{N-1}$)

# Wave 1

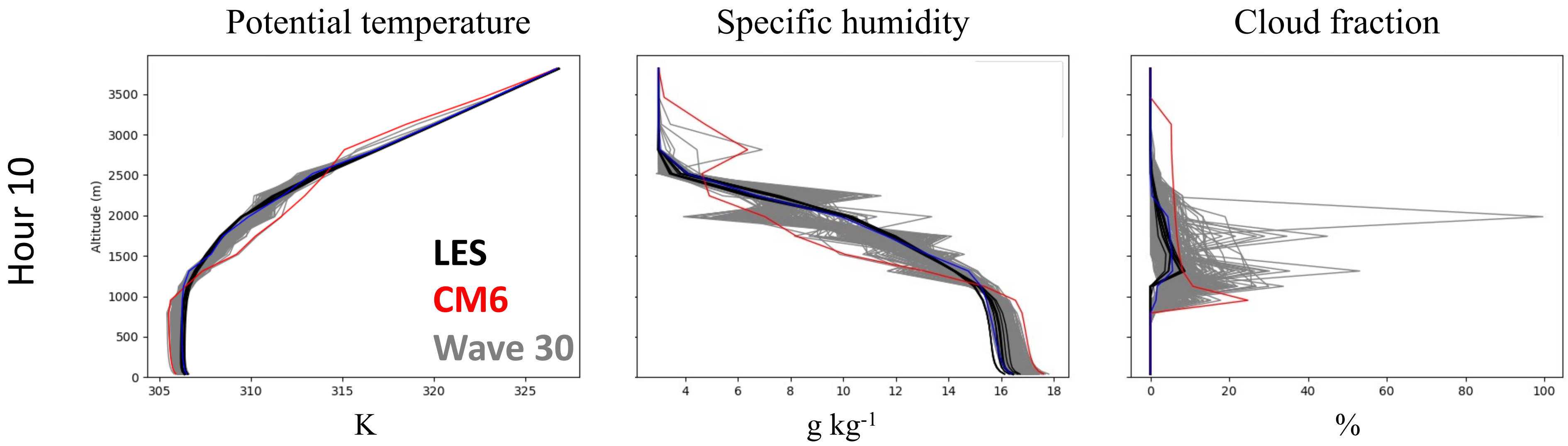
### *Tolerance to error*

- Potential temperature: 0.5 K except at 3400 m (0.1 K)
- Specific humidity: 0.5 g kg$^{-1}$
- Cloud fraction: 5 %



# Wave 33

- Several configurations much better than default.
- Convergence not fully achieved (esp. for cloud fraction).
- ***Intrinsic limits of the model physics***:
  - ➢ Some irregularities in the profiles seem intrinsic (esp. $q_v$)

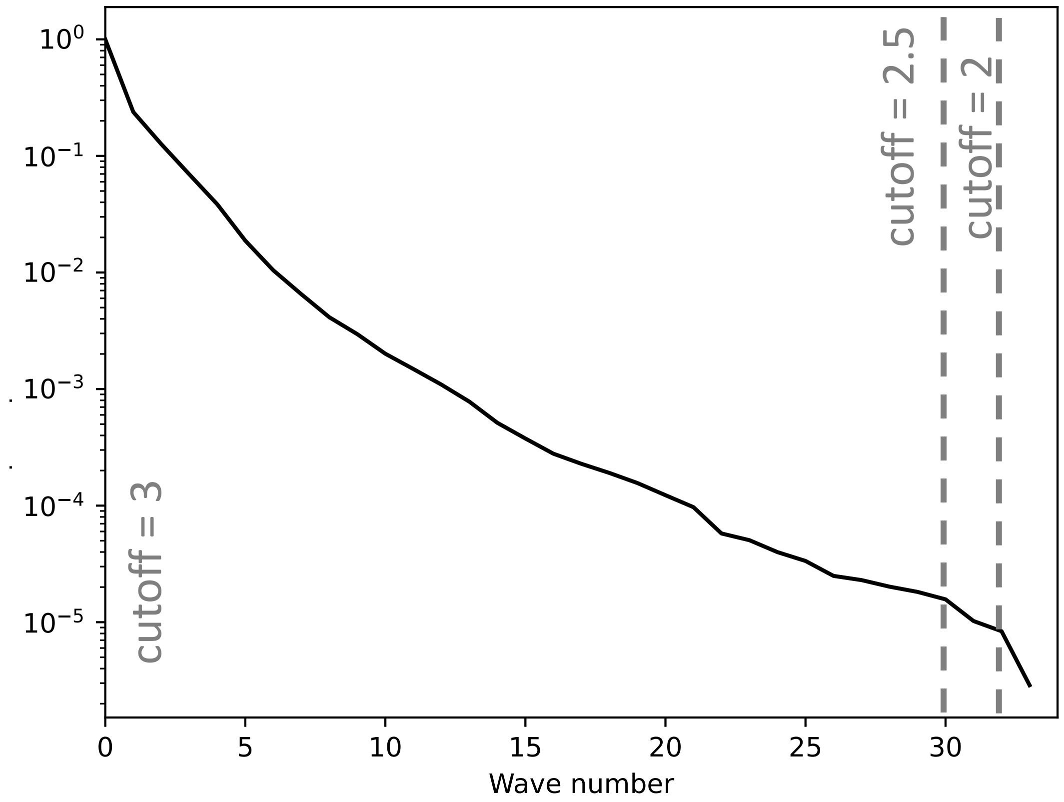


# NROY space evolution and convergence

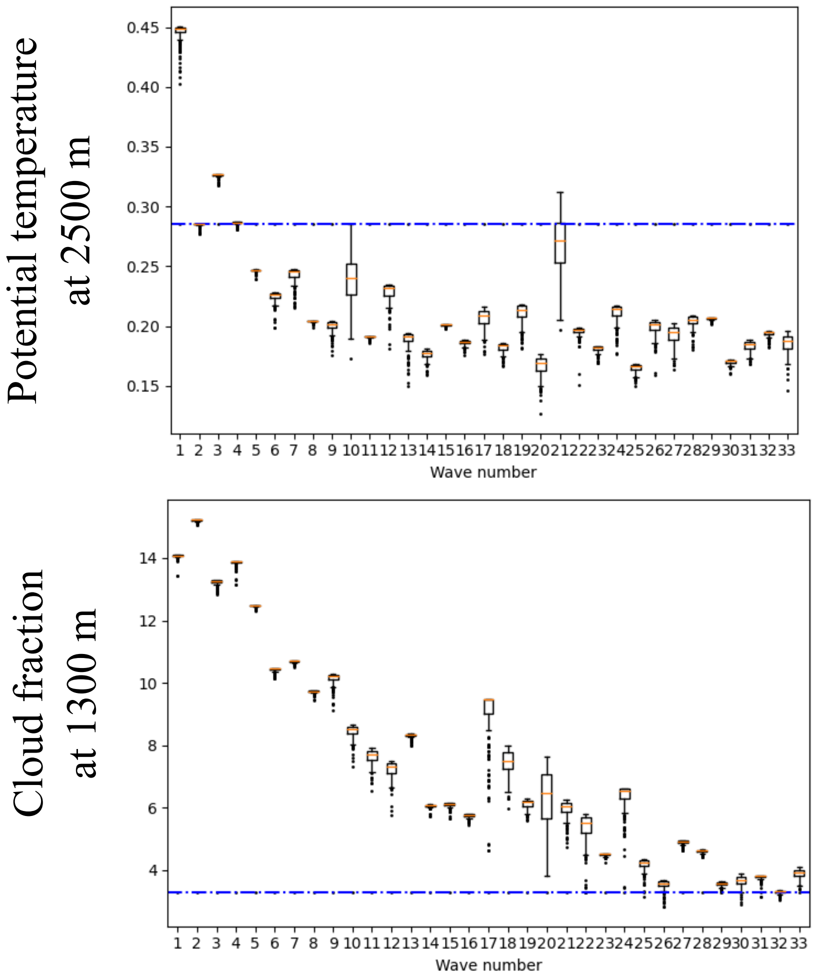
- Decrease of cutoff
  - when emulator uncertainty comparable/lower than reference uncertainty/tolerance-to-error
  - when NROY space size approximately stable
- After 33 waves, NROY $\sim 2.9\times10^{-6}$ of the input parameter space

  >> $\sim$290 over $10^8$ configurations

NROY space fraction




GP standard deviation (Leave-One-Out)

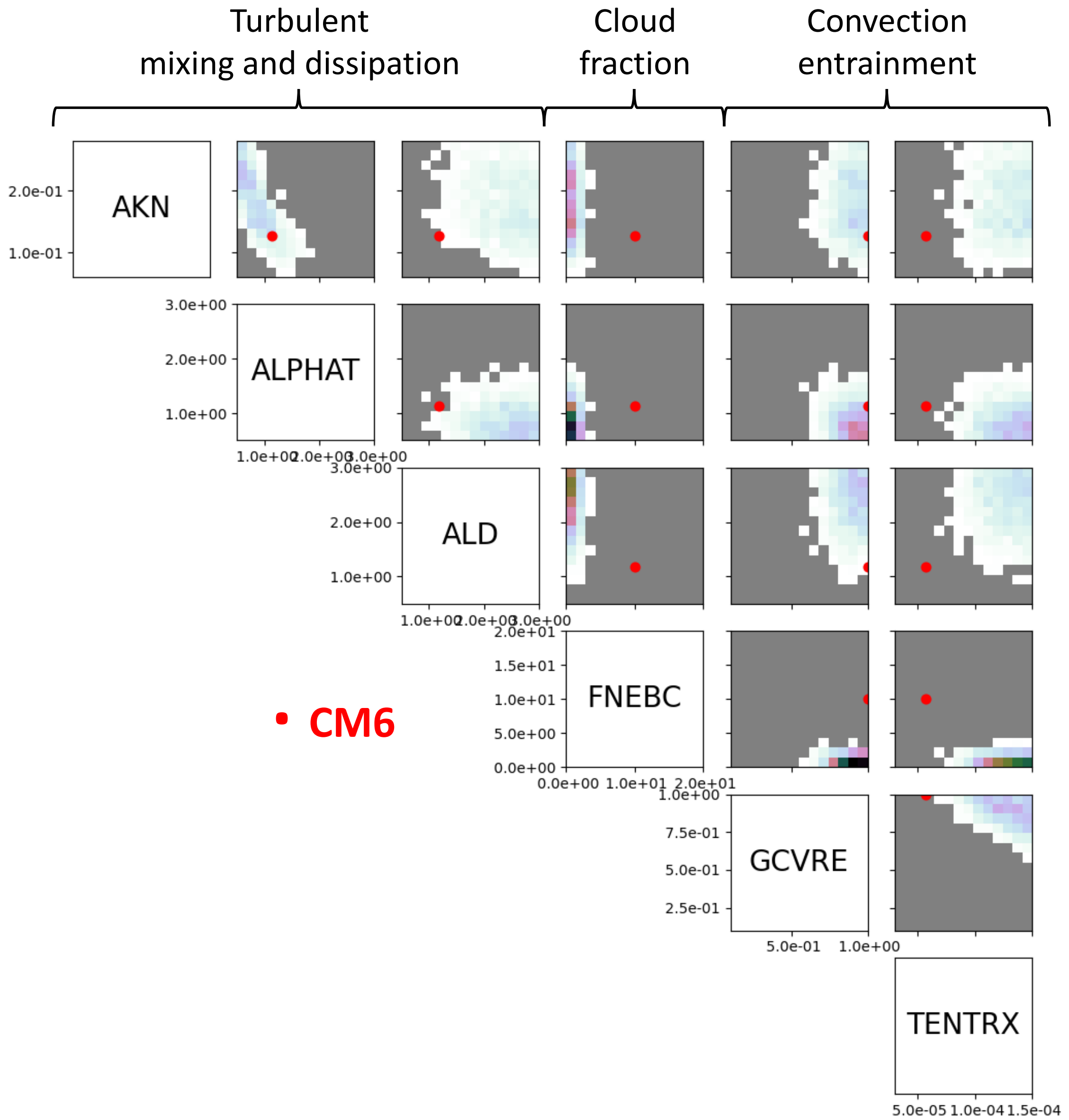


# Representing the NROY space

***Numerical characterization*** of the NROY space:

- (very) large sampling (LHS) of the input parameter space
- Use emulators to compute associated implausibilities
- Compute densities of points within NROY space as a function of parameters
- 1D or 2D representations

# Dominant parameters



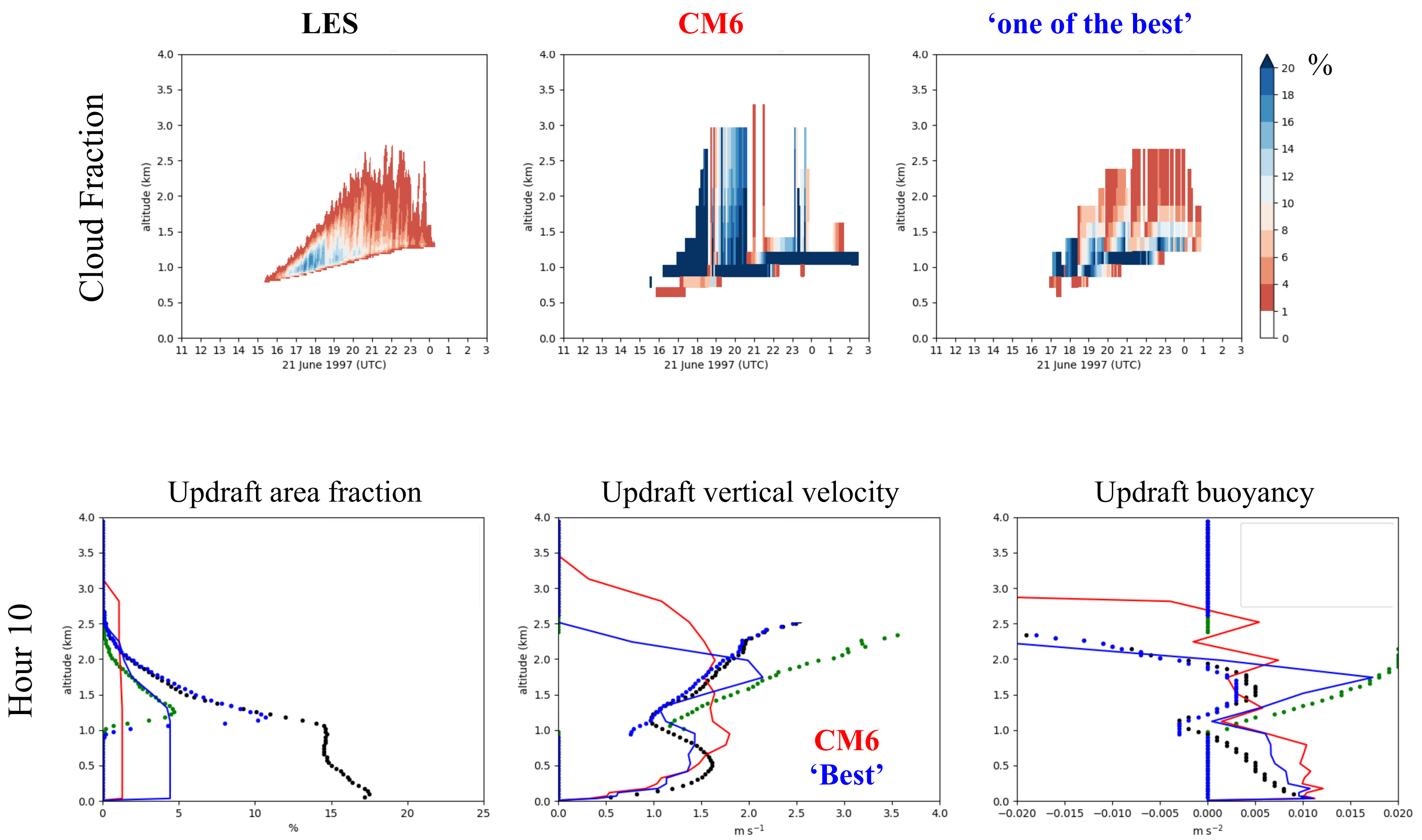

***Dominant parameters***

- Turbulent mixing (AKN and ALPHAT)
- TKE dissipation (ALD)
- Convective cloud fraction (FNEBC)
- Organized entrainement modulation factor (GCVRE)
- Maximum turbulent entrainment (TENTRX)

***Strong constraints on turbulent mixing and convective cloud fraction***

***High entrainment rates*** required for convection

# One configuration within the NROY space



# Calibration vs. structural limits

During the development and tuning of CNRM-CM6-1, hard to capture both shallow and deep convection (unified approach)

- ***Is the CNRM-CM6-1 unified approach for convection parameterization appropriate?***

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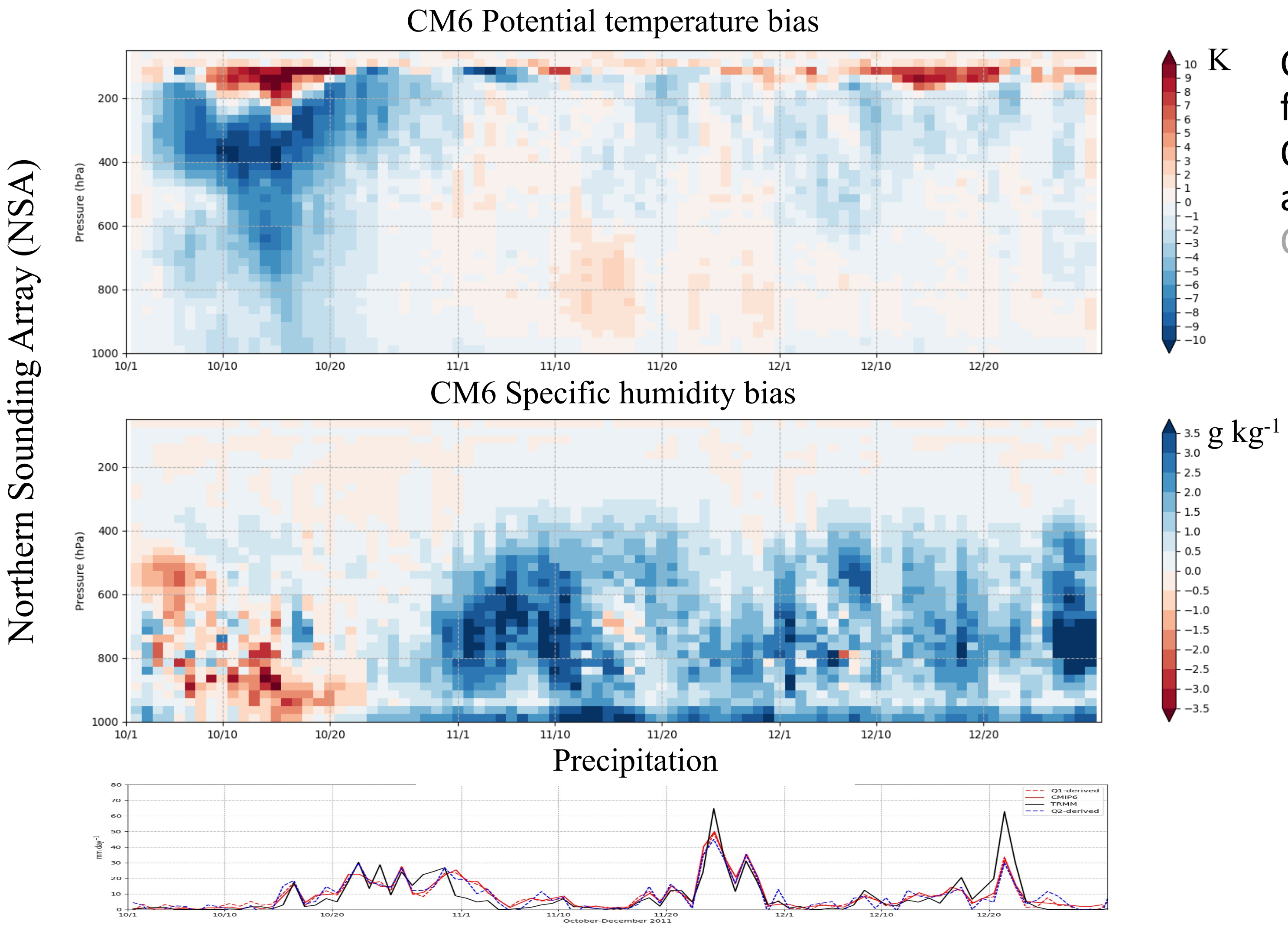
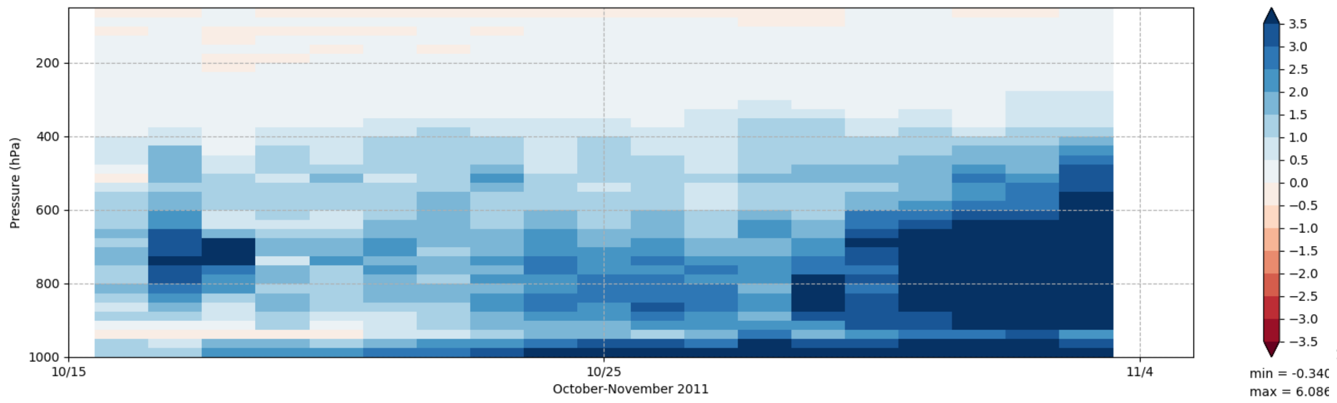



Consider the DYNAMO 1D case, based on a field campaign in OND 2011 in the Indian Ocean, and with alternating convectively-active and suppressed phases (Johnson and Ciesielski, 2013)

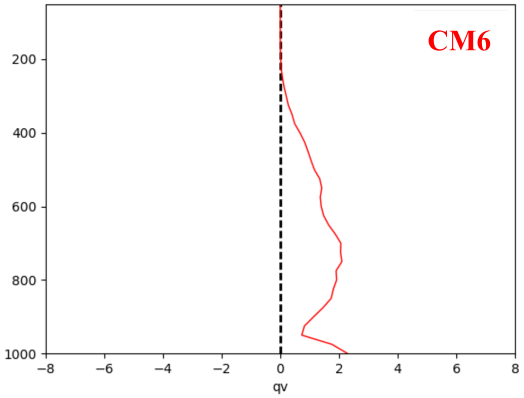
# Metrics, parameters and experimental design

- Focus on the first MJO event (15 October to 4 November 2011)
- **Metrics**: temperature/humidity average profiles
  - 3 levels for θ: 925, 600 and 200 hPa
  - 2 for $q_v$: 925 and 700 hPa
  - 4 for RH: 850, 700, 500 and 300 hPa
- **Reference** (field campaign observations):
  - temperature uncertainty ~0.1 K; tolerance 1 to 5 K
  - $q_v$ uncertainty ~0.1 g kg$^{-1}$; tolerance 0.2/0.1 g kg$^{-1}$
  - RH uncertainty ~2 %; tolerance 5 to 20%
- **Parameters**: same 26 parameters as for ARM-Cumulus
  + 13 for ice microphysics
  + 4 for cloud radiative properties
- Wave 1 and following: 200 simulations

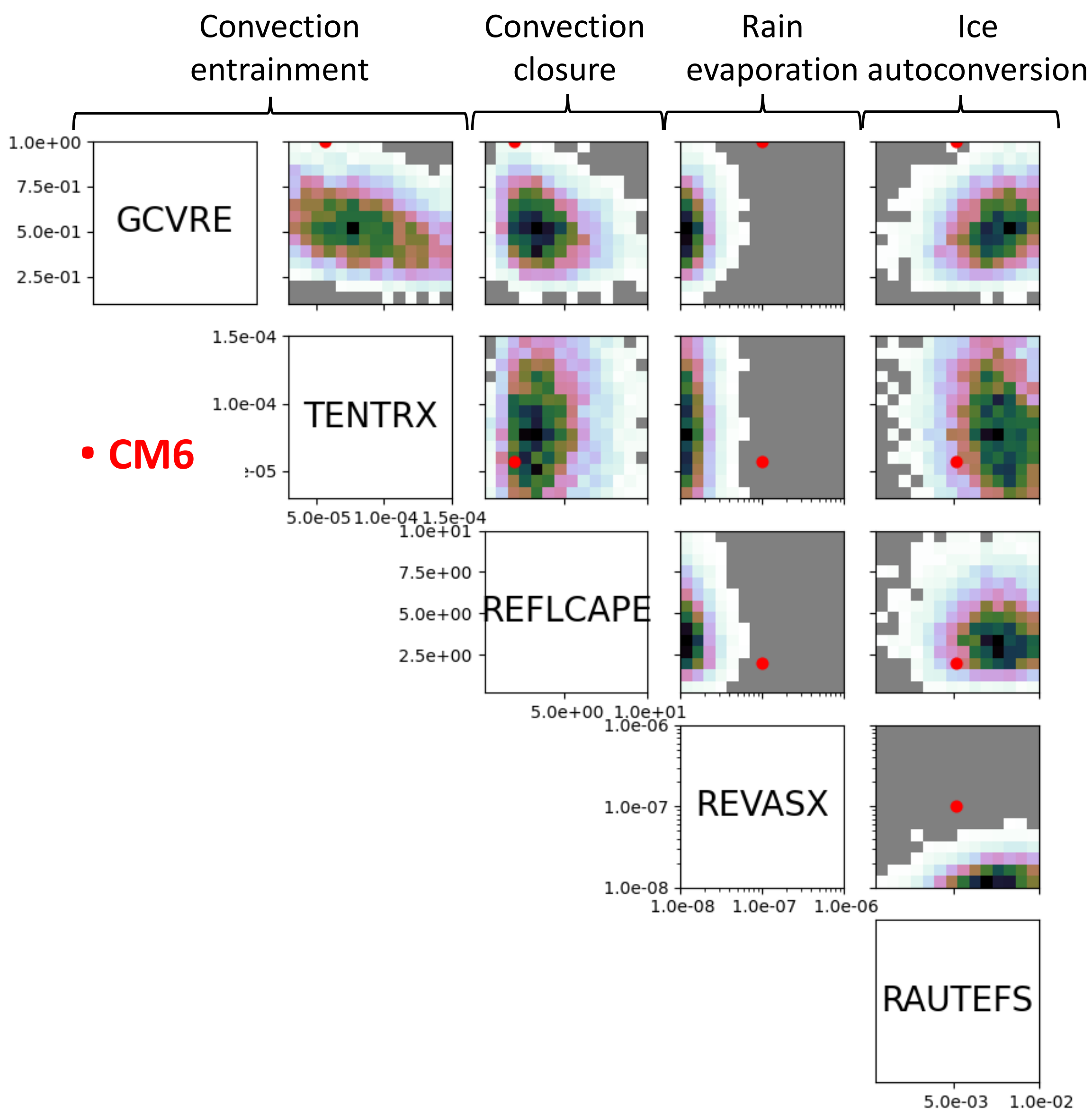
Specific humidity bias




20-day average bias



# Wave 29



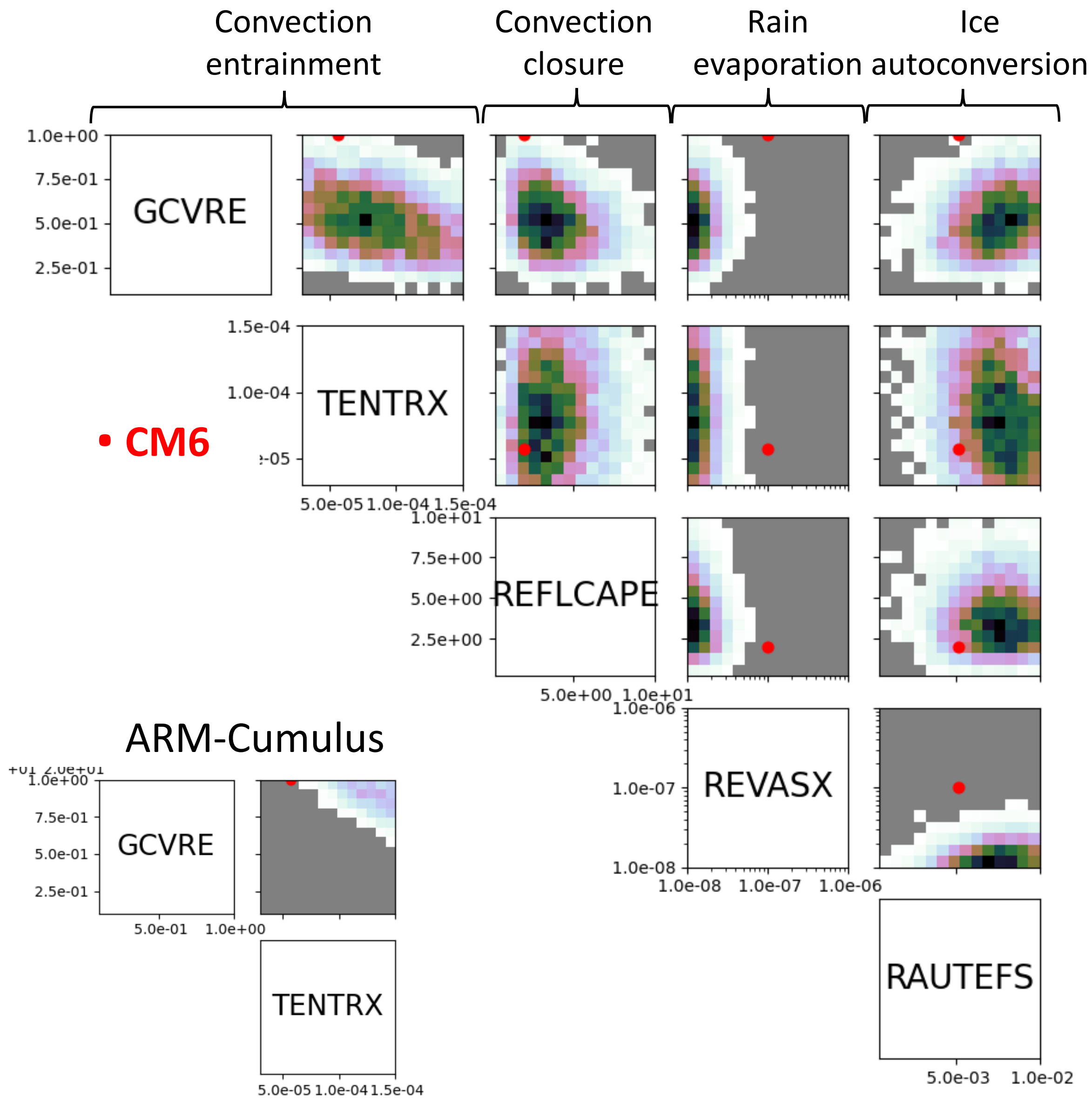

***Wave convergence not yet fully achieved.***

NROY$^{29}$ $\sim 6.9\times10^{-5}$ of the input space

***Dominant parameters*:**

- ***Rain evaporation*** rate key to get the moisture vertical profile right
- Reduced ice autoconversion required >> ***longer life cycle of (high-level) ice clouds***. Feedback through LW heating?
- ***Convection intensity*** (closure) is important
- ***Convective entrainment*** still key, towards more moderate values compared to shallow convection.

# Deep vs. shallow convection

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- ***Convection intensity*** (closure) is important
- ***Convective entrainment*** still key, towards more moderate values compared to shallow convection.
- ***Weak overlap between the entrainment parameter NROY spaces for shallow and deep cases***

# What did we learn from 1D configurations?

- ***History Matching with Iterative refocusing:*** framework to rigorously explore the ***parametric calibration*** of a parameterization/model physics, and identify its ***structural limits***

- Better tuning of the CNRM convective parameterization (in fact the CNRM physics) can be achieved for each of the two 1D cases addressed here.

- The combination of a shallow convection case and a deep convection case emphasizes the difficulty to make the CNRM “unified” convection parameterization work for both.
  - ***The CNRM-CM6-1 single-plume mass-flux approach is structurally limited.***

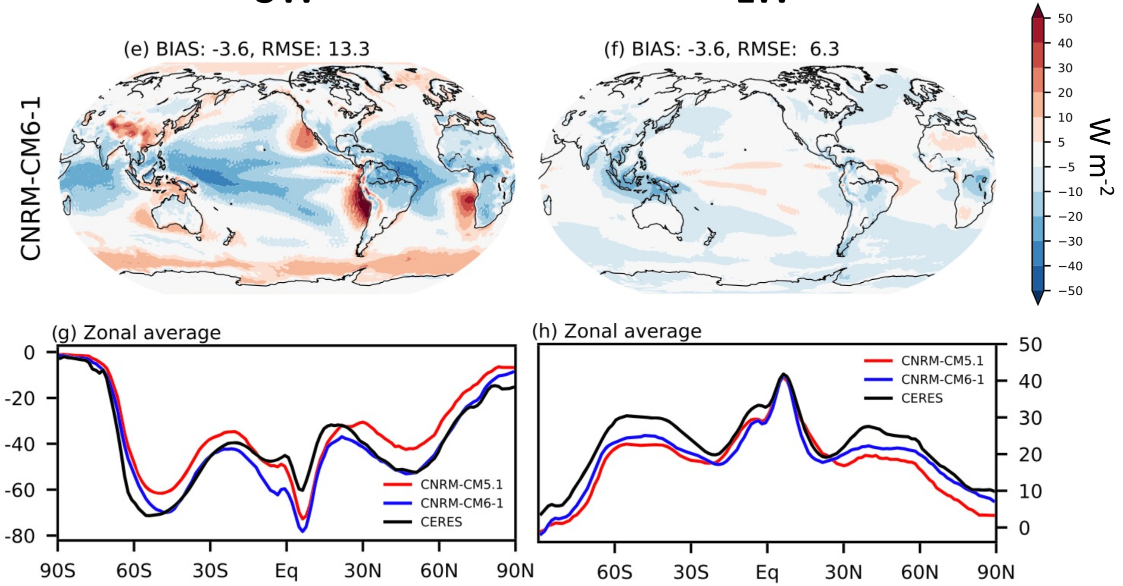
- Shallow and deep convection regimes require significantly different entrainment rates.

➢ ***What about more ‘realistic’ (3D) configurations?***

# Calibrating the 3D (atmospheric) configuration of CNRM-CM6-1

CRE at TOA

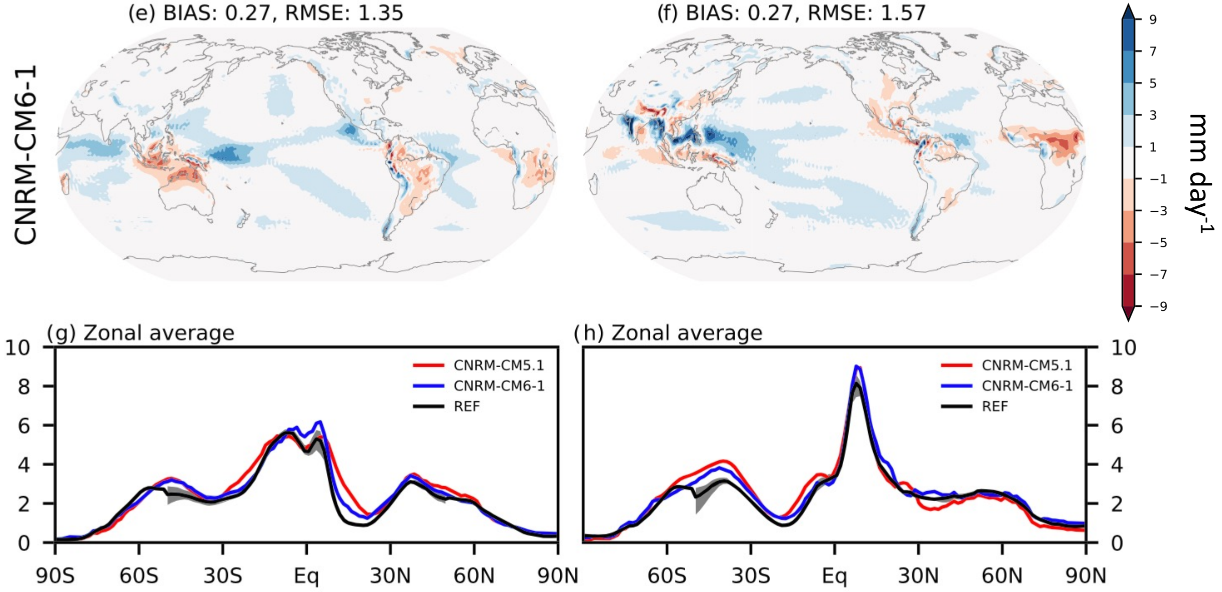
SW LW




Reference: *CERES-EBAF Ed. 4.1*

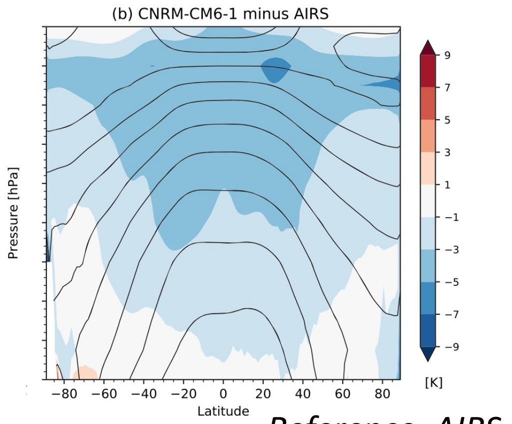
Precipitation

DJFM JJAS




*Reference: MSWEP v1.2 + GPCP v2.3 + TRMM 3B42 v7*

Annual Temperature

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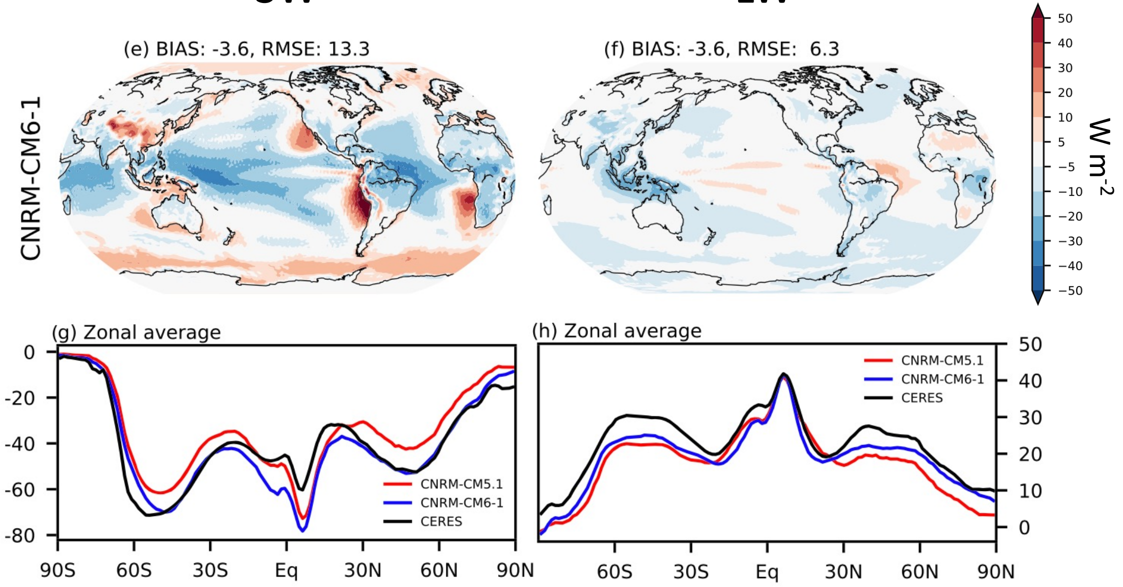


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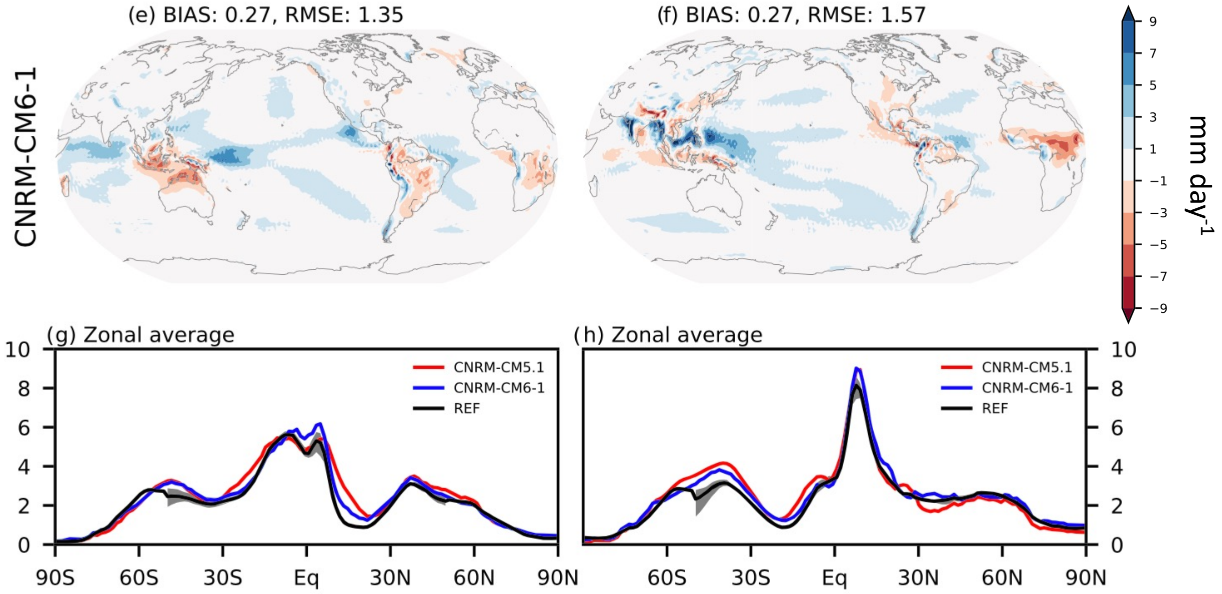


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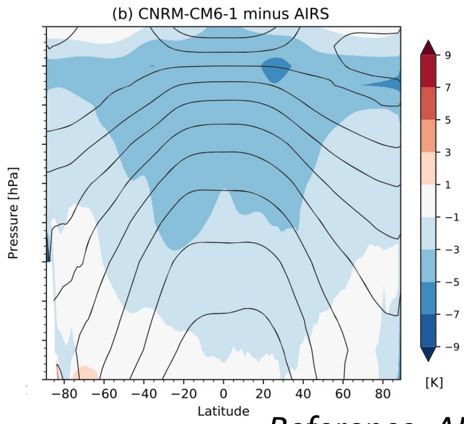


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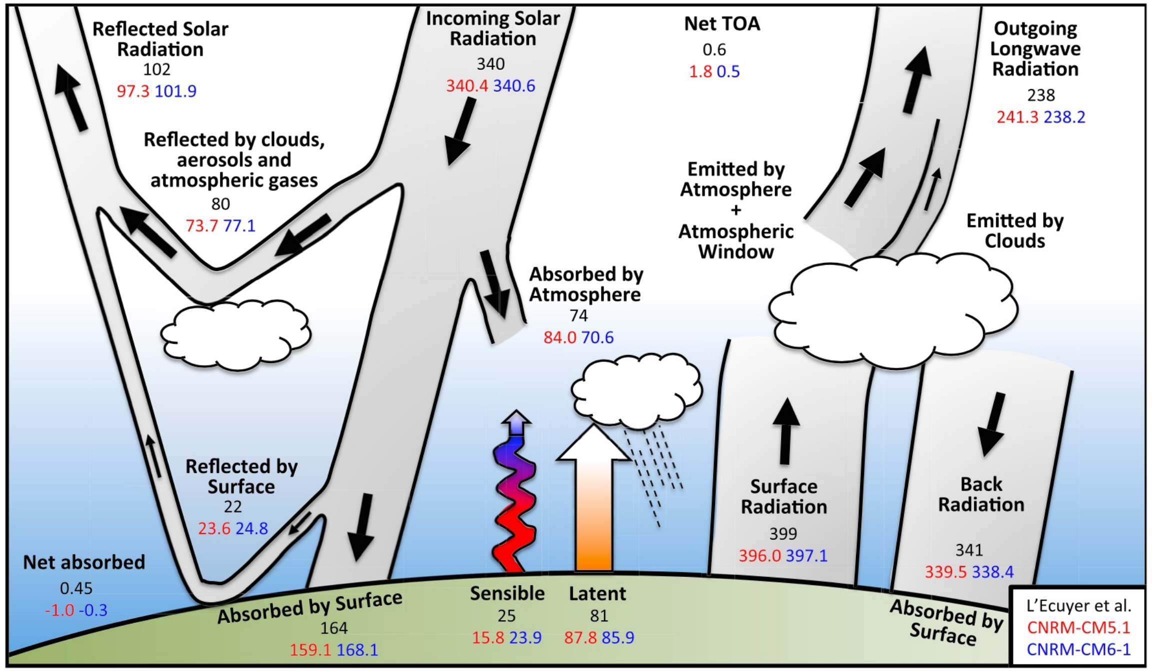
➢ ***Can we reduce CNRM-CM6-1 biases through better calibration?***

*Roehrig et al. (2020)*

# Metrics, references and uncertainty estimates

Following the CNRM-CM6-1 tuning strategy, 3 classes of metrics:

1. ***Global averages of the energy budget components***
   - at TOA: OLR, OSR, Net, SW/LW CRE
   - at the surface ocean: Net, SWdn, LWdn
   - Values from CERES-EBAF, uncertainties based on the literature
   - Except Net at surface/TOA = 0 +/- 0.1 W $m^{-2}$ : the model has to be equilibrated.
   - Tolerance to error: 0.5 W $m^{-2}$




Roehrig et al. (2020)

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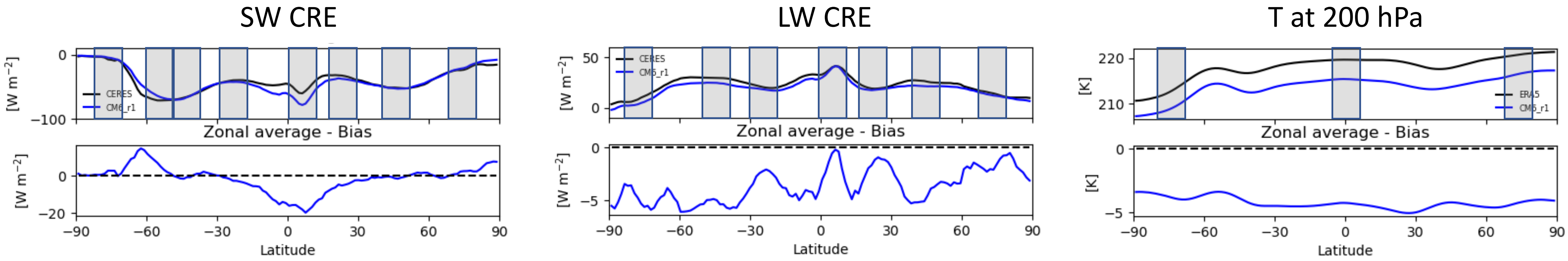
1. Global averages of the energy budget components
2. ***Zonally average profiles*** of SW/LW CRE + Temperature at 200 hPa
   - SW/LW CRE: CERES-EBAF with uncertainty of 2 W $m^{-2}$ + tolerance of 1 W $m^{-2}$
   - T200: based on ERA5/JRA55/MERRA/CFSR ensemble mean and std, tolerance 1.5 K



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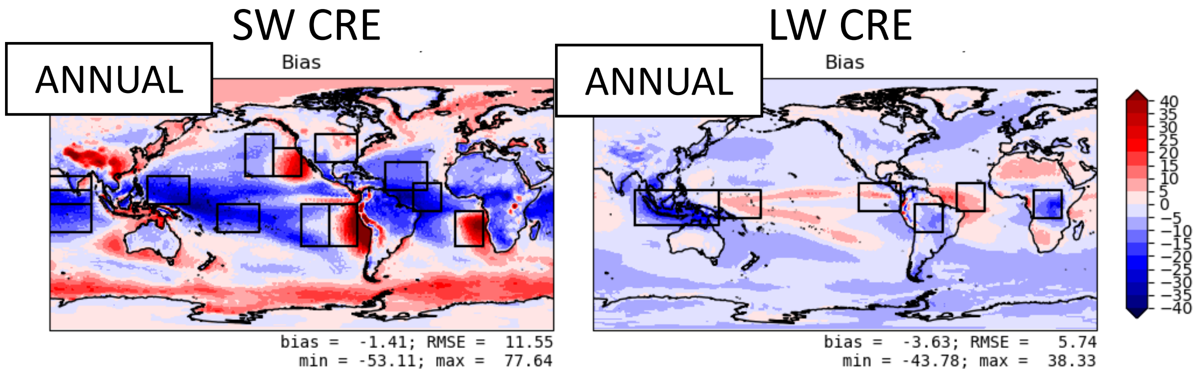
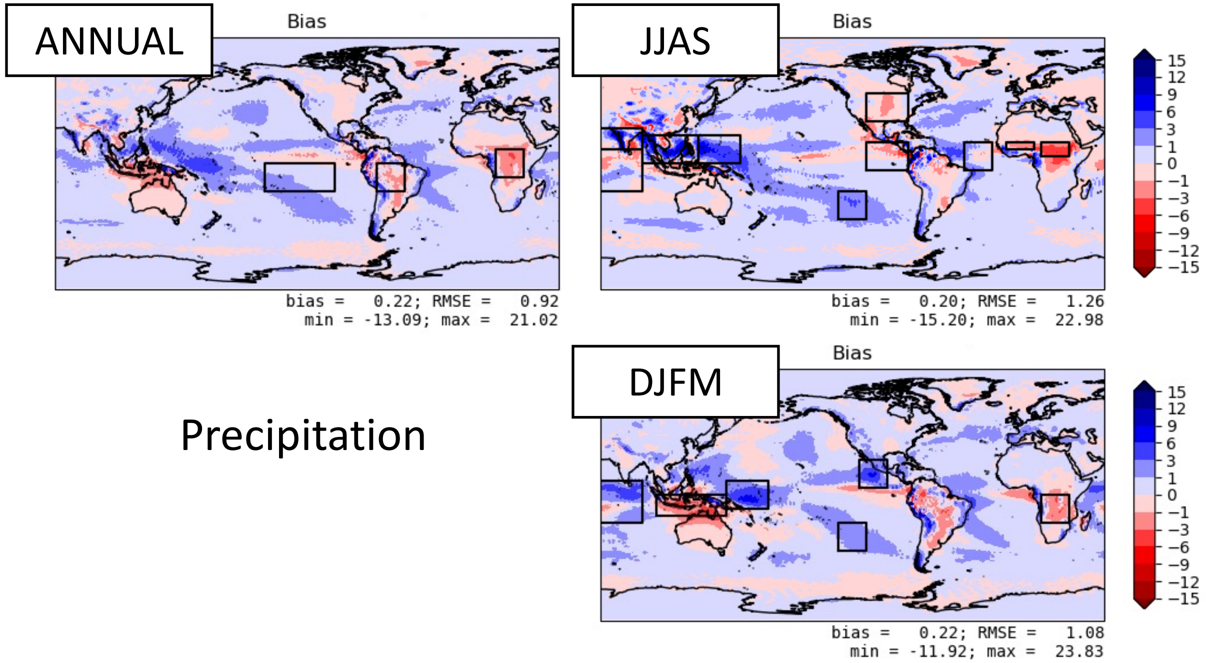
1. Global averages of the energy budget components
2. Zonally average profiles of SW/LW CRE + Temperature at 200 hPa
3. ***Regional and seasonal averages*** of SW/LW CRE and precipitation
   - SW/LW CRE: CERES-EBAF, uncertainty of 2 W $m^{-2}$, tolerance of 5 W $m^{-2}$
   - Precipitation: MSWEP/GPCP/TRMM 3B42 ensemble mean and std, tolerance between 0.5 and 1 mm $day^{-1}$



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- ***63 (scalar) metrics***

# Model parameters and simulation strategy

***46 model parameters***

- 7 from turbulence (TKE scheme + PBL-top entrainment)
- 16 from microphysics (1-moment, 5 hydrometeors)
- 19 from the unified dry, shallow and deep convection scheme
- 4 from cloud radiative properties (heterogeneity)

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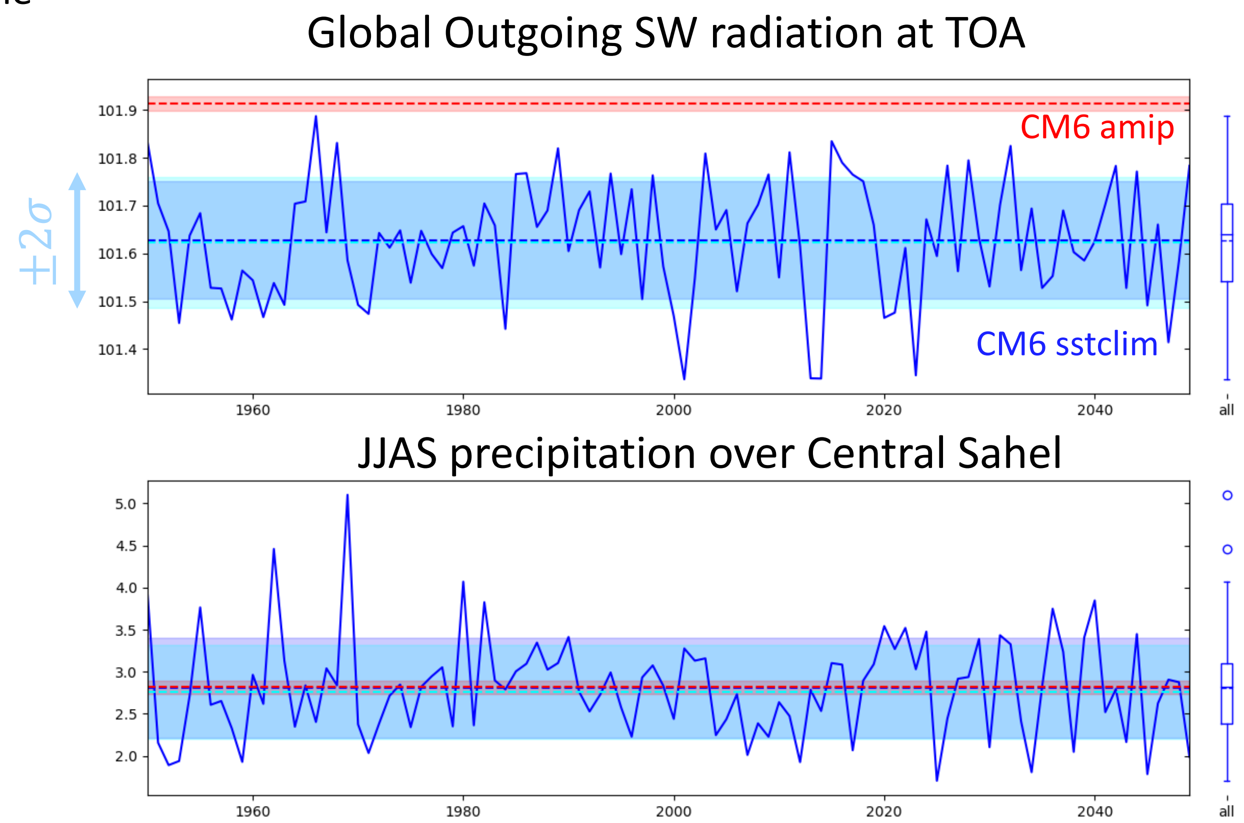
### ***Waves of 400 simulations***

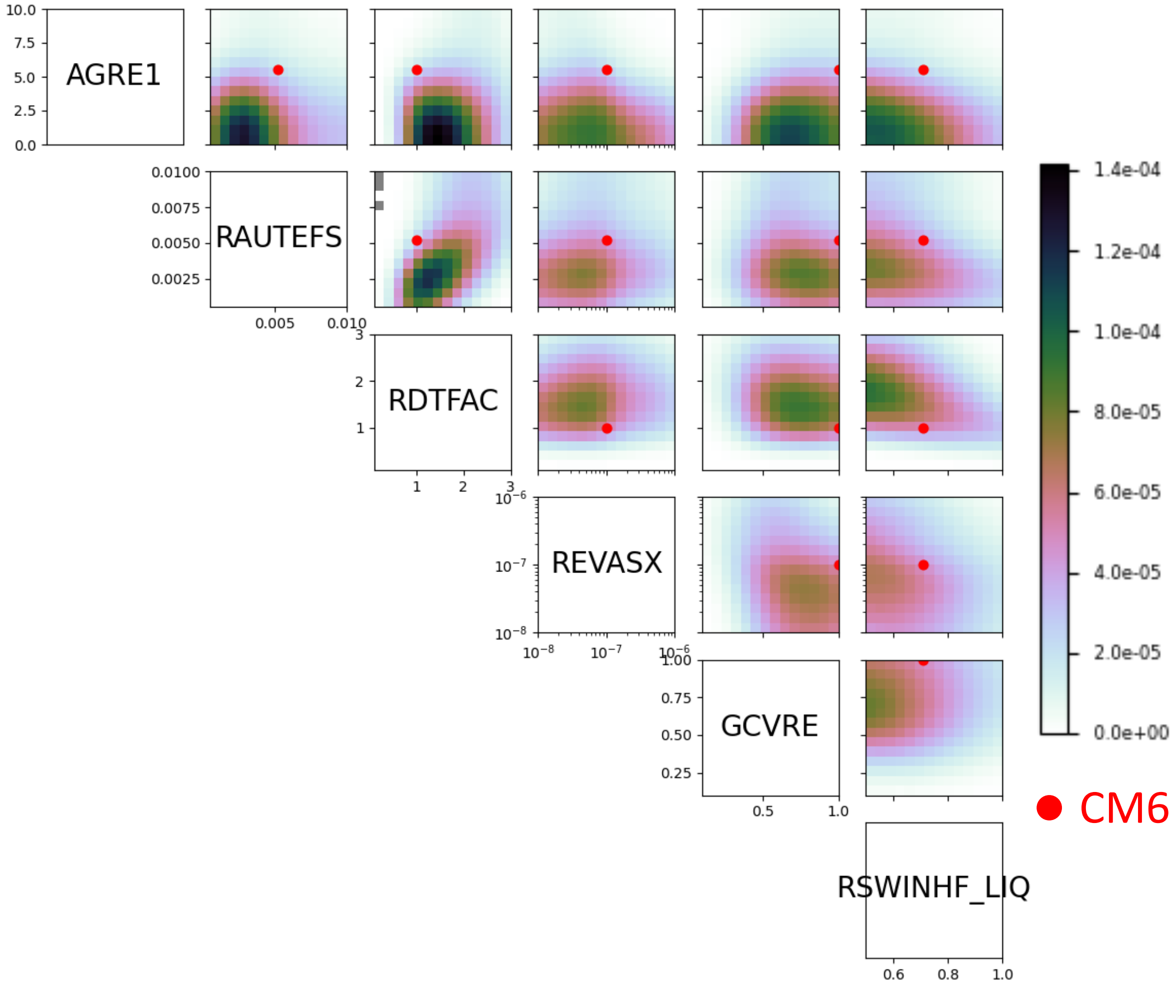
- 1-year ***sstclim*** simulations + 3-month spin-up
- sstclim vs amip correction of the reference target
- Consideration of ***internal variability uncertainty*** based on a 100-year sstclim simulation with CNRM-CM6-1.
- Latin Hypercube sampling for 1st wave



# Wave 1 results

- NROY[1] space: 0.66% of the input space
- Cloud (esp. ice) and convection parameters are critical

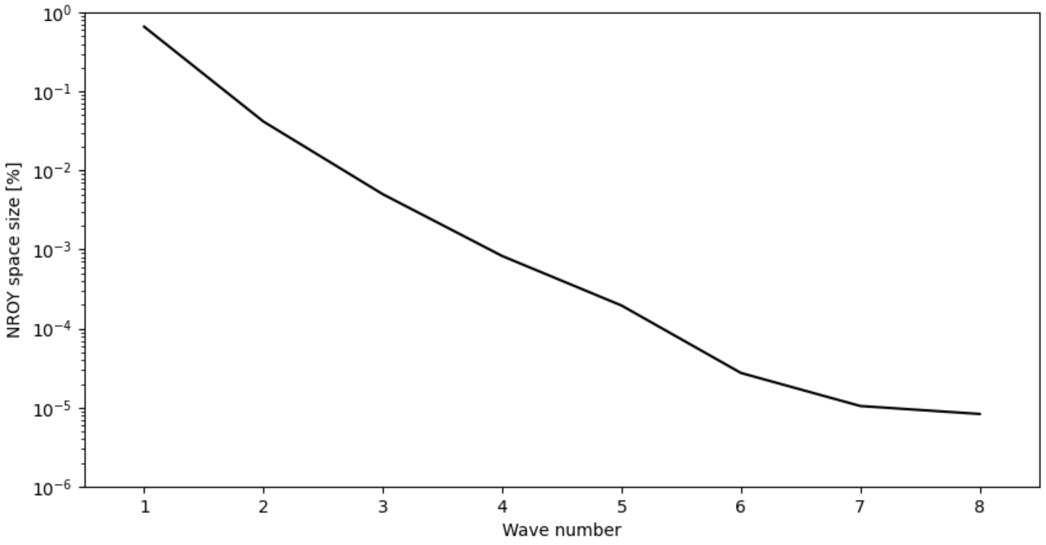
NROY[1] density within input parameter space
For some of the dominant parameters



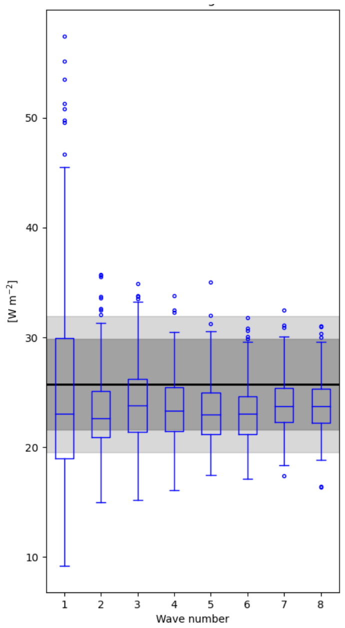
# From Wave 1 to Wave 8

- Large shrinking of the NROY space size (8 orders of magnitude)
- Some metrics have converged, some are more demanding

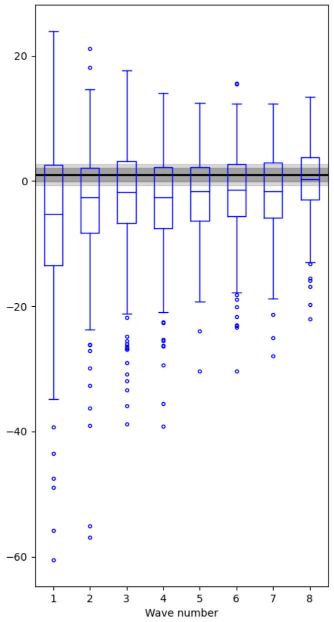
NROY space fraction of the input space




Global LW CRE at TOA

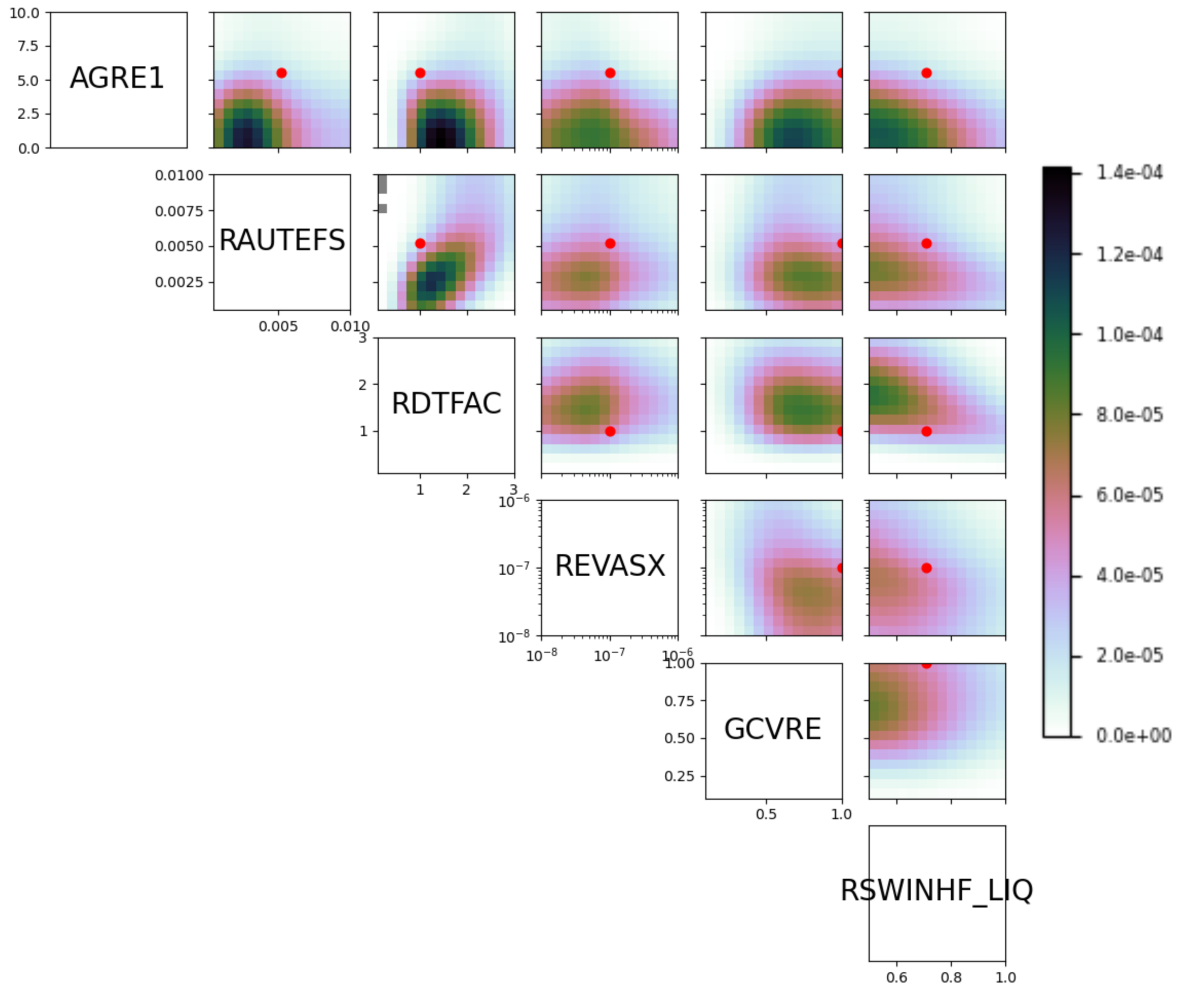



Ocean net energy flux

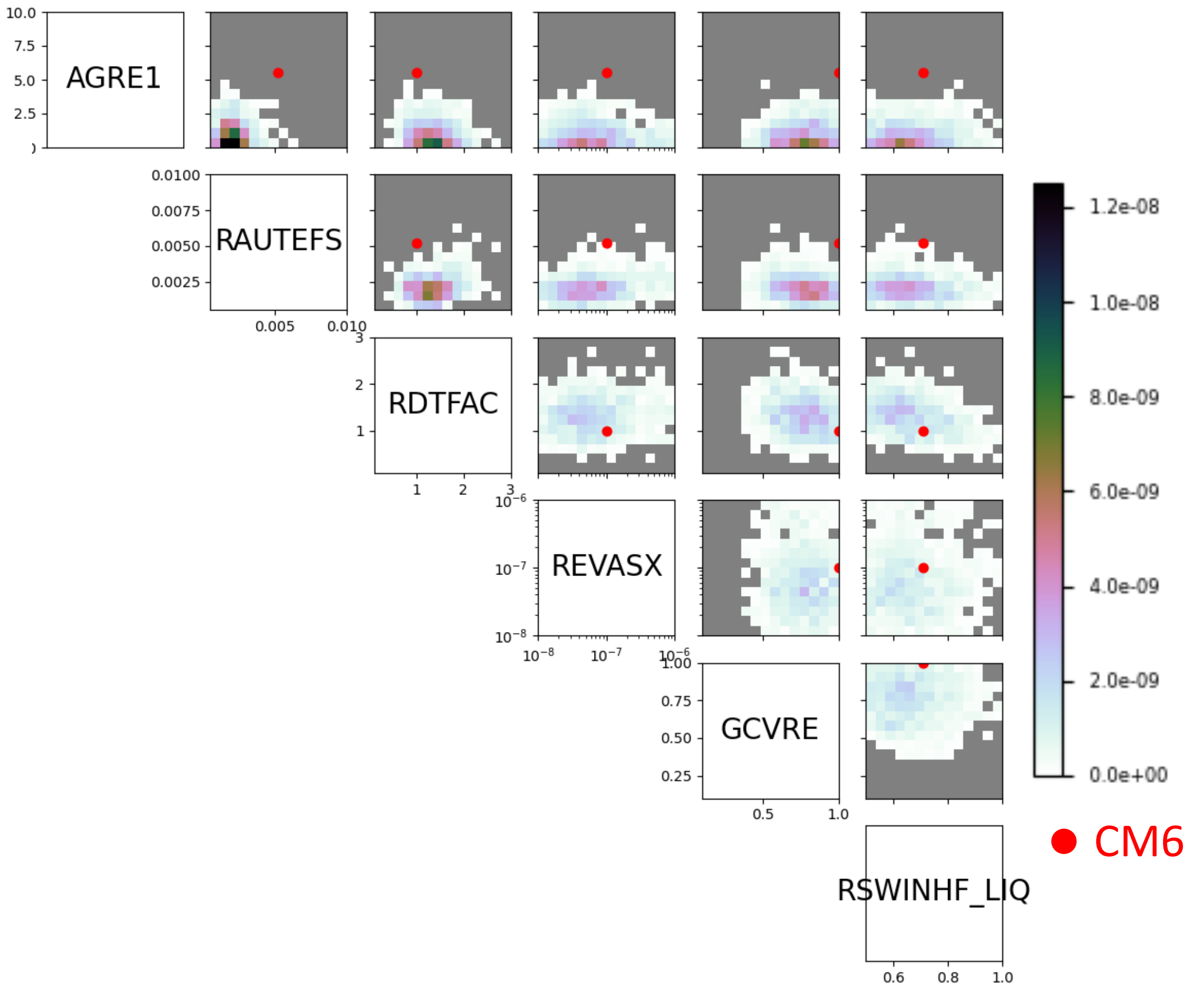


# From Wave 1 to Wave 8

NROY[1] density within input parameter space
For some of the dominant parameters




NROY[8] density within input parameter space
For some of the dominant parameters




+ some new dominant parameters have emerged

# Choosing configurations of interest

***Unfortunately, none of Wave 1-8 simulations fulfils all the metrics***

- Convergence is not yet achieved
- Appropriate sampling of small NROY spaces is difficult and requires further work
- Some tolerances to error are likely too weak and require to be revisited.

***Nevertheless***

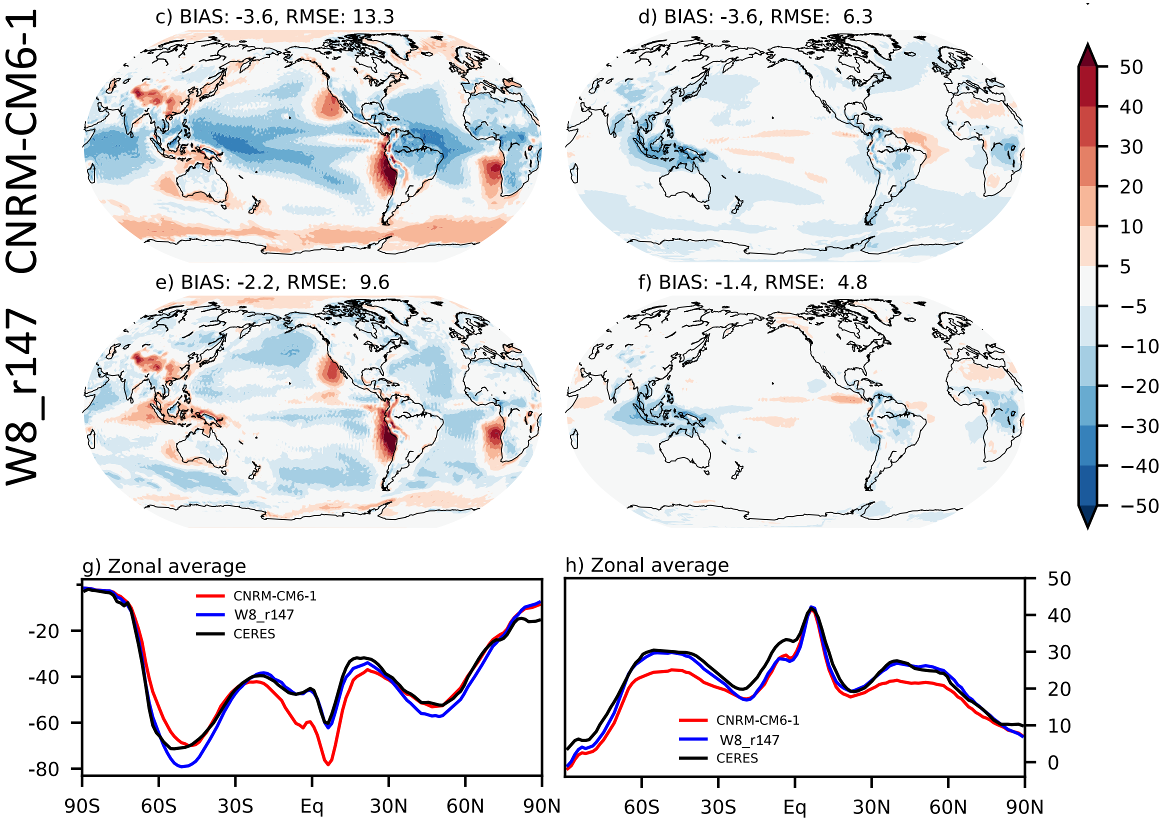
- A few simulations fulfil all the metrics but one (for a cutoff of 3)
- A few have interestingly low RMSEs for targeted variables

➢ A selection of these simulations is further analysed with 10-year amip-style simulations.

# Improved performance?

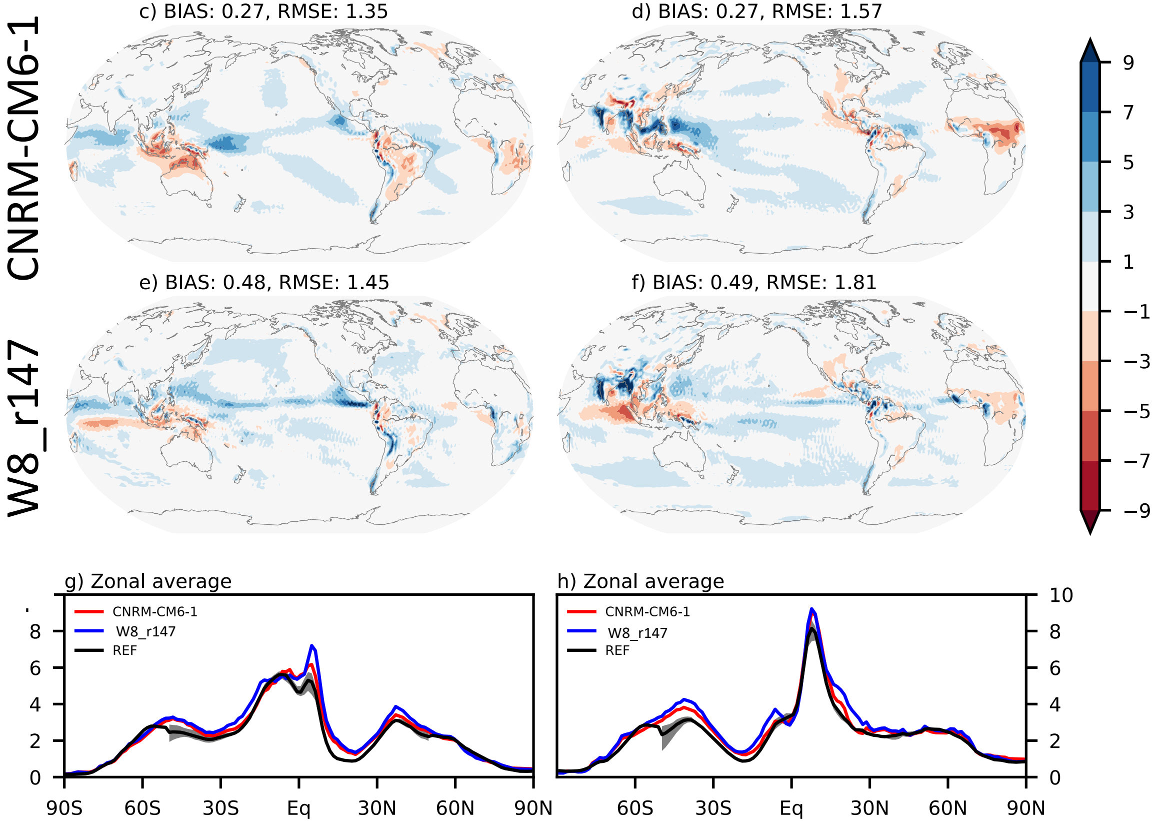
## CRE at TOA

SW LW




## Precipitation

DJFM JJAS



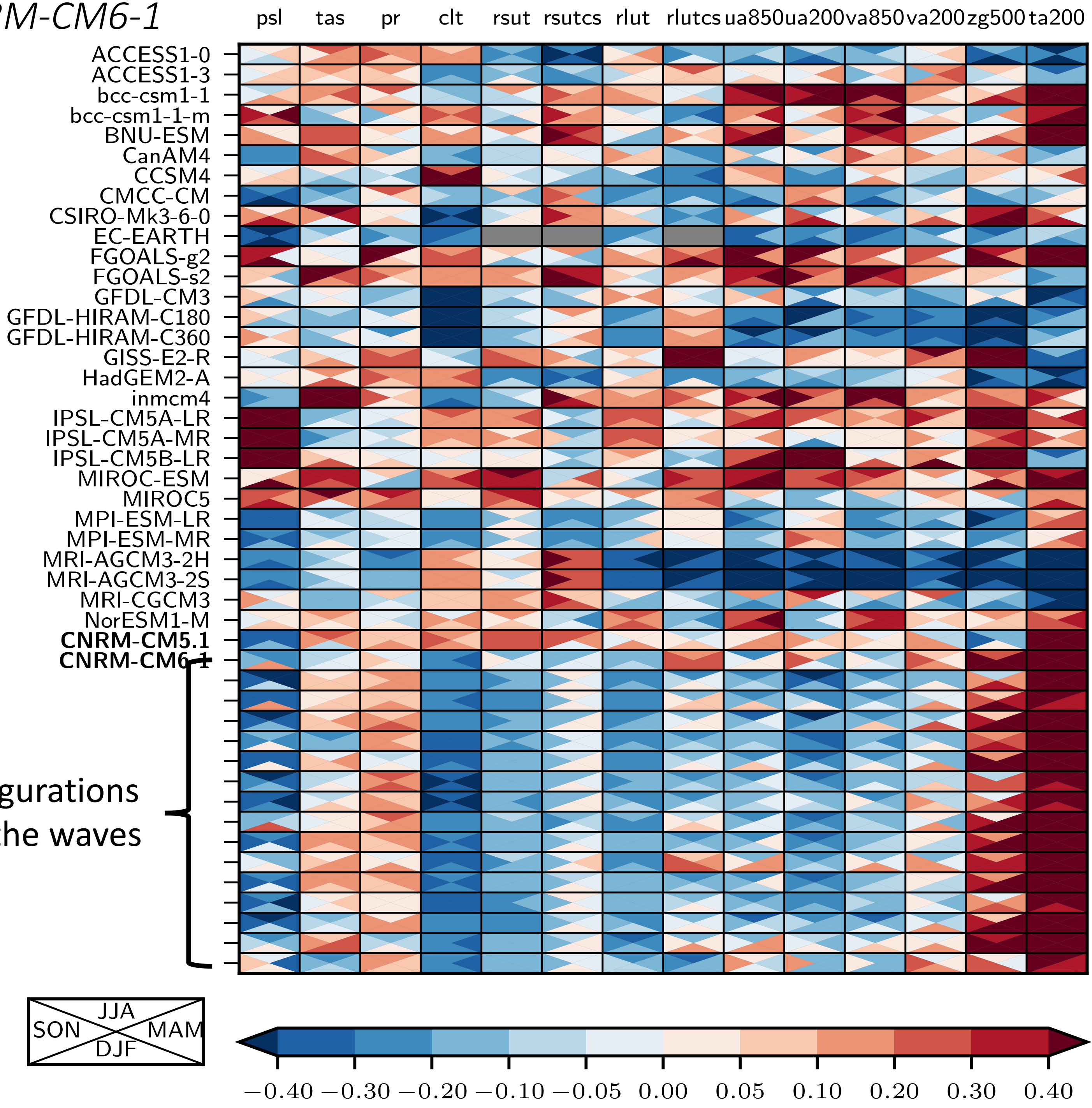

- ***Improved or similar performance*** on several mean state features
- Some errors seems truly structural: clouds/radiation over eastern part of ocean basins

# Improved performance?

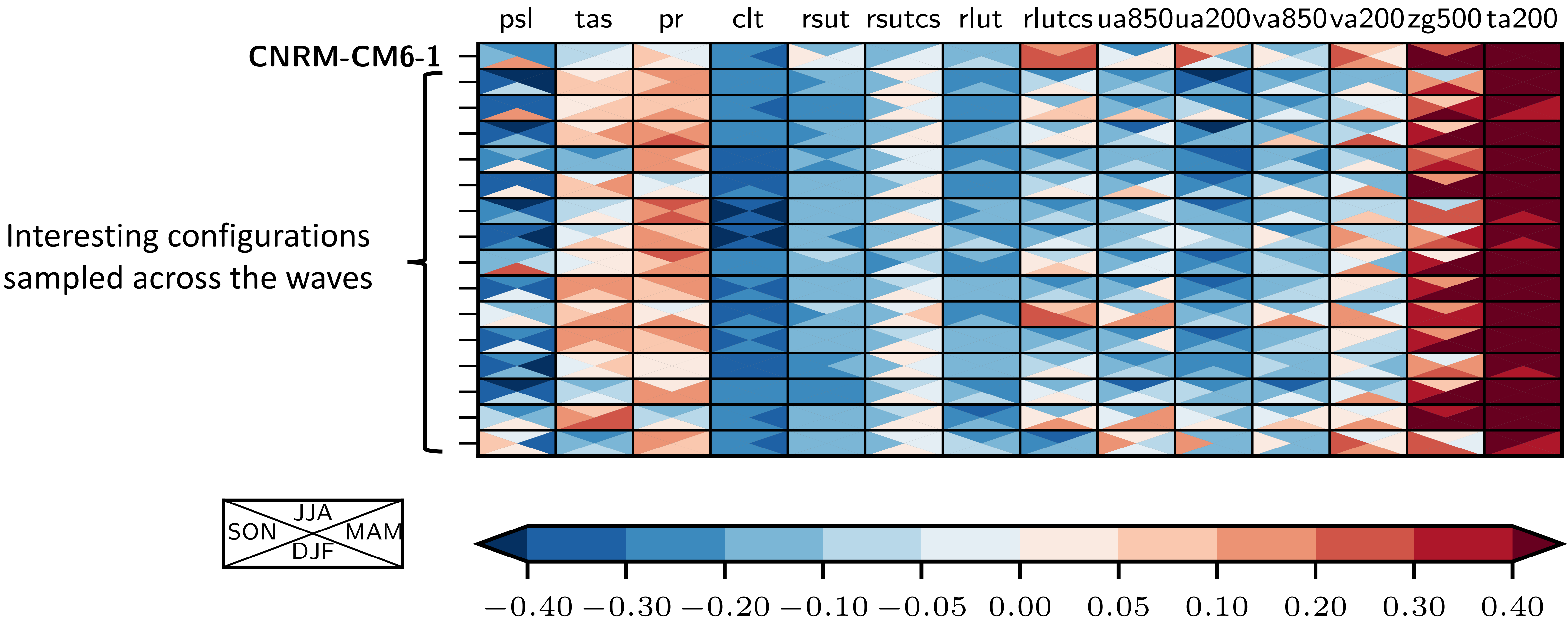
Relative score within the CMIP5 ensemble
*(Gleckler et al. 2016)*

$$\text{score} = \frac{\text{RMSE} - \text{RMSE}_{\text{median}}}{\text{RMSE}_{\text{median}}}$$

Interesting configurations sampled across the waves



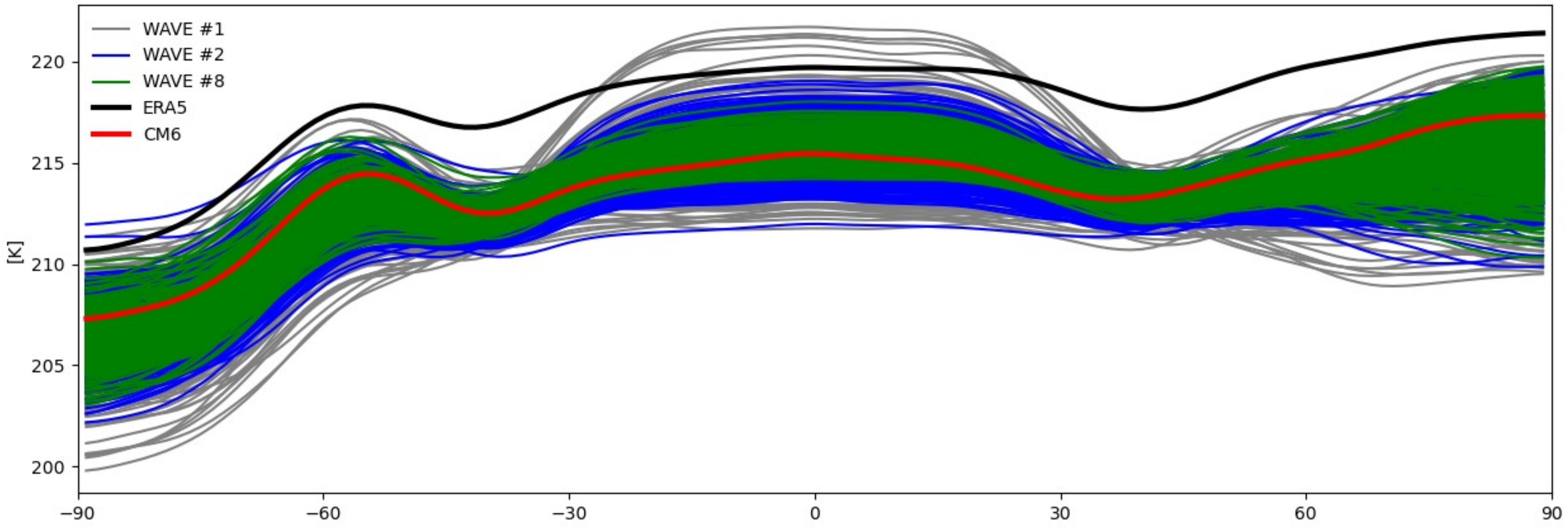
# Improved performance?




- ***Improved or similar performance*** on several mean state features
- Some errors seems truly structural: clouds/radiation over eastern part of ocean basins, upper-tropospheric temperature
- Some ***trade-offs*** are required

# Upper-tropospheric temperature bias: structural limit?

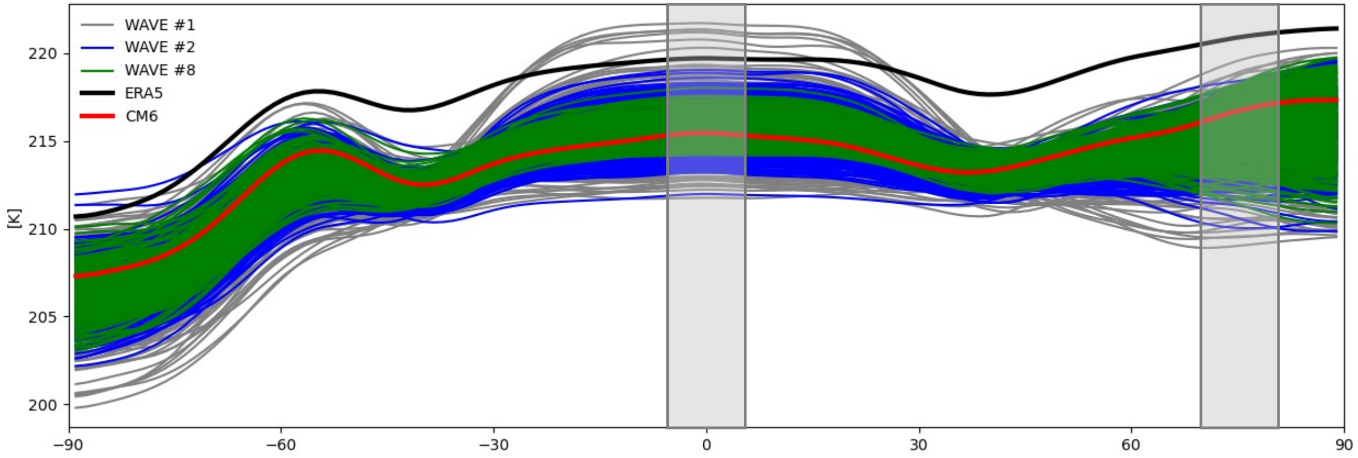
Zonally-average 200-hPa Temperature

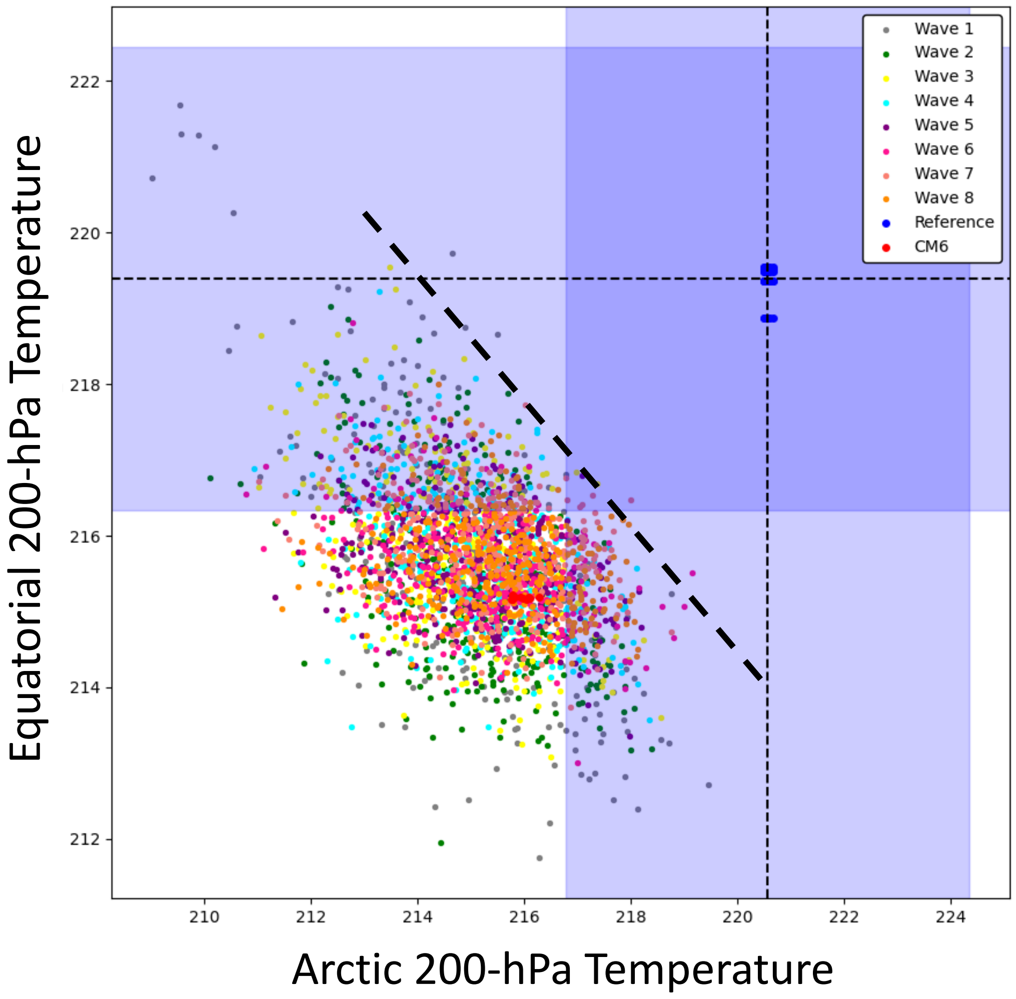



- Simulations performing well (beyond the chosen tolerance to error) in the equatorial regions disappear with successive waves
  - ➢ Incompatible with other metrics

# Upper-tropospheric temperature bias: structural limit?

Zonally-average 200-hPa Temperature




- Simulations performing well (beyond the chosen tolerance to error) in the equatorial regions disappear with successive waves
    - ➢ Incompatible with other metrics
- The model can most likely not capture both equatorial and arctic upper-tropospheric temperatures within uncertainty ranges, while remaining compatible with other metrics.

# From 1D and 3D: the High-Tune philosophy

- ***Start calibration at the process level*** (1D vs. LES) to ***pre-condition*** calibration of more realistic configurations
  - Keep the representation of processes right

- Requirement: have ***high-quality references*** (observations, LES or CPM) for the targeted processes.
  - Some are available (LES for boundary-layer convection/clouds, stable boundary layers)
  - Some are currently being developed (radiation for boundary-layer clouds)
  - Some are not fully appropriate or missing (e.g., microphysics)

# Proof of concept with LMDZ

### *Multi 1D case approach (boundary-layer clouds) :*

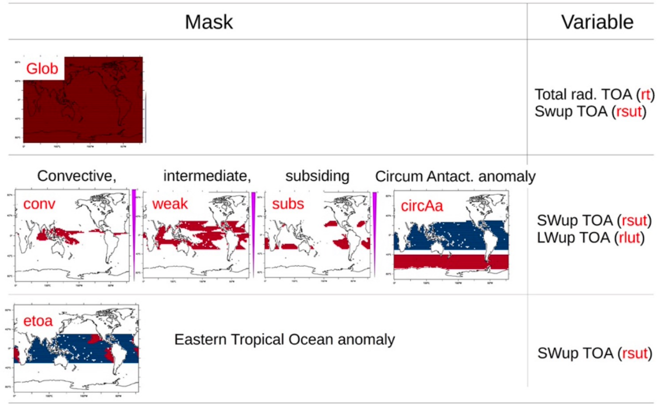
- Dry convective boundary layer (IHOP, Couvreux et al. 1996)
- Continental cumulus (ARMCU, Brown et al. 2002)
- Marine cumulus (RICO, van Zanten et al. 2011)
- Stratocumulus-cumulus transition (SANDU, Sandu et al. 2011)
- Reference LES: Meso-NH ou UCLA

*Metrics Retained for the SCM/LES Tuning*

| Case | IHOP | ARMCU | RICO | SANDU | SANDU | SANDU |
|---|---|---|---|---|---|---|
| Subcase | REF | REF | REF | REF | SLOW | FAST |
| Time | 7–9 | 7–9 | 19–25 | 50–60 | 50–60 | 50–60 |
| $\theta_{400-600\ \mathrm{m}}$ | X | X | - | - | - | - |
| $q_{v,400-600\ \mathrm{m}}$ | - | X | - | - | - | - |
| $\alpha_{cld,\mathrm{max}}$ | - | X | X | - | - | - |
| $z_{cld,\mathrm{ave}}$ | - | X | - | X | - | - |
| $z_{cld,\mathrm{max}}$ | - | X | - | X | X | X |

### *Metrics*

- 11 1D metrics: potential temperature, humidity averaged in the boundary layer, cloud fraction
- 11 3D metrics: TOA radiative budget components, global/regional averages




| Metrics | target $\mathrm{W\ m^{-2}}$ | error $\mathrm{W\ m^{-2}}$ |
|---|---|---|
| glob.rt | 2.5 | 0.2 |
| glob.rsut | 99.6 | 5 |
| circAa.rsut | 24.0 | 5 |
| circAa.rlut | -48.6 | 5 |
| subs.rsut | 84.9 | 5 |
| weak.rsut | 81.8 | 5 |
| conv.rsut | 103.2 | 5 |
| subs.rlut | 274.6 | 5 |
| weak.rlut | 264.3 | 5 |
| conv.rlut | 235.8 | 5 |
| etoa.rsut | 11.0 | 5 |

### *LMDZ model parameters*

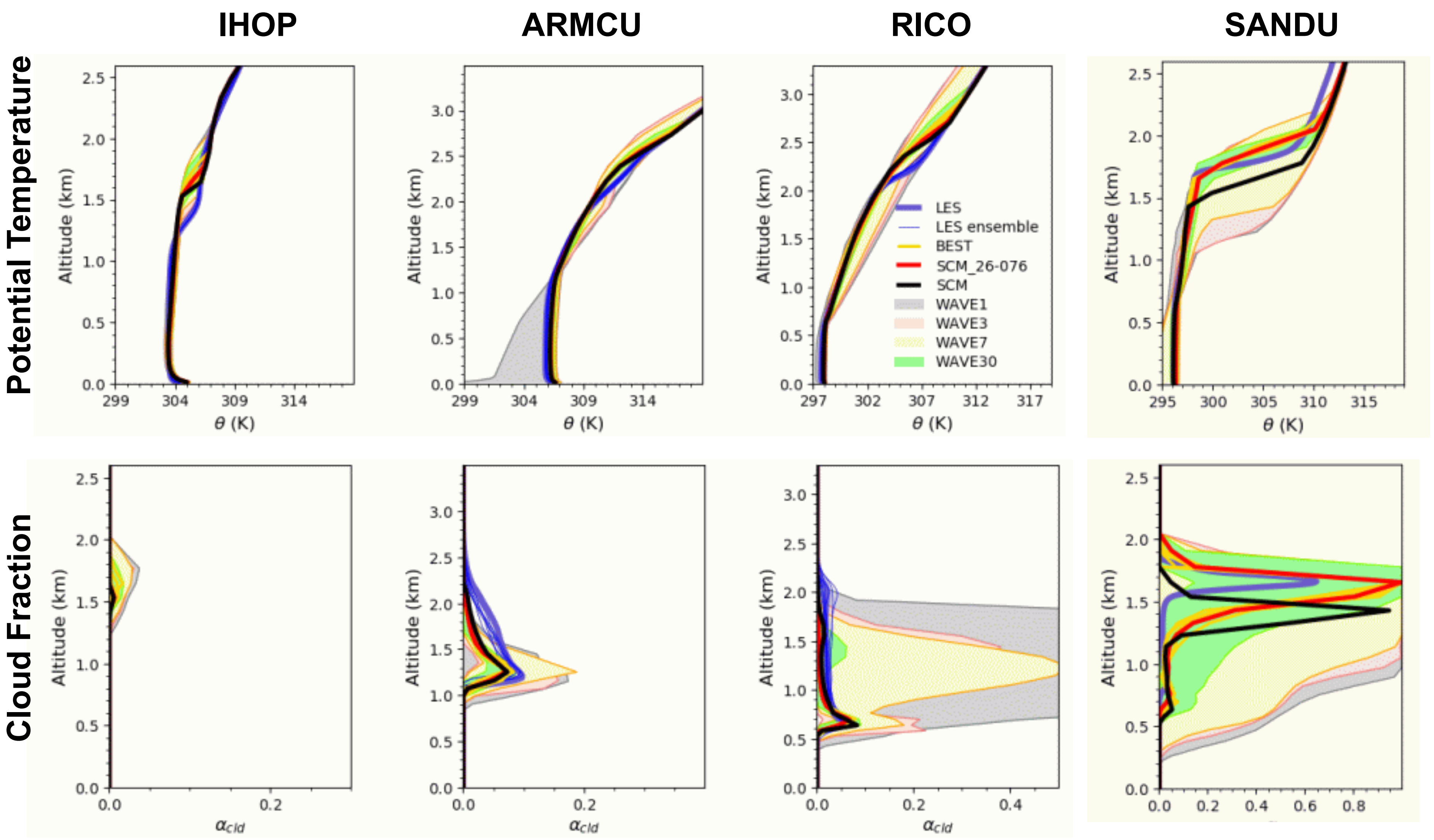
- 9 parameters from cloud, shallow convection and microphysics parameterizations

### *Waves*

- 30 waves with 1D configuration, progressive reduction of the implausibility cutoff (from 3 to 2)
- 2 waves with 3D configuration

*Hourdin et al. (2020, 10.1029/2020MS002225)*

# 30 Waves in 1D

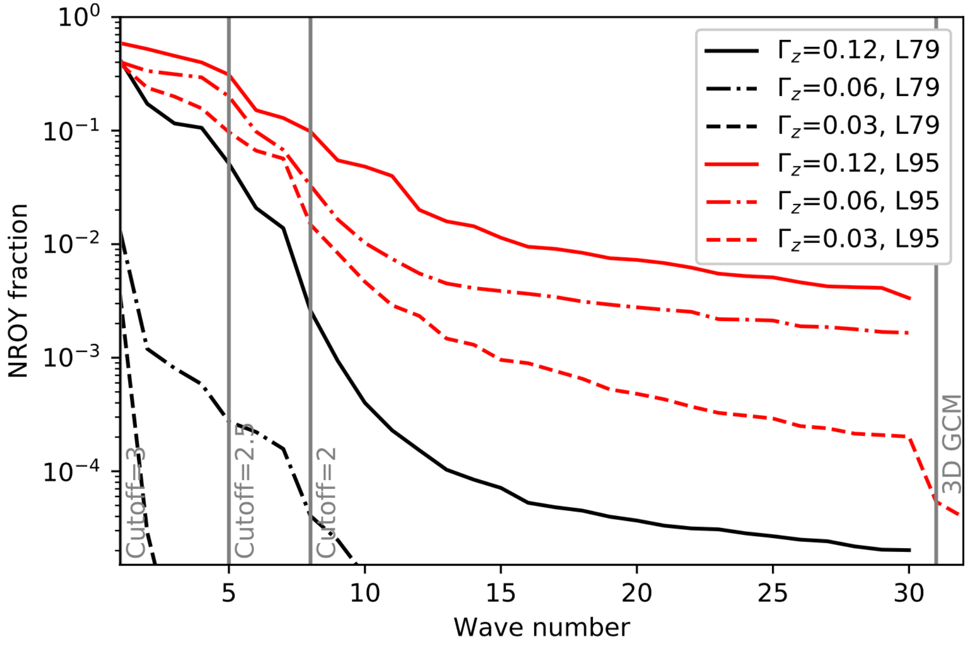


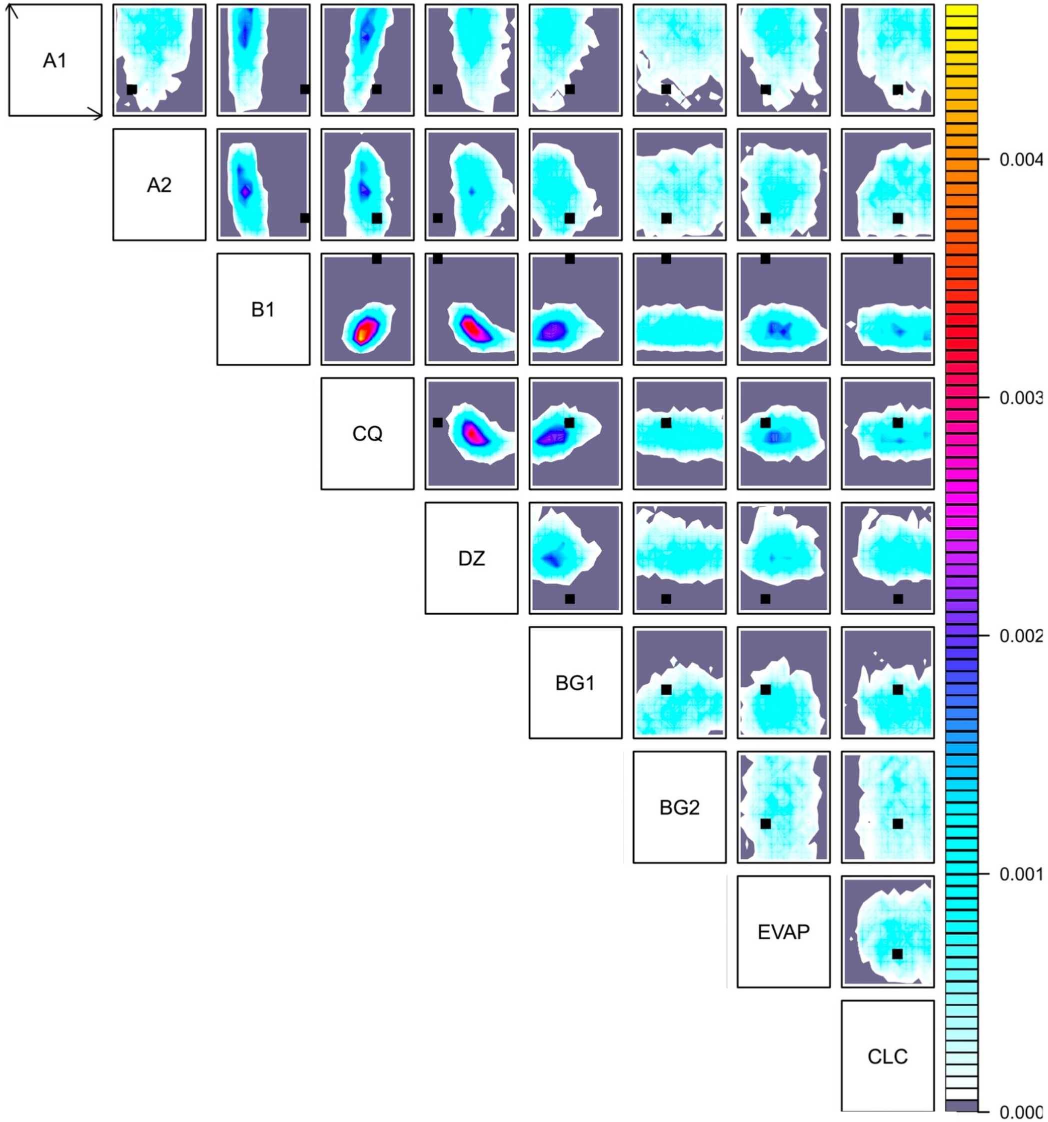

*Hourdin et al. (2020, 10.1029/2020MS002225)*

# 30 Waves in 1D

***NROY space***

- Approximate convergence
- Non-empty space (0.02% of the *input space*)
- LMDZ6 calibration non optimal



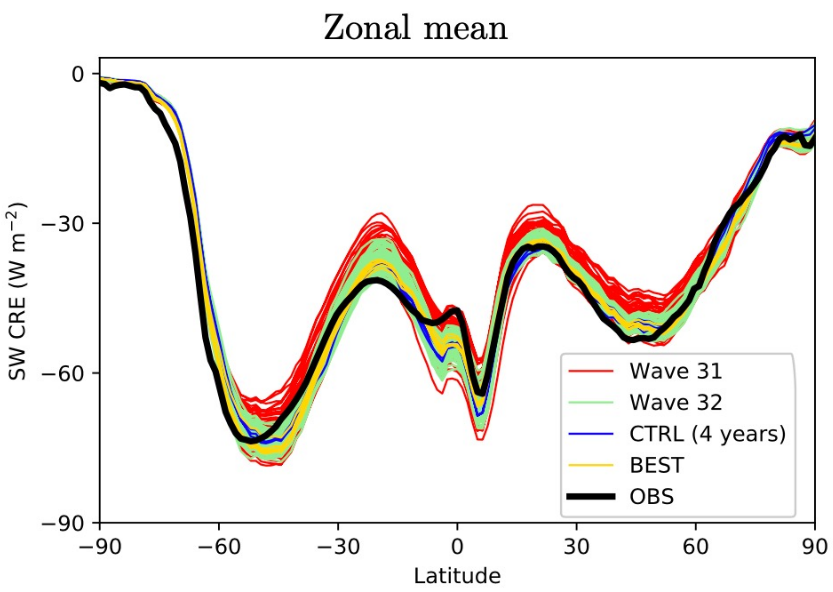



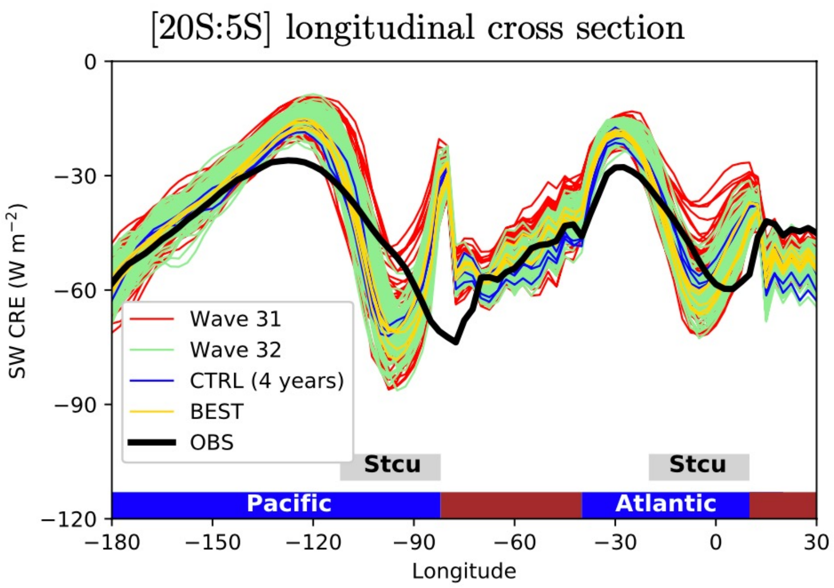

Hourdin et al. (2020, 10.1029/2020MS002225)

# 2 waves in 3D

***Continuing calibration in 3D, starting from 1D NROY space***

- Non-empty space (0.004% of the input space)
- 1D calibration resulted in an efficient pre-conditioning of the 3D model
- LMDZ6 calibrated 'by hand' relatively skilfull, though non optimal
- Probably necessary to add a few more waves (but dependent on computing resources)



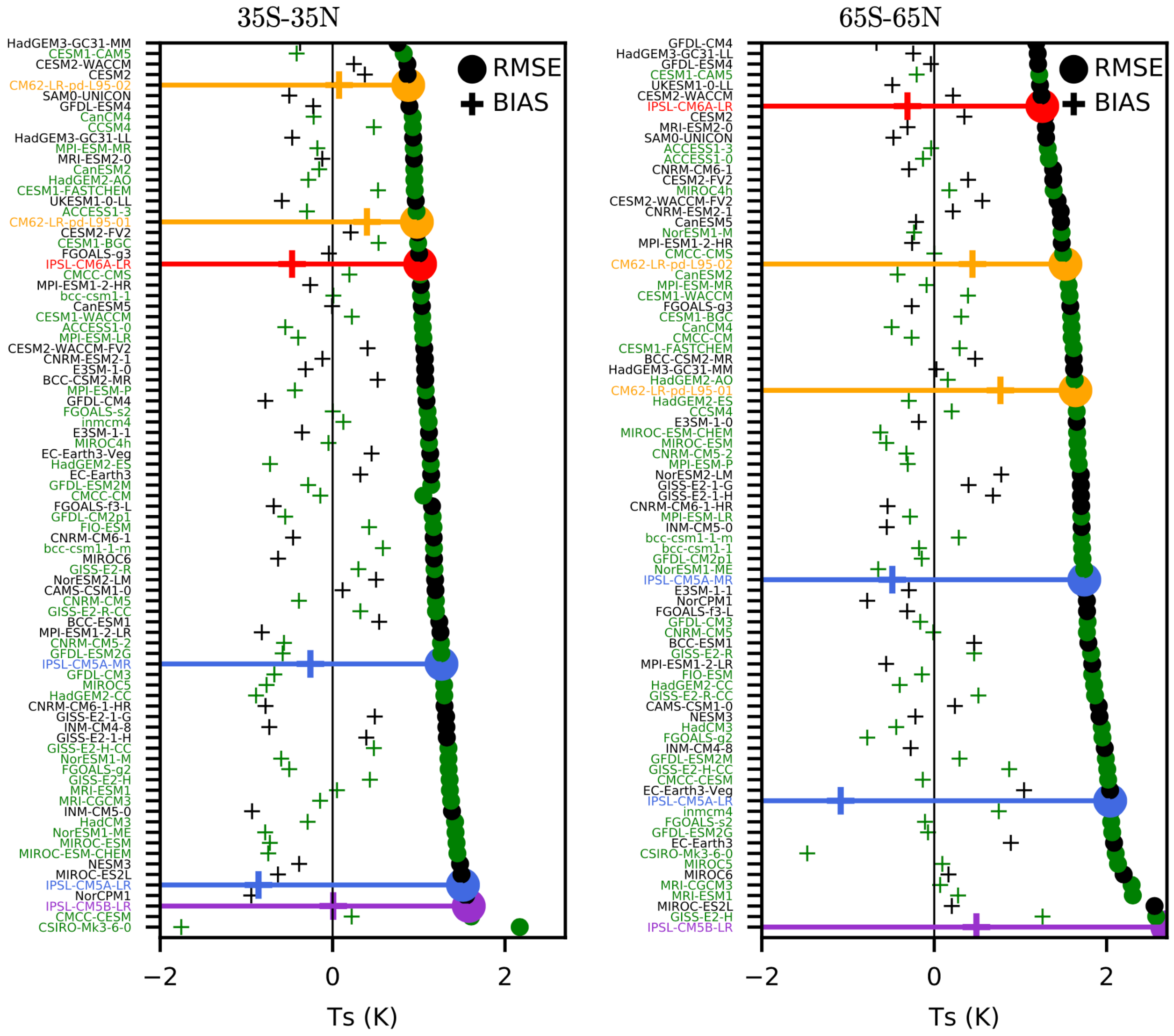




*Hourdin et al. (2020, 10.1029/2020MS002225)*

# Testing in ocean-atmosphere coupled configurations

***From atmosphere-only to OA coupled configration***

- Calibration by hand of the TOA energy budget (1 parameter)
- Behaviour similar to the version calibrated by hand over 2-3 years.




*Hourdin et al. (2020, 10.1029/2020MS002225)*

# Conclusions, Perspectives

## *History matching with iterative refocussing*

- Provides a ***relevant and efficient framework for model calibration in the presence of uncertainties***
- Can help accelerate model development by comparing calibrated model version
    - *Assessing the true added value of a new development*
- Helps better ***identify and quantify model structural errors***, and thereby helps focus on bias understanding/model development
- ***Overall questions the scientific content of a climate model***

## *Next steps*

- Play with tolerances to error to better identify/quantify model structural errors and trade-offs to be made
- Add new metrics, e.g., variability: can we get both mean state and variability right?
- Pre-conditioning with cheaper model configurations

  e.g., 1D/LES for preserving process-level performance *(Couvreux et al. 2020, Hourdin et al. 2020)*.
- Towards calibration of ocean-atmosphere coupled configurations:

  accelerating spin-up, use of intermediate resolutions, fast/slow processes…
- Develop physical interpretations of what is happening in the calibration process.

## *More on the technical/statistical aspects*

- Develop strategies to better sample particularly small NROY spaces.
- Going beyond scalar metrics, emulate directly vectors/maps (e.g., using EOFs, *Salter et al. 2019*)
- Emulate the expert judgment (‘subjective metrics’, Xu et al. 2023)