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ESCAPE 2

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WP4 Verification Validation Uncertainty Quantification (VVUQ)

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Dissemination workshop, 3rd September 2021, Bluejeans

The ESCAPE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671627.

WP Objectives

- **Based on the URANIE platform, WP4 aims to:**
  - Develop a **generic European VVUQ package** for weather and climate simulations that is deployable on supercomputers preparing workloads of pre-exascale computations on many-core configurations.
  - **Demonstrate the VVUQ package for both dwarf and full forecasting system workloads** and optimise the performance of the VVUQ package for the use cases based on the available VVUQ methodologies.
  - **Enhance the URANIE platform** to capitalise and disseminate the approaches learned from the weather and climate community to other science disciplines and use cases

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T4.1 – VVUQ framework

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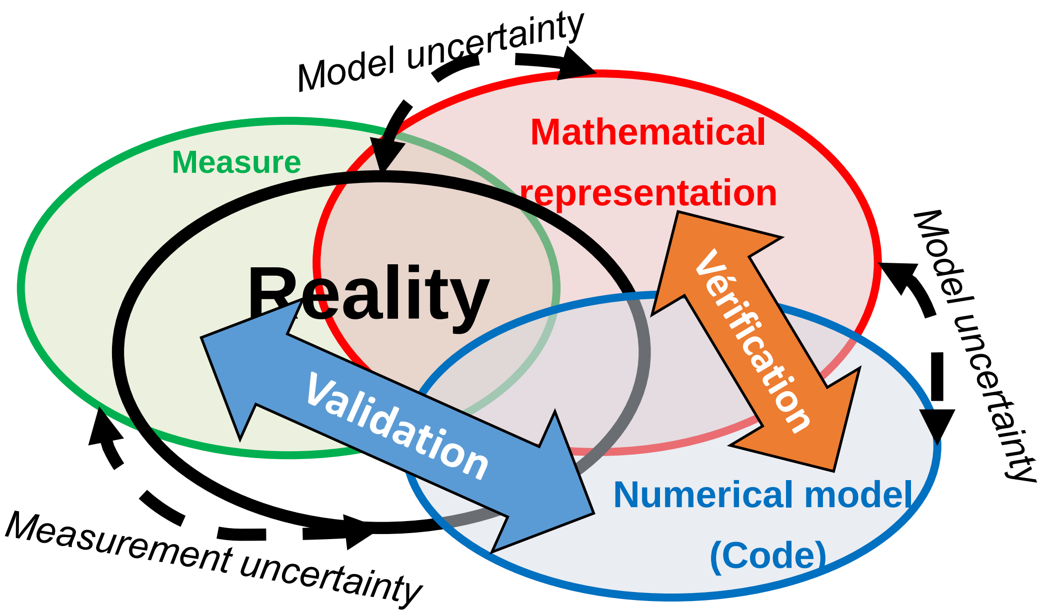
- **Goal**
  - Definition of common VVUQ framework between both communities for the following of the project
- **Concepts**
  - **Reality** (ou truth): Phenomenon what we want to simulate
  - **Measure**: Information that we collect
    - Error from measure tools
  - **Mathematical representation**: How we model the truth
    - Error of the model
  - **Numerical model**: Approximation to solve the mathematical equations
    - Error of approximation



- **VVUQ**
  - **Validation**: Quantify how accurate the numerical model is able to predict the reality
  - **Verification**: testing whether the model is “solving the equation correctly”.
- **Uncertainty Quantification**
  - Uncertainty propagation
  - Sensivity analysis
  - Quantify the input uncertainties

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T4.1 – VVUQ framework

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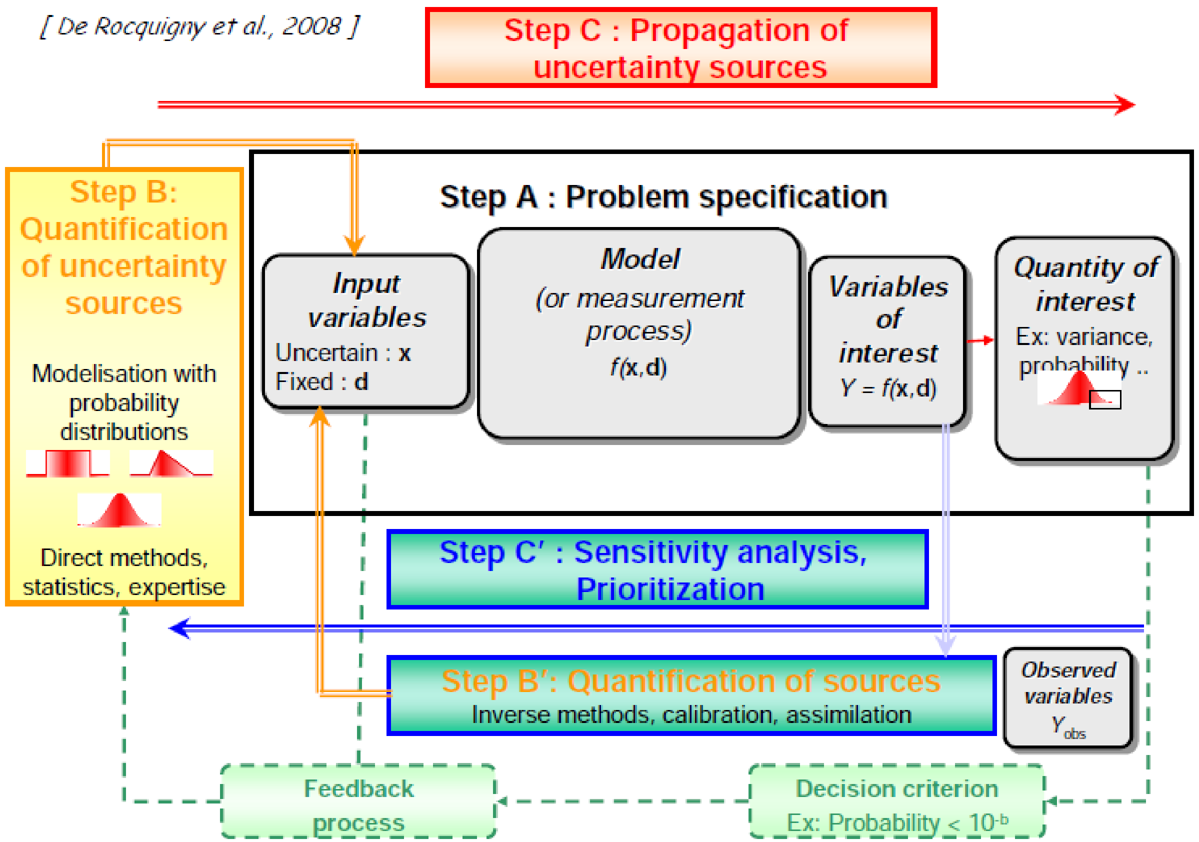
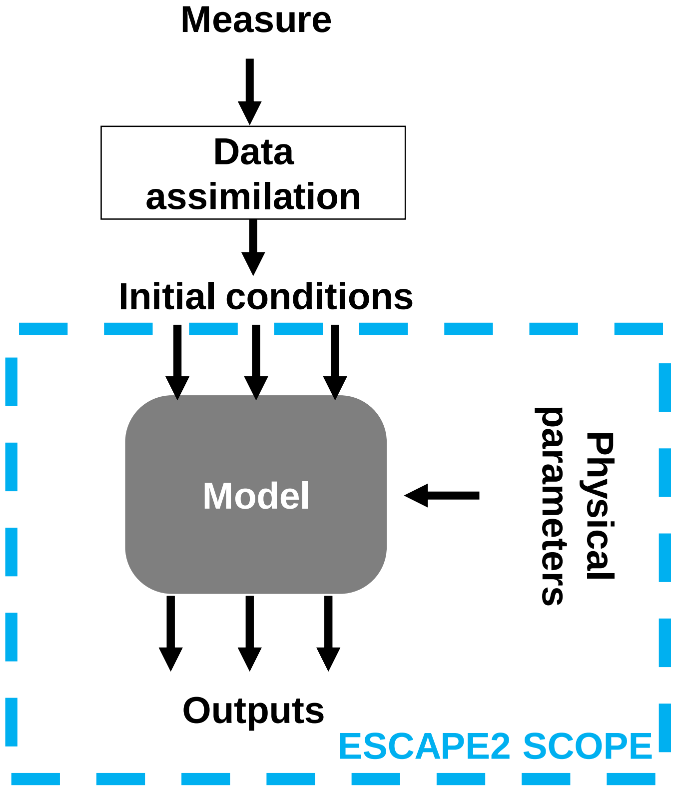
- The **URANIE platform**
  - Dedicated for **Uncertainty Quantification**
  - Developed by CEA/DES (nuclear/defense fields)
  - C++ (2 releases a year), based on ROOT (cern)
  - Multi platform (Unix / Windows)
  - Advanced visu tools (on top of ROOT's ones)
  - **Black-box** approach (non intrusive)
  - Parallelism (fork, pthread, MPI, GPU)
  - Main purposes:
    - construction of **Design Of Experiments (DOE)**
    - **uncertainty propagation**
    - **sensitivity analysis**
    - **surrogate model** building
    - **optimisation** problem
    - **calibration**
    - **reliability** analysis



- Link: https://sourceforge.net/projects/uranie and description paper: https://arxiv.org/abs/1803.10656

T4.1 – VVUQ workshop

- Organisation of **VVUQ workshop**
  - Held in Paris, April 2019
  - inputs from URANIE and NWP communities
- Definition of a **common working basis**
  - VVUQ
    - **Verification** done at the code level (typically unit tests)
    - **Validation** comparison with measurements (business-specific)
    - URANIE → Mainly dedicated of **Uncertainty Quantification**
  - Distinction between **physical parameters** and **initial conditions**
- Weather forecast → complex process
  - Data assimilation to generate the forecast initial condition
  - Uncertainty Quantification based on the Ensemble Prediction System (EPS)
- URANIE
  - **focus will be on the physical parameters**
  - Example: parametrisation of the radiation model as in ACRANEB-2



T4.2 – VVUQ for weather/climate toy model

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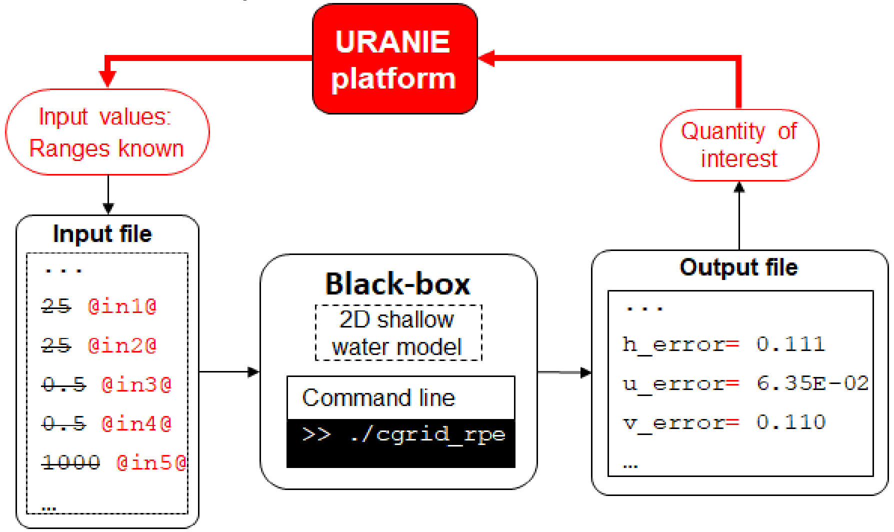
- **Shallow water toy model**
  - provided by ECMWF
  - Black box (meaning is unknown)
  - 5 inputs
  - Only the variation is given
  - → Uniform distribution
  - 3 outputs: Errors with reference solution



Definition (common for all SW anaylisis)

```
//// ================== UNCERTAINTY DEFINTION ======================
    TDataServer *tds = new TDataServer("SW_model","oat"); // Defining the dataserver to store all the information
    // Creating the input with their distribution
    tds->addAttribute( new TUniformDistribution("in1", 0 , 50 ) );
    tds->addAttribute( new TUniformDistribution("in2", 0 , 50 ) );
    tds->addAttribute( new TUniformDistribution("in3", 0 , 1 ) );
    tds->addAttribute( new TUniformDistribution("in4", 0 , 1 ) );
    tds->addAttribute( new TUniformDistribution("in5", 0 , 5000 ) );

//// ================== LINK WITH CODE ======================
    TString sIn = TString("namelist"); // Input file...
    tds->getAttribute("in1")->setFileFlag(sIn,"@in1@");
    tds->getAttribute("in2")->setFileFlag(sIn,"@in2@");
    tds->getAttribute("in3")->setFileFlag(sIn,"@in3@");
    tds->getAttribute("in4")->setFileFlag(sIn,"@in4@");
    tds->getAttribute("in5")->setFileFlag(sIn,"@in5@");
    // Defining the code
    TCode *mycode = new TCode(tds, gSystem->Getenv("PWD")+TString("/runSW.sh") );
    // Define the output file and what to find in it
    TOutputFileKey *_fout = new TOutputFileKey("cgrid_rpe.out");
    // Adding the output
    _fout->addAttribute(new TAttribute("h_error"));
    _fout->addAttribute(new TAttribute("u_error"));
    _fout->addAttribute(new TAttribute("v_error"));
    // Add the output file to the TCode object
    mycode->addOutputFile( _fout );
```

Analysis (movable)

```
//// ================== DOE GENERATION ======================
    // Set the Morris method parameters
    Int_t ndoe = 10000; // Size of the DOE
    TString typeDOE = "lhs";// "srs" is also possible

    TSampling *tsam = new TSampling(tds, typeDOE, ndoe); // Create the TSampling object
    tsam->generateSample(); // Generation of the sample of inputs
    TLauncher *tlch = new TLauncher(tds, mycode);
    tlch->run(); // Evaluation of the DOE

    // export the tds in a data file
    tds->exportData("mydoe.dat");
```

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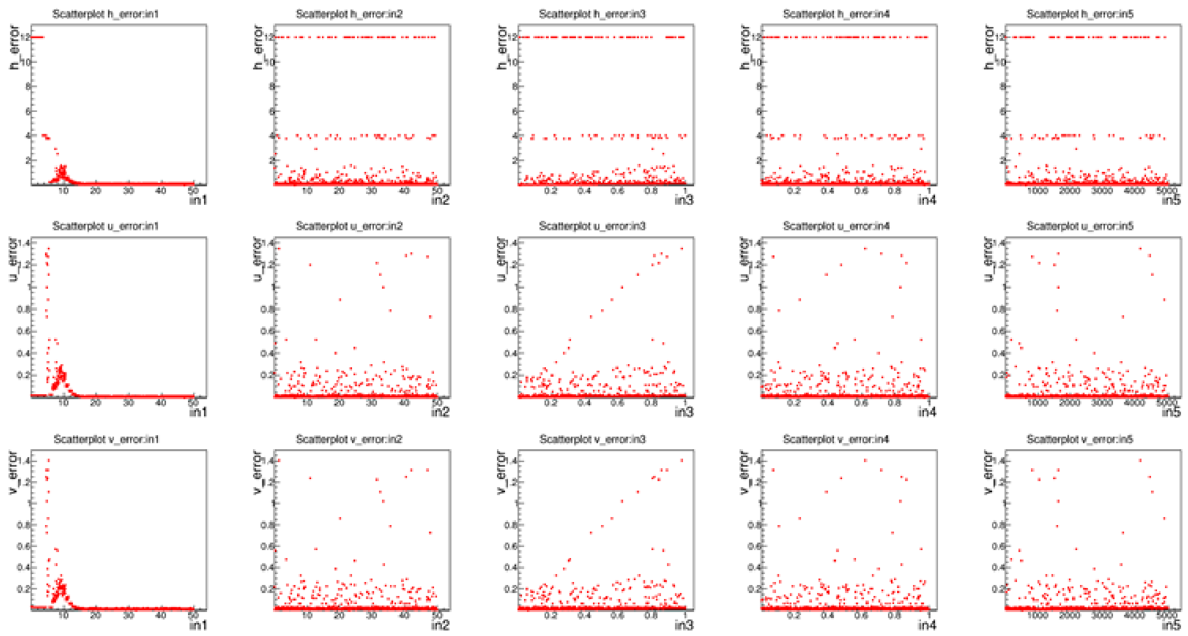
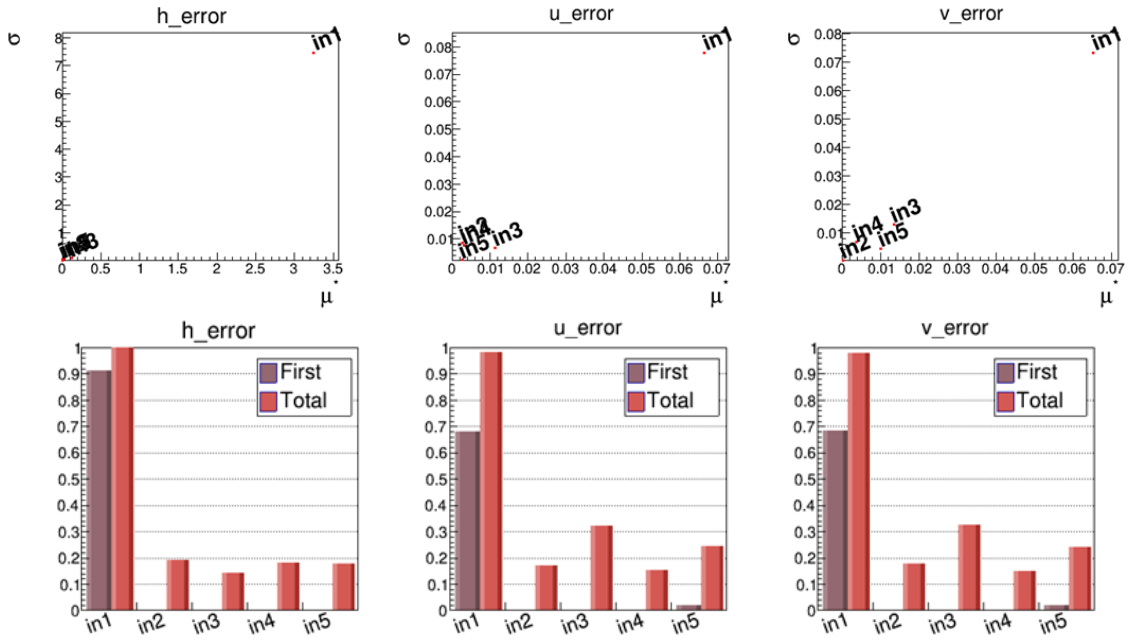
T4.2 – VVUQ for weather/climate toy model

- **Sensitivity analysis**
  - Design of Experiments → trends of the model
  - Qualitative Morris indices → Hierarchy between inputs
  - Quantitative Sobol indices → Influence of input variances on outputs





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T4.2 – VVUQ for weather/climate toy model

- **Sensitivity analysis**
  - Design of Experiments → trends of the model
  - Qualitative Morris indices → Hierarchy between inputs
  - Quantitative Sobol indices → Influence of input variances on outputs
- **Calibration by optimization**
  - URANIE
  - Non linear algorithms
  - Multi starting point strategy

	Range	URANIE	TRUE	Meaning	
in_1	$[0; 50]$	32.665	52 (integer)	Number of bits	VERIFICATION
in_2	$[0; 50]$	20.43	20 (integer)	Seed of the random generator	
in_3	$[0; 1]$	0.05	0.05	Amplitude of the initial perturbation in the h direction	
in_4	$[0; 1]$	1.0	1.0	Slippyness along the coast-line (0 free-slip, 1 no slip)	
in_5	$[0; 2000]$	470.23	470.23	Viscosity of the fluid	

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T4.3 – Enhancement of URANIE workflow management

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- **Main goals:**
  - Implement a new workflow management system, the Autosubmit tool, which is the workflow management tool developed at BSC for operating large-scale and diverse applications on HPC systems.
  - Enhance the I/O management of URANIE to process large data workloads across multiple tasks efficiently without affecting the scalability of the application.
  - Perform tests and produce performance assessments using the BSC tools Extrae and Paraver, and to identify potential bottlenecks in the processing.
  - Testing with node allocation patterns beyond today's limits of URANIE.
- **Main outcome:**
  - Output of this task will be an upgraded workflow management environment for URANIE that allows running large-scale applications in parallel and on large HPC node allocations.
  - Deliverable D4.3 summarizing the developments done to improve the workflow in URANIE.

T4.3 – Enhancement of URANIE workflow management

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- **Main tasks performed**
  - Study, install and deploy Uranie Code as developer
  - Launch code on remote clusters
    - Add support for Marenostrum 4 (adding SLURM support)
    - Launch a design of experiment from the workstation
    - Enable to launch multiple code on the same macro
    - Enable sensitivity, optimizer and modeler modules to be launched on remote
  - Compilation of heavy intensive code
  - Local compilation + remote launch

- **New features**
  - Integrate remote functionalities to URANIE launcher
  - Based on the Autosubmit workflow manager experience
  - Allow send and launch design of experiment from remote
  - Allow send and launch a binary with static libraries
  - Allow send multiple launches within a single macro.
  - Compile and launch a code within a macro.
  - Grant usage flexibility to user
  - Allow to configure cluster, launcher and compiler parameters.
  - Job management

T4.4 - VVUQ of ACRANEB2 dwarf

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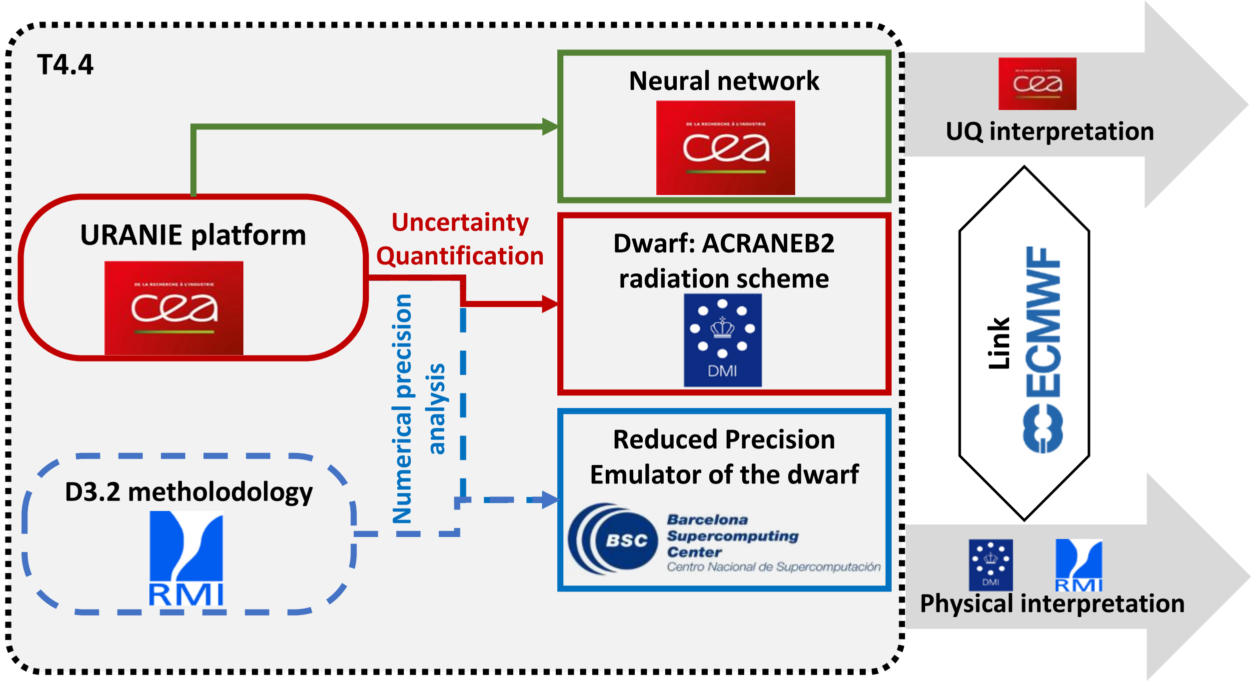
- **ACRANE dwarf**
  - Radiation scheme
  - 12 input physical parameters
  - Fast to run (<1s)
  - 300 columns of 48 layers
  - Summarized in 6 norms with a reference solution
  - Reference solution from another model



- **Complete VVUQ analysis**
  - Sensitivity analysis for each column (CEA)
  - Global sensitivity analysis (CEA)
- **Calibration**
  - Reference solution from DMI
  - Optimal parameters determined by optimization (CEA)
- **Numerical precision analysis**
  - Building a reduced precision emulator (BSC)
  - UQ URANIE analysis (CEA)
  - D3.2 methodology application (RMI)
- **Neural Network**
  - Artificial Neural Network based on data (URANIE - CEA)
    - Main trends identified
    - Lack of physical meaning for improving quality

T4.5 - New calibration techniques for URANIE

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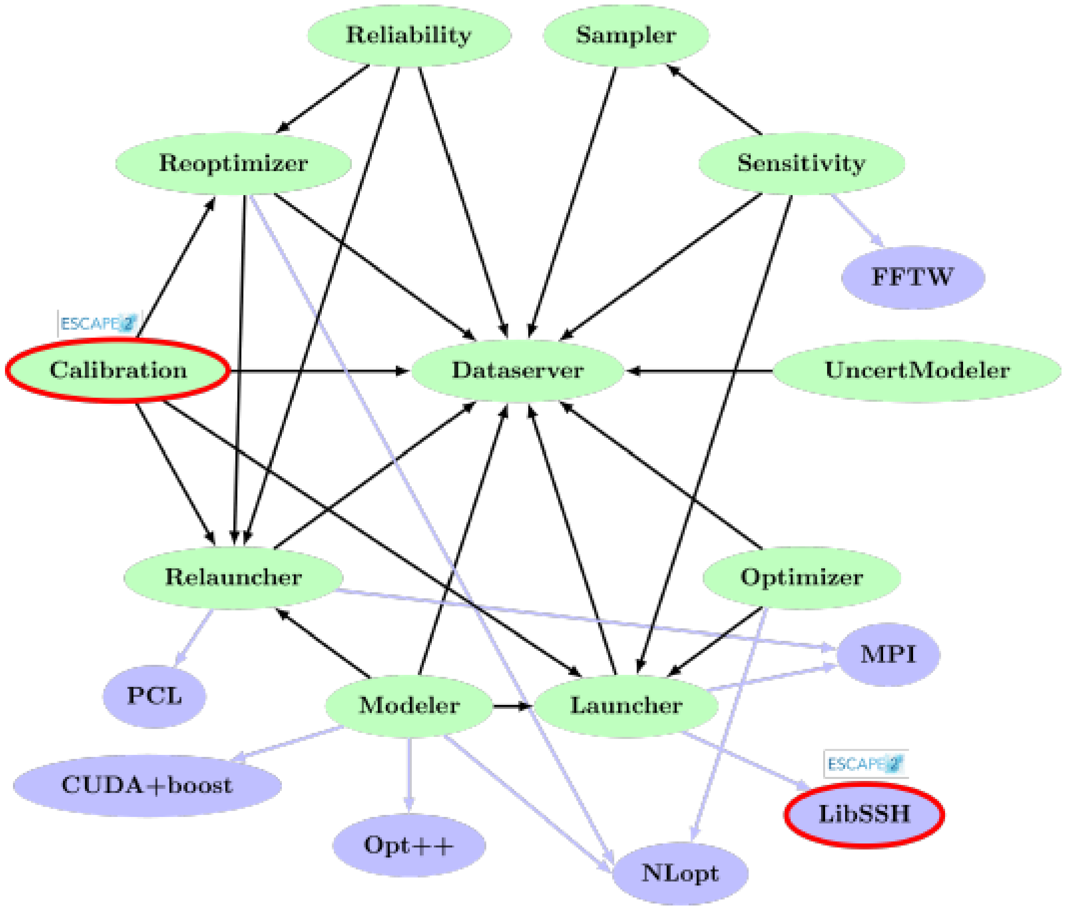
- **Context**
  - Provided the optimal set of parameters targeting the reference solution
- **New module**
  - Calibration by optimization (URANIE)
  - Calibration techniques for identifying inputs stochastic model
    - Bayesian methods
      - Strong experiment from URANIE team
      - Sequential approach for MCMC
    - Approximate Bayesian Calibration (ABC)
      - Easy to parallelize → HPC



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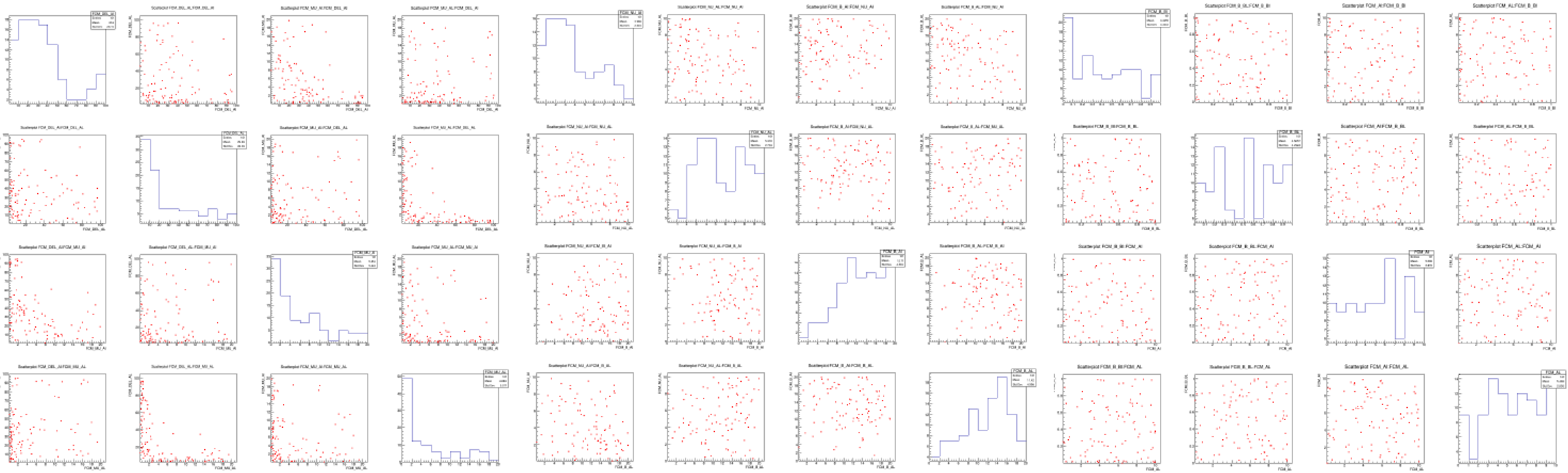
T4.5 - New calibration techniques for URANIE

- **ABC on ACRANEB2 → Quantification of the input uncertainties**



T4.6 - VVUQ on HARMONEPS

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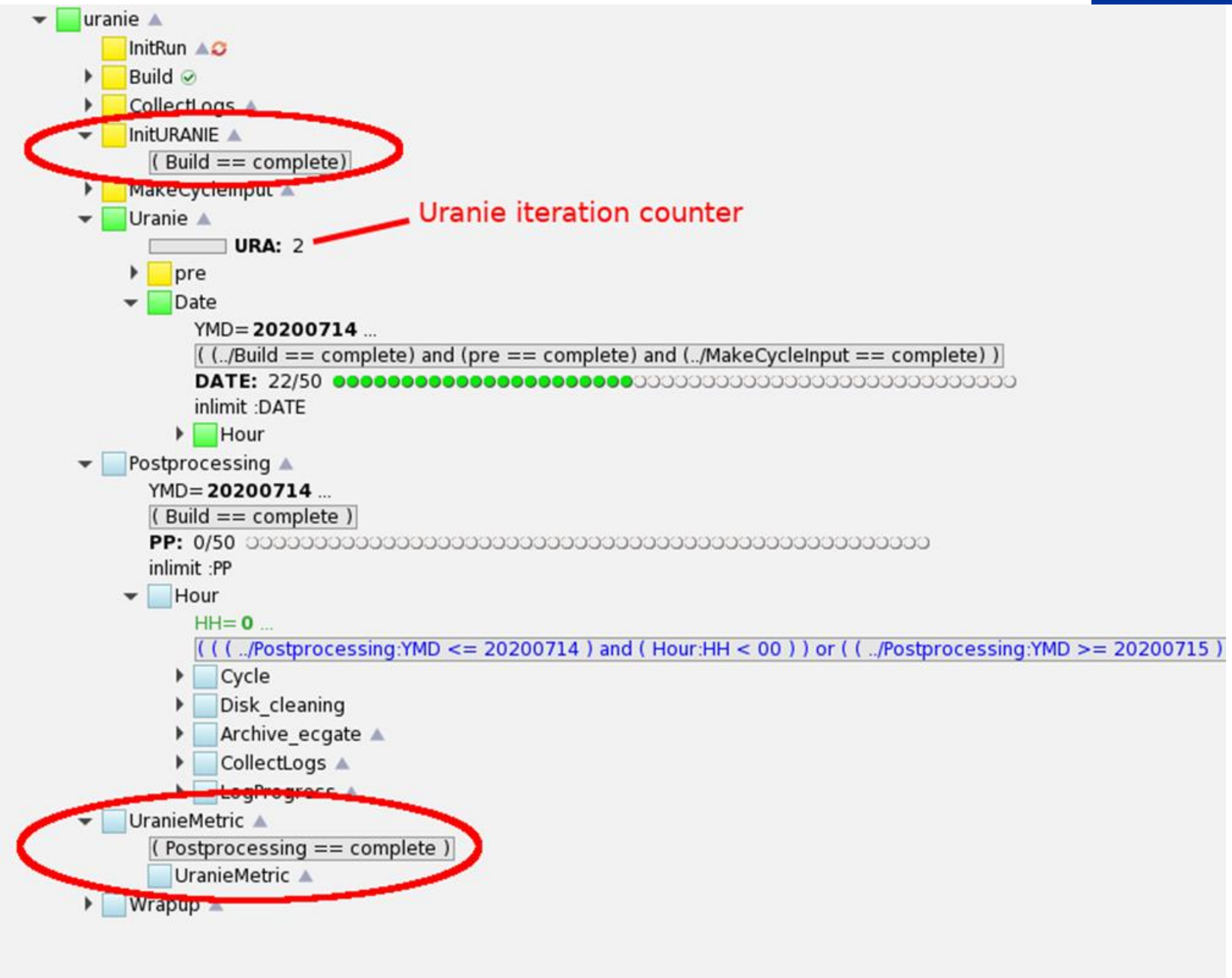
HarmonEPS

- Limited Area Model Ensemble Prediction System

  → used operationally in several ACCORD countries
- 11 members
- Initial and boundary condition perturbations coming from IFS (ECMWF) ensemble
- Tendency perturbations (SPPT)
- Parametrization parameter perturbations (SPP)
- Surface field perturbations



Complex scripting structure (HARMONIE + ECFLOW) for data staging and data-assimilation cycling

- ➢ Typical URANIE black box approach no longer feasible
- ➢ Split URANIE workflow in different tasks
- ➢ Each task now part of HarmonEPS scripting system

T4.6 - VVUQ on HARMONIE EPS

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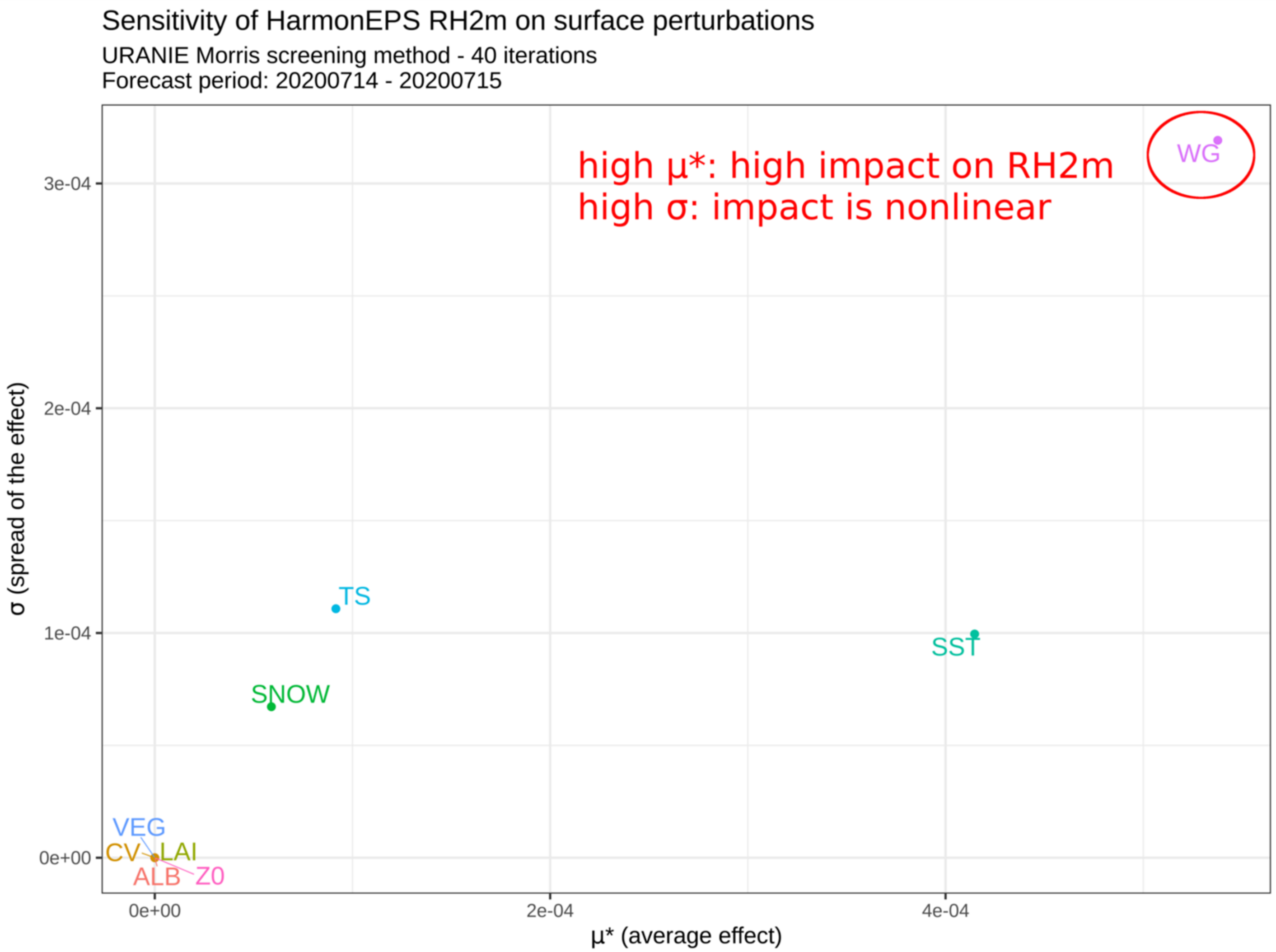
First Experiment:

- Problem with too dry perturbed members when surface perturbations are active
- After numerous experiments SOIL MOISTURE (WG) perturbations were identified as culprit
- Perform sensitivity study with URANIE Morris screening method
- → confirms 2m relative humidity bias as most sensitive to soil moisture perturbations



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T4.6 - VVUQ on HARMONIE EPS

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Second experiment (in progress):

- Identify sensitivity of typical surface variables (T2m, RH2m, S10m, …) on tendency and perturbation length scales (done)
- optimize/calibrate the perturbation correlations length scales for most important length scale – surface variable combination (in progress)

Conclusions:

- URANIE can be combined with Ensemble prediction system
- Most useful for sensitivity and calibration experiments
- Allows systematic screening of characteristics of the EPS
- Bottleneck lies in many iterations some of the URANIE methods require

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Conclusions

- 6 deliverables + 1 workshop
- A common VVUQ framework is defined
  - ✓ Validation : to solve the right equations
  - ✓ Verification : to solve the equations right
  - ✓ Uncertainty Quantification : measurement of the uncertainties introduce at each step
- VVUQ analysis using URANIE on increasing complexity model
  - ✓ Shallow water toy model → Black-box analysis, macros
  - ✓ ACRANEB2 dwarf → Complete analysis: UQ, numerical precision analysis
  - ✓ Harmonie EPS → Full complex system
- Improvement of the URANIE platform
  - ✓ Launcher based on Libssh library for multi-cluster running
  - ✓ Calibration module → specifically Approximate Bayesian Computation
- *Participation of ESCAPE2 summer school*

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Questions?

The ESCAPE-2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 800897.
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