



# eFlows4HPC

Next-generation HPC workflows for natural hazards

## Overview of eflows4HPC Pillar “Urgent Computing” workflows

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eFlows4HPC workshop – Barcelona, September 13th 2023



This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union’s Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway.

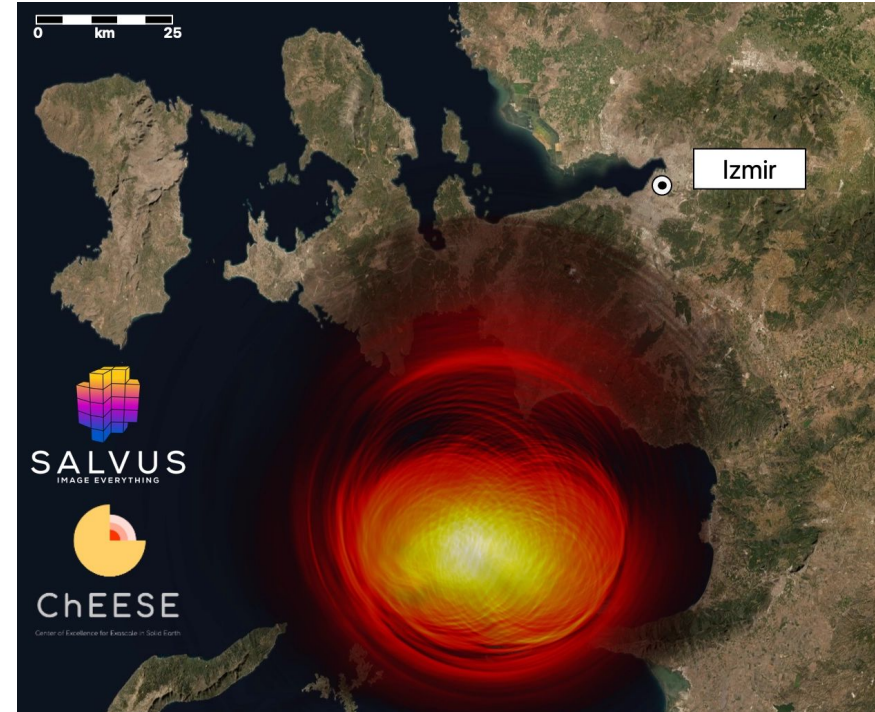
# URGENT COMPUTING

Links the advantage on:

- COMPUTING CAPACITY
- OPTIMIZED SIMULATION CODES
- DATA AVAILABILITY
- HPDA, ML

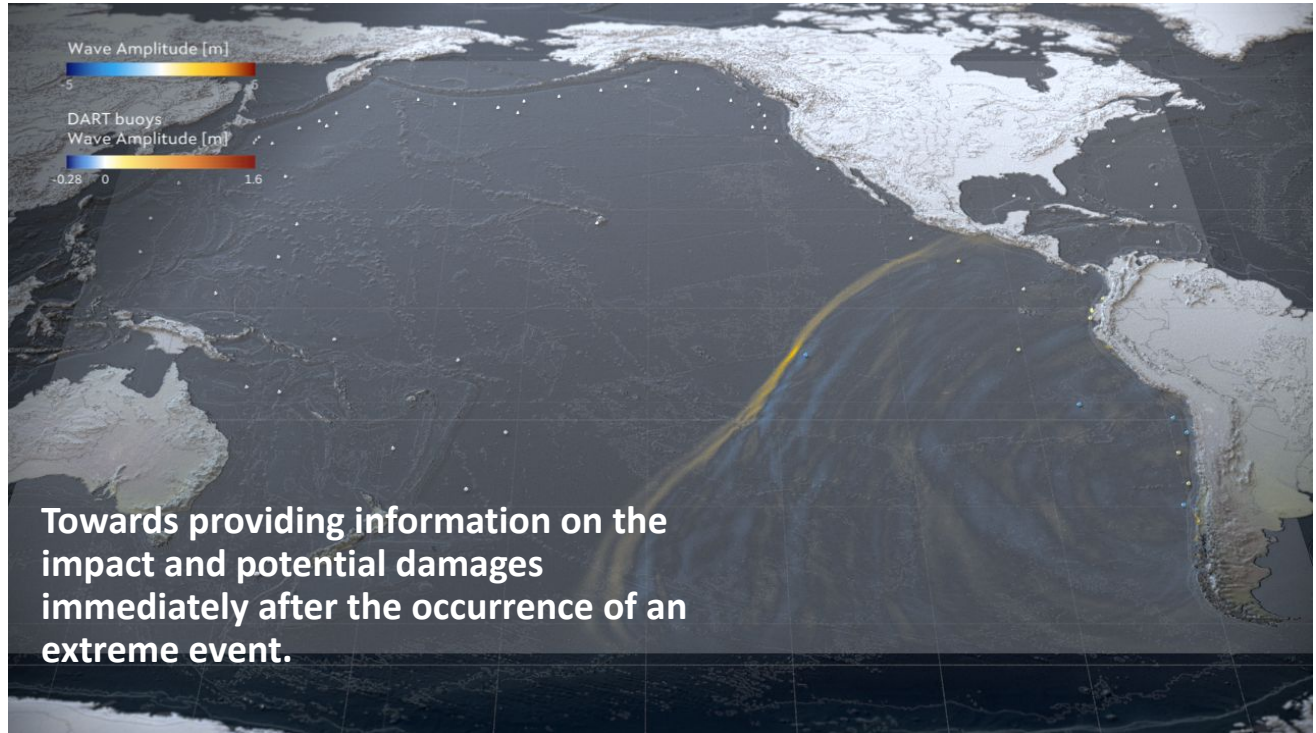


1. The computation operates under a strict deadline after which the computational results may have little practical value.
2. The onset of the **events** that need the computation is mostly **unpredictable**.
3. The computation requires **significant** computational resource usage.



# URGENT COMPUTING FOR NATURAL HAZARDS

Earthquakes and tsunamis are unpredictable and devastating events that can have catastrophic socioeconomic impacts.



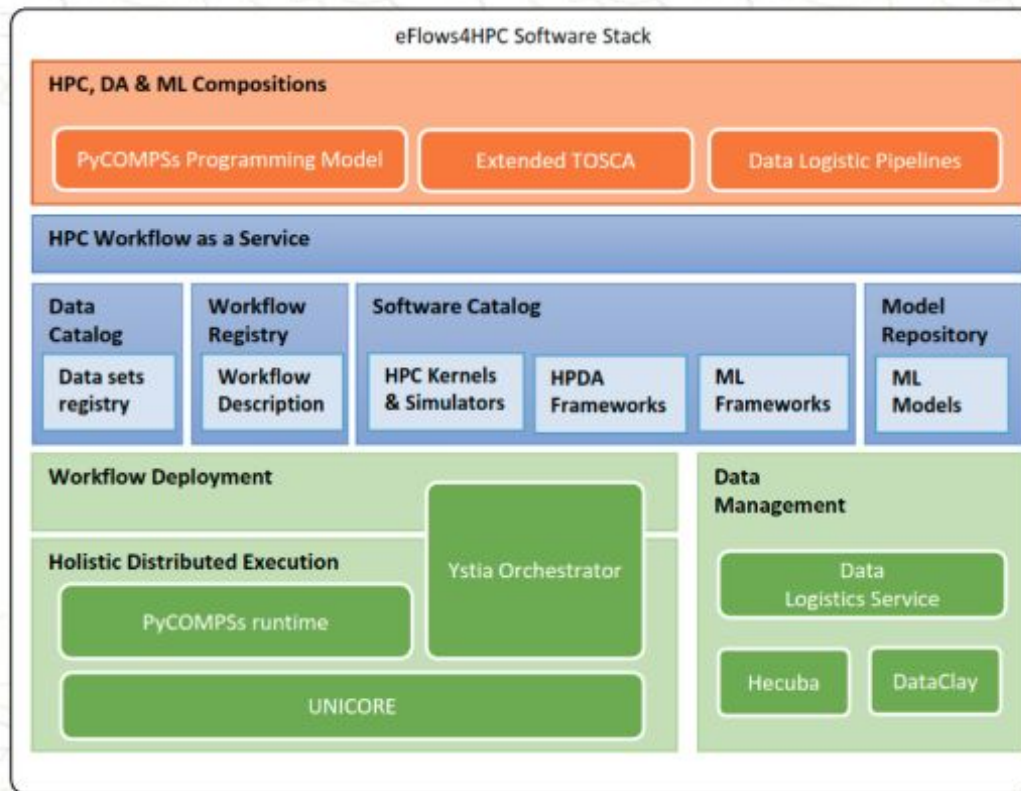
## Pillar III: Urgent computing for natural hazards Earthquakes and Tsunamis

The development of UC workflows for earthquakes and tsunamis involves the deployments of advanced tools and developments of complex tasks to ultimately bring them to an operational level.

# Challenges

- Obtaining **high-resolution Earth models** (velocity models that define the properties of the subsurface).
- Rapidly **constraining source parameters** and accurately estimating the impact of parameter variations in the outcome of simulations, i.e. sensitivity to parameter uncertainties.
- Ensuring fast and reliable results with **urgent access to computational resources** and smart management of all workflow components.

# Software Stack



# Natural hazard workflows and components

- **Workflows involved:**
  - Tsunami: PTF
  - Earthquakes: UCIS4EQ, MLEsmap
- **Software Stack Components used:**
  - DA and ML: Dislib, EDDL, Ophidia
  - HPC Kernels: Salvus, HySEA
  - HPC, DA & ML Compositions: PyCOMPSSs

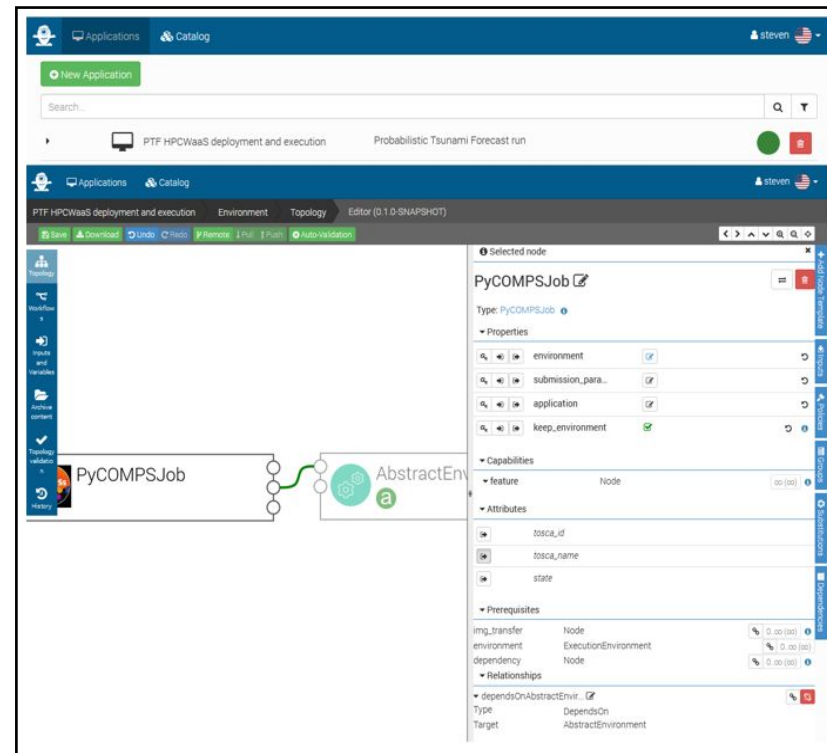
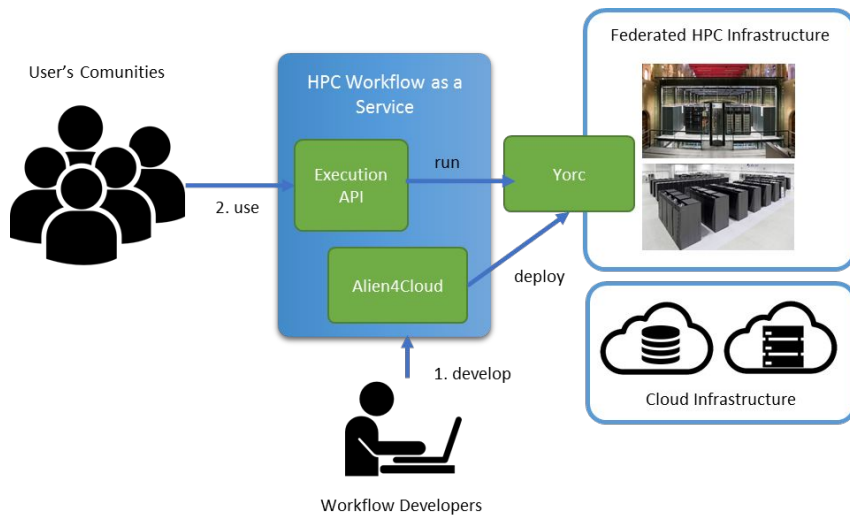
Software stack components	UCIS4EQ Workflow	MLEsmap	PTF/FTRT Workflow
HPC Workflows	PyCOMPSSs		
ML / AI	dislib	dislib EDDL	EDDL
Data Analysis			Ophidia



# Deployment with HPC Workflows as a Service (HPCWaaS)

## HPCWaaS:

- TOSCA: description of the workflow
- Alien4Cloud: development interface







# Earthquake workflows

**UCIS4EQ**

**MLESmapp**



# **Urgent Computing Integrated Services for Earthquakes**

## **UCIS4EQ workflow**

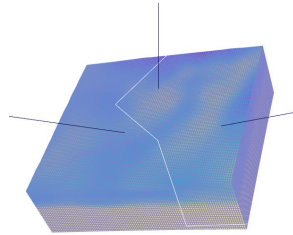
# Urgent Computing for Seismic simulation

Resilience Workflow: to provide fast outcomes using a fully automatic workflow



analysis

Source location  
Magnitude estimation  
Grid generation  
Ask for resources

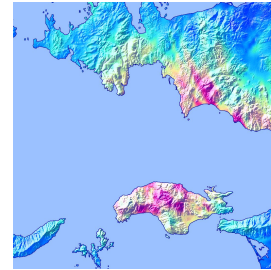


pre-processing



HPC  
simulations

Launch in supercomputer  
Filter data  
Build maps  
Uncertainty quantification  
Reach conclusions



post-processing

## 3D-physics based seismic simulations:

- Full time-histories
- Uniform sampling in space
- Sensitive in different ways to uncertainties than current approaches

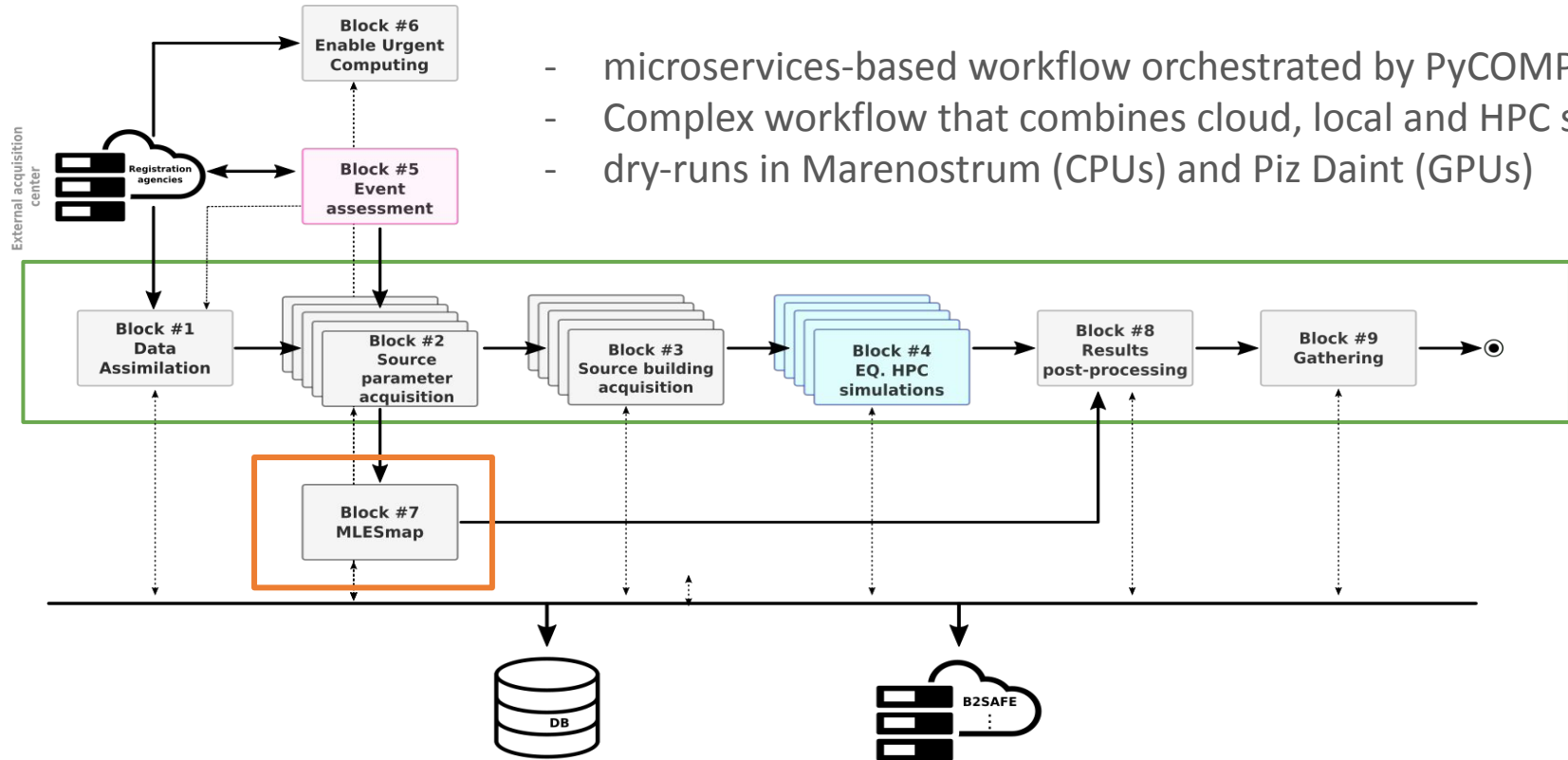
The high resolution of this approach can complement the information of the GMM.

minutes / hours



# UCIS4EQ: Urgent Computing Integrated Services for Earthquakes

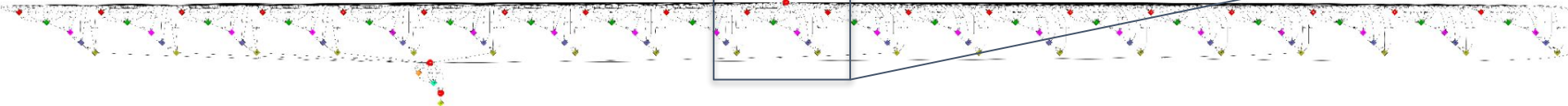
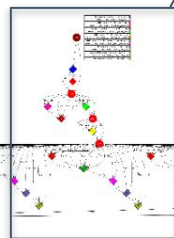
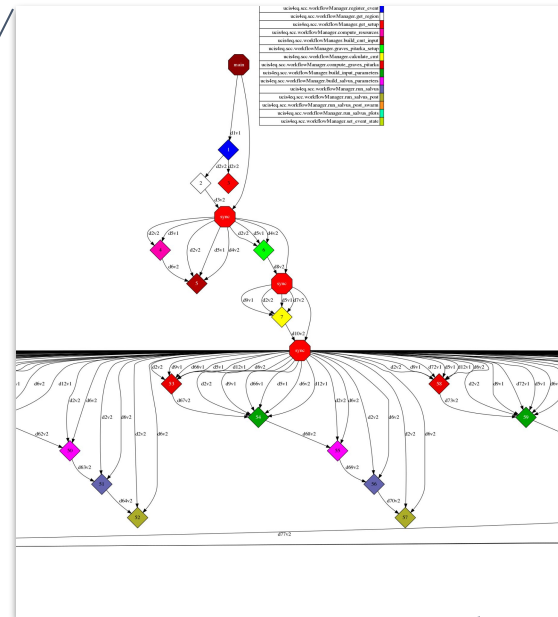
- microservices-based workflow orchestrated by PyCOMPSs
- Complex workflow that combines cloud, local and HPC services
- dry-runs in Marenostrum (CPUs) and Piz Daint (GPUs)



# PyCOMPSs orchestration of microservices

- PyCOMPSs adapted to the micro-services design structure and integrated into UCIS4EQ.
- PyCOMPSs has been extended with the **@http decorator**. It allows developers to define a task that performs an HTTP request

```
@on_failure(management='CANCEL_SUCCESSORS')
@http(request="POST", resource="Graves-Pitarka", service_name="slipgen",
      payload={'event' : {{alert}}, "id" : {{event_id}}, "CMT" : {{cmt}}, \
              "trial" : "{{path}}", "region": {{region}}, "setup" : {{setup}}, \
              "resources" : {{resources}}, "ensemble" : "{{ensemble}}"}, \
      produces={'result' : "{{return_0}}"})
@task(returns=1)
def compute_graves_pitarka(event_id, alert, path, cmt, region, setup, resources, ensemble):
    pass
```



# HPC Workflow implemented in PyCOMPSs



## PyCOMPSs workflows to orchestrate different HPC executions

### Before:

→ every execution in the HPC system was performed in a separate service call with its corresponding overhead

→ every system has its own job scheduler, the original UCIS4EQ workflow implements a set of adaptors to submit the job in the HPC schedulers of every machine

### Now:

→ This Workflow is called from the microservices workflow which submits the HPC Workflow using the **PyCOMPSs queuing scripts** which already **supports different schedulers that has the same execution interface**

- *slipgen* which runs the slip generation using a singularity image
- *salvus\_prepare* and *salvus\_post* which executes the Salvus preprocessing and postprocessing as normal python tasks,
- and *salvus\_run* which performs the simulation with Salvus defined as an MPI application

```
@container(engine="SINGULARITY", image="$SLIPGEN_IMAGE", options="-e --bind {{workingdir}}:/workspace/ --pwd /workspace")
@binary(binary="/opt/scripts/launcher.sh", args="-o rapture --dt {{dt}} -v {{fk_file}} -s {{input_src}}", working_dir="{{workingdir}}")
@task(input_src=FILE_IN, fk_file=FILE_IN, workingdir=DIRECTORY_INOUT)
def slipgen(input_src, dt, fk_file, workingdir):
    pass

@task(input_data=FILE_IN, rapture=DIRECTORY_IN, salvus_setup=FILE_IN, working_dir=DIRECTORY_INOUT)
def salvus_prepare(input_data, rapture, salvus_setup, working_dir):
    rapture_file = rapture + "/scratch/outdata/rapture/rapture.srf"
    os.chdir(working_dir)
    pre_process(input_data, rapture_file, salvus_setup, working_dir)

@mpi(runner="mpirun", binary="$SALVUS_BINARY", args="compute {{prepare_path}}/salvus_input_rapture.toml", processes="$SALVUS_PROCESSES",
processes_per_node= "$SALVUS_PPN", working_dir="{{working_dir}}")
@task(prepare_path=DIRECTORY_IN, working_dir= DIRECTORY_INOUT)
def salvus_run(prepare_path, working_dir):
    pass

@task(UC_input = FILE_IN, salvus_setup= FILE_IN, grid_coordinates= DIRECTORY_IN, simu_folder=DIRECTORY_IN, output_path=DIRECTORY_INOUT)
def salvus_post(UC_input, salvus_setup, grid_coordinates, simu_folder, output_path):
    process_outputs_grid( UC_input, salvus_setup, grid_coordinates, simu_folder, output_path=output_path)

if __name__ == "__main__":
    slip_id, input_path, salvus_setup, slip_input_src, region_fkld, dt = parse_arguments()
    slipgen_dir, salvus_wrapper_dir, salvus_dir, salvus_post_dir = create_output_dirs()

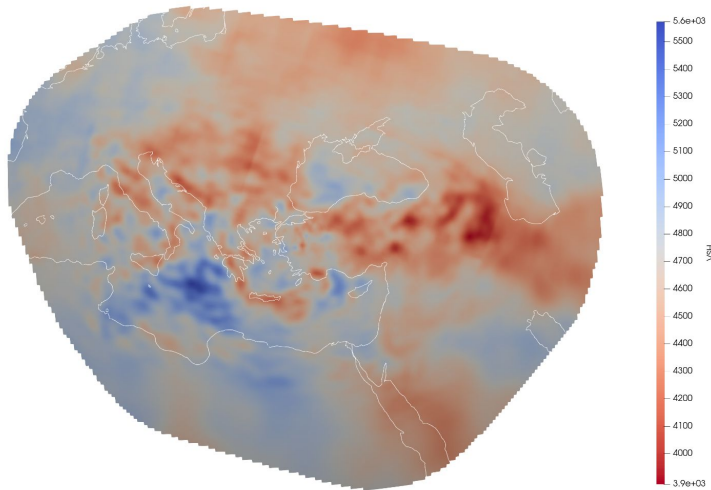
    slipgen(slip_input_src, dt, region_fkld, slipgen_dir)
    salvus_prepare(input_path, slipgen_dir, salvus_setup, salvus_wrapper_dir)
    salvus_run(salvus_wrapper_dir, salvus_dir)
    salvus_post(input_path, salvus_setup, salvus_wrapper_dir, salvus_dir, salvus_post_dir)
```

## Simulations are sensitive to model inputs

- Earth models (HPC or remote repository)

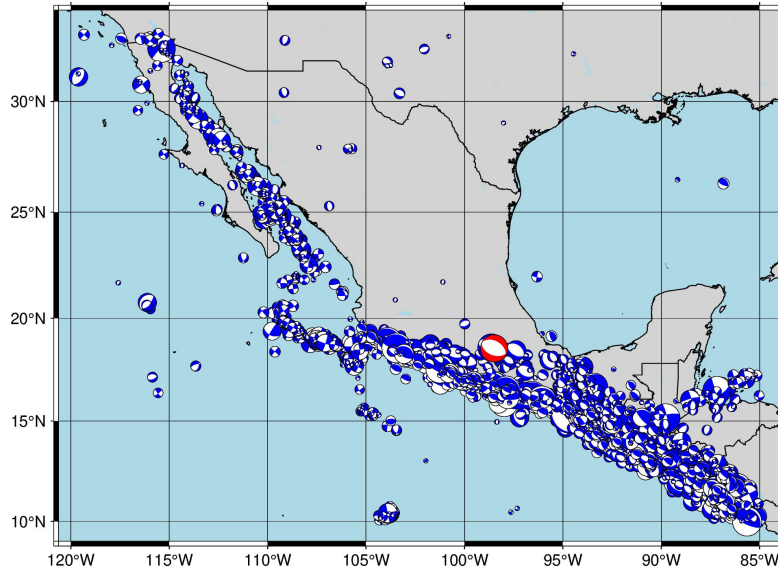
UCIS4EQ requires reliable Earth models for the forward modelling of ground motions.

The second generation Collaborative Seismic Earth Model (CSEM) – a multiscale global tomographic Earth model that incorporates a range of local-, regional- and global-scale updates – has been integrated into the UCIS4EQ workflow



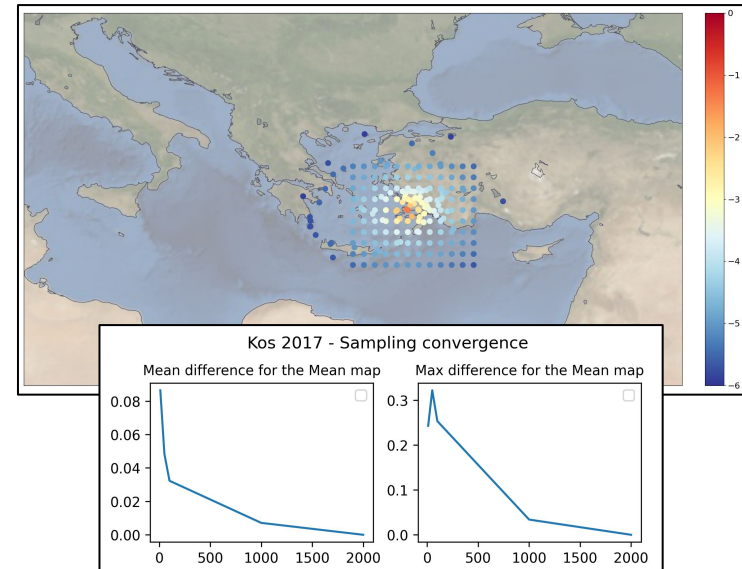
- Ensemble methodologies

## Statistical based on historical events



Monterrubio-Velasco, M., et al. (2022). *Frontiers in Earth Science*, 339.

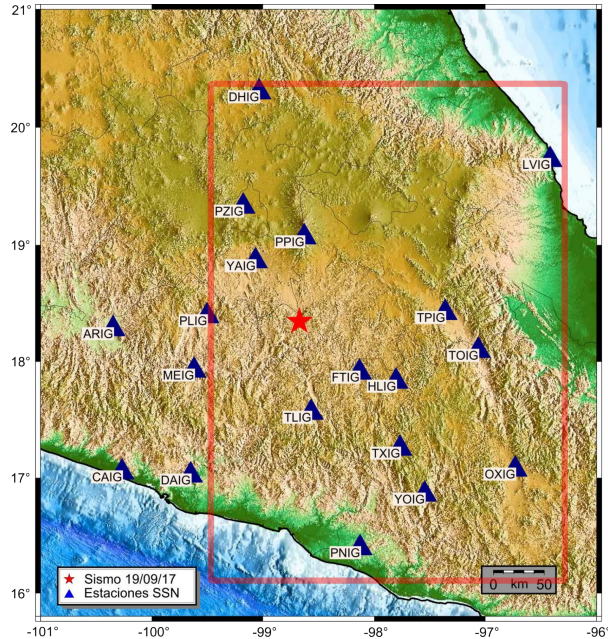
## Probabilistic approach: SeisEnsMan



Stallone, A., et al., *International Union of Geophysics and Geodesy General Assembly 2023*

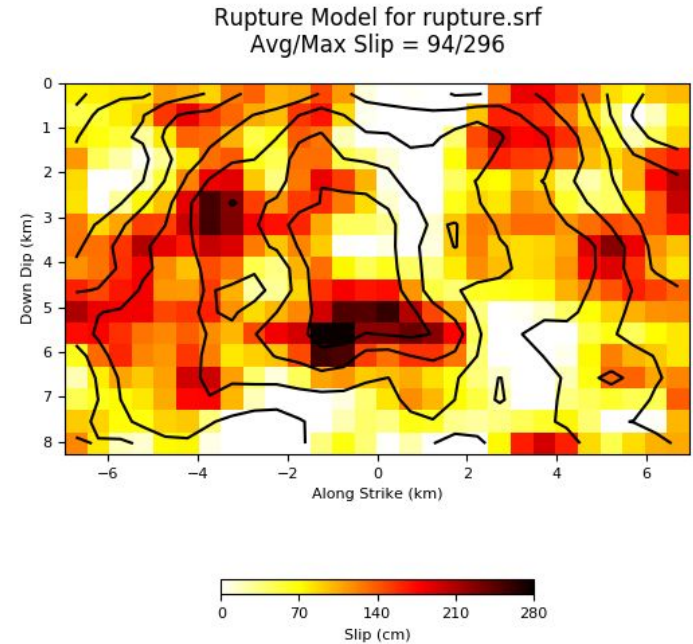


- Receivers



Selecting the stations and the receivers on the simulation domain.

- Kinematic finite-fault



Generating the kinematic finite-fault history using the Graves-Pitarka rupture code

# UCIS4EQ Front-end -- GUI

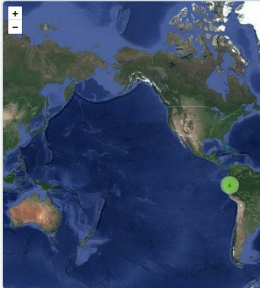



## UCIS4EQ Portal

Monitor dashboard provides real-time information about urgent computing EQ simulations


Alerts
User Event
System Monitor
Results

Origin	Source	Magnitude	Latitude	Longitude	Depth (m)	Time (UTC)	Elapsed Time (hours)
Northern Peru [Land: Peru]	INGV	7.6	-4.43072	-76.7883	108594	28/11/2021, 18:52:13	1105.93
NORTHERN PERU	IRIS	7.5	-4.4528	-76.8189	126860	28/11/2021, 18:52:14	1105.93
Northern Peru	SCEC	7.5	-4.4898	-76.8461	112480	28/11/2021, 18:52:13	1105.93
Northern Peru	GEOFON	7.42	-4.426	-76.758	101900	28/11/2021, 18:52:13	1105.93
Indonesia [Sea]	INGV	7.1	-7.62338	133.314	8266	14/12/2021, 03:38:32	738.46





Center of Excellence for Earthquake Simulation



Enabling dynamic and intelligent workflows in the future Earthquake ecosystem

## UCIS4EQ Portal

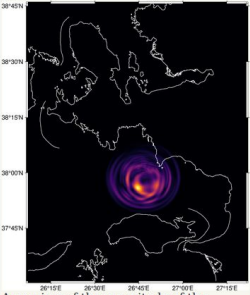
Monitor dashboard provides real-time information about urgent computing EQ simulations

Alerts
User Event
System Monitor
Results

Status	Origin	Site	Latitude	Longitude	Min. Mw	Max. Mw	Min. Depth	Max. Depth	# Alerts	Run
REJECTED	East Nusa Tenggara		-7.63	122.23	7.1	7.3	7.1	7.3	4	61e539ec739c12a603c903a7
REJECTED	Lautem		-7.58	127.57	7.27	7.3	7.27	7.3	4	61e539ec739c12a603c903a8
REJECTED	Loreto	Datem Del Maranon	-4.45	-76.8	7.42	7.6	7.42	7.6	4	61e539ec739c12a603c903a9
LAUNCHED	North Aegean	Nomos Samou	37.92	26.79	7	7	7	7	1	61e53a97739c12a603c903ae

43 %

Service	Status	InitTime	EndTime
EventDomains	SUCCESS	2022-01-17 09:44:55	2022-01-17 09:44:55
CMTInputs	SUCCESS	2022-01-17 09:44:55	2022-01-17 09:44:55
ComputeResources	SUCCESS	2022-01-17 09:44:55	2022-01-17 09:44:55
CMTCalculation	SUCCESS	2022-01-17 09:44:55	2022-01-17 09:45:06
SourceType	SUCCESS	2022-01-17 09:45:06	2022-01-17 09:45:06
SlipGenP	SUCCESS	2022-01-17 09:45:06	2022-01-17 09:46:44
InputParametersBuilder	SUCCESS	2022-01-17 09:46:44	2022-01-17 09:46:44
SalvusPrepare	SUCCESS	2022-01-17 09:46:44	2022-01-17 09:49:02
SalvusRun	RUNNING	2022-01-17 09:49:02	



A preview of the magnitude of the (unfiltered) velocity field.

- **Mediterranean Sea:**
  - 2017 M6.6 Kos-Bodrum earthquake, 120 km x 100 km
  - **2020 M7.0 Samos-Izmir earthquake, 140 km x 110 km**
  
- **Iceland:**
  - **2000 (June 17) M6.4 SISZ earthquake, 135 km x 85 km domain**
  - 2000 (June 21) M6.5 SISZ earthquake, 135 km x 85 km domain
  
- **México:**
  - 2017 M7.1 Puebla earthquake, 200 km x 150 km

# Mediterranean Sea

## Mw 7.0 Samos-Izmir, 2020

- Off-shore the North coast of Samos Island in the eastern Aegean Sea
- 2020-10-30 11:51:27 (UTC)
- 118 fatalities, ~ 100 injuries, collapse of structures
- Local high-intensity effects, Tsunami run-up



Source: <https://earthquake.usgs.gov/earthquakes/eventpage/us7000c7y0/shakemap/pga>

# Mw 7.0 Samos-Izmir, 2020

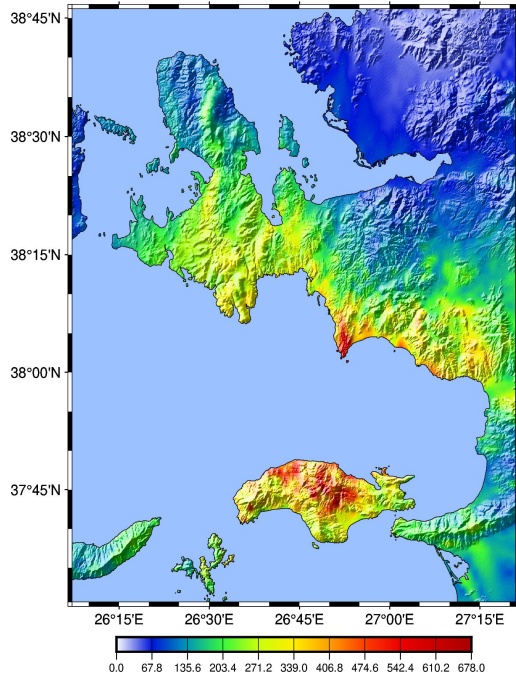
## UCIS4EQ configuration

- 4,012,250 number of mesh elements
- Domain: 110km in longitude, 140km in latitude, and 35km in depth
- **Up to 5 Hz**
- 22 simulations in the ensemble
- 90 GPUs (Piz Daint) per WF execution

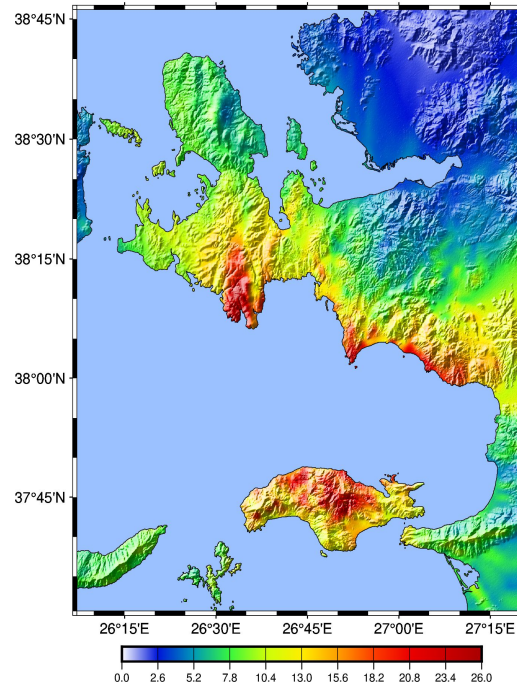
# Use cases: Mw 7.0 Samos-Izmir, 2020

- 1h20m wallclock per WF execution

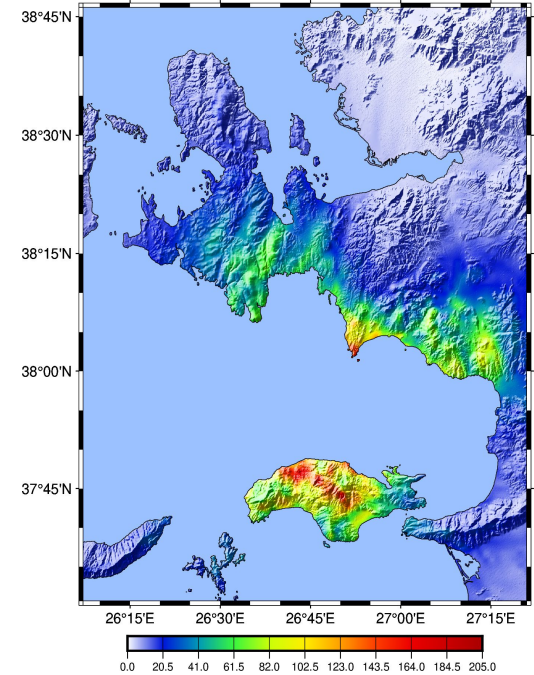
**PGA\_horizontal\_max (cm/s/s)**



**PGV\_horizontal\_max (cm/s)**



**Arias\_horizontal\_max (cm/s)**





# Use cases: 2000 doublet SISZ earthquakes

1.  $M_w$  6.5, 17/06/2000

Lat:  $63.98^\circ$

Lon:  $-20.34^\circ$

Depth: 6.3 km

Focal mechanism:

{strike:273 , dip:74, rake:-3}

2.  $M_w$  6.4, 21/06/2000

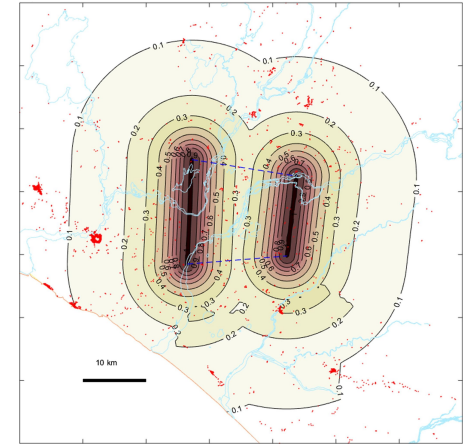
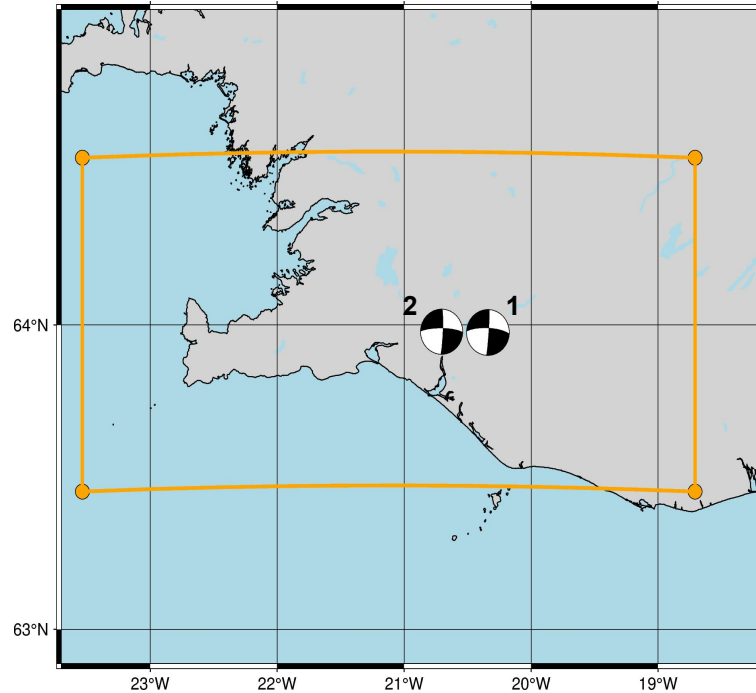
Lat:  $63.98$

Lon:  $-20.70^\circ$

Depth: 5.1 km

Focal mechanism: :

{strike:271 , dip:77, rake:-5}



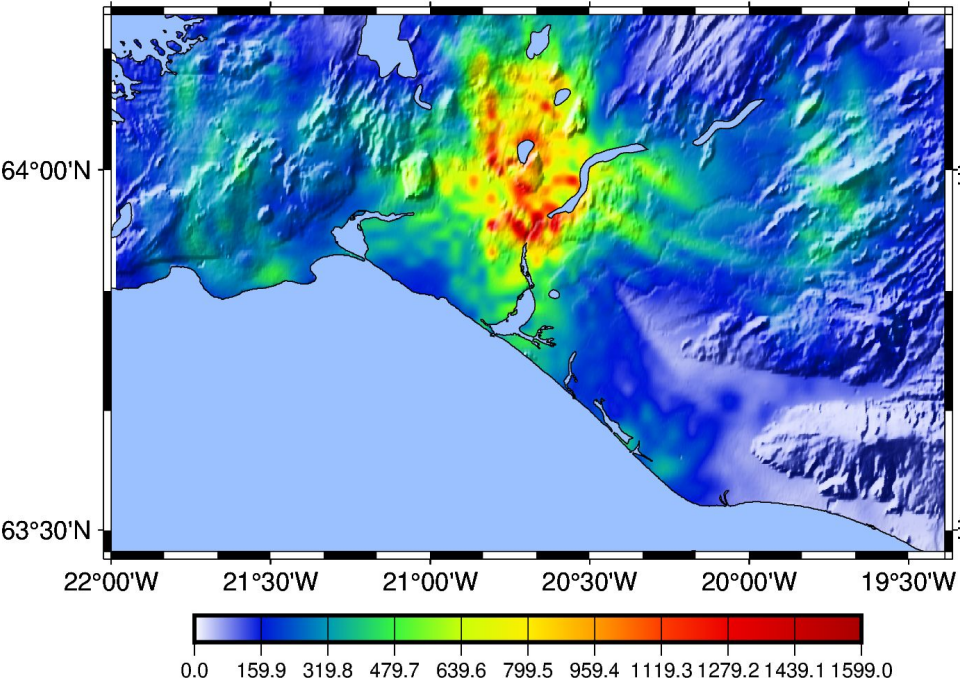
Source: **Shake map for the two June 2000 earthquakes in South Iceland in Bessason, B., Bjarnason, J. Ö., & Rupakhety, R. (2020)..**



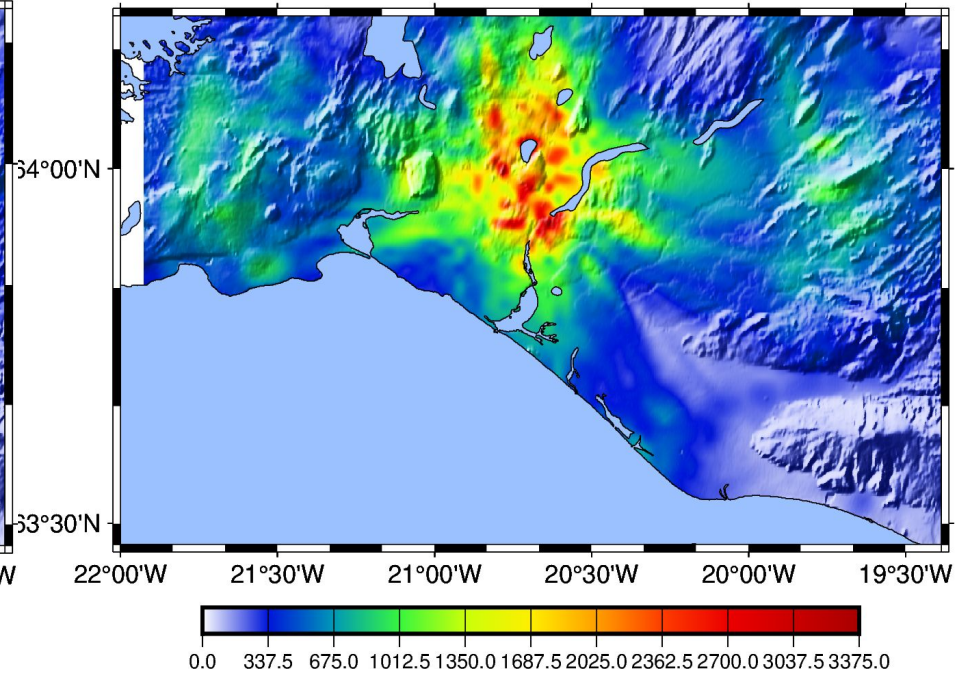
# Mw 6.4, 21/06/2000

- 4,400,001 number of mesh elements
- Domain: 127km in longitude, 84km in latitude, and 25km in depth
- Up to 5 Hz
- 14 simulations
- **44m** wallclock per execution of WF
- 90 GPUs (Piz Daint) per execution

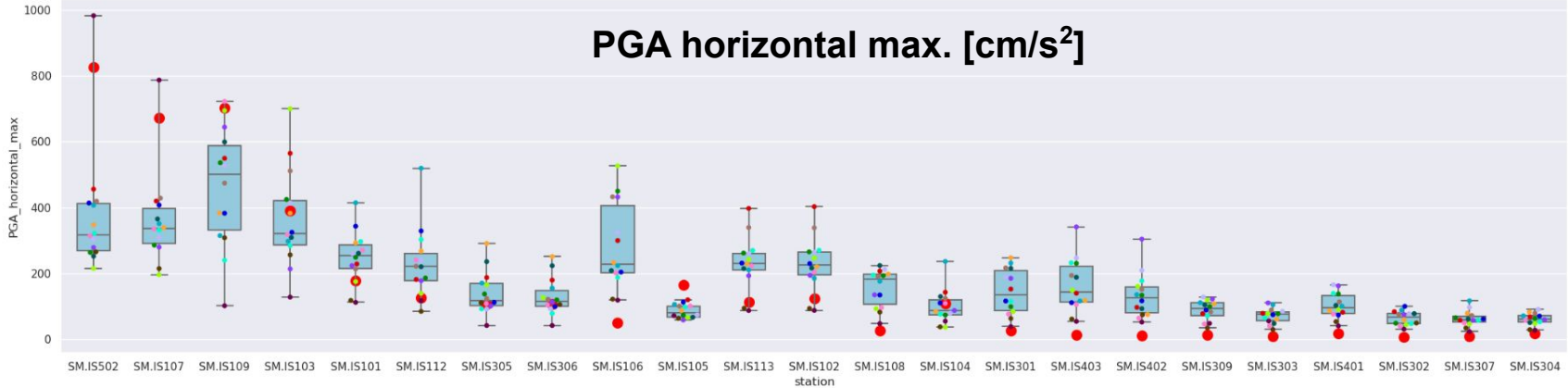
## PGA horizontal max. [ $\text{cm/s}^2$ ]



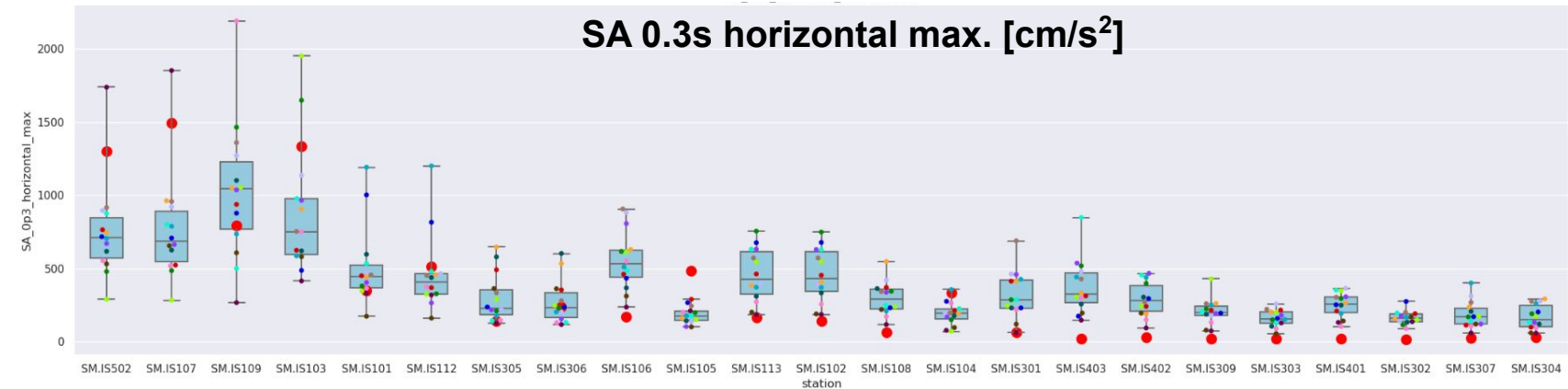
## SA 0.3s horizontal max. [ $\text{cm/s}^2$ ]



## PGA horizontal max. [cm/s<sup>2</sup>]



## SA 0.3s horizontal max. [cm/s<sup>2</sup>]



- Successful end-to-end executions of the UCIS4EQ using PyCOMPSs workflow manager
- The results are encouraging, with synthetics reproducing the right orders of magnitude observed in the recorded data.
- When well-calibrated, our results could complement or replace GMPEs for rapid hazard assessment.



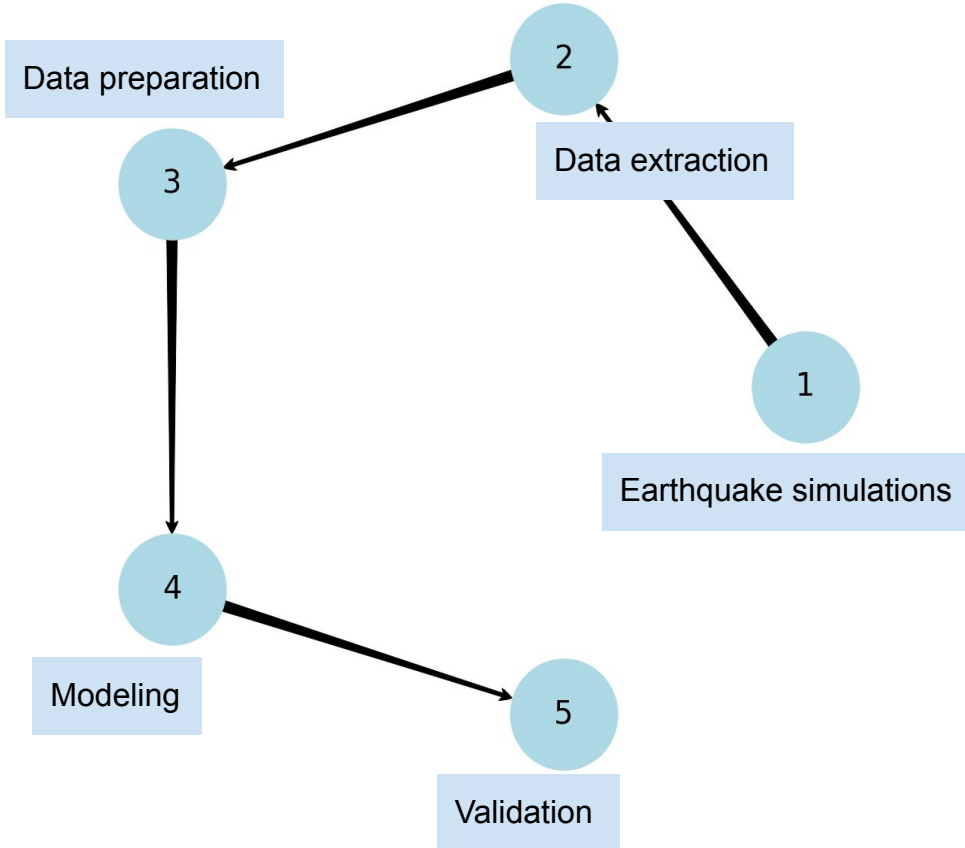
# **Machine Learning based Estimator for ground Shaking maps**

## **MLESmap workflow prototype**

# Machine Learning based Estimator for ground Shaking maps (MLEsmap)



Developing a novel methodology based on **analogous ML models** trained by a **large data set of physics-based** seismic simulations to fast-generate intensity maps in a given region **few seconds after an earthquake occurs**.



**features:** {  
"Site Lat", "Site Lon",  
"Magnitude",  
"EQ Lat", "EQ Lon", "EQ Depth",  
"Distance EQ-Sta", "Azim\_EQ-Sta" }  
**target:** "PSA"

Regression

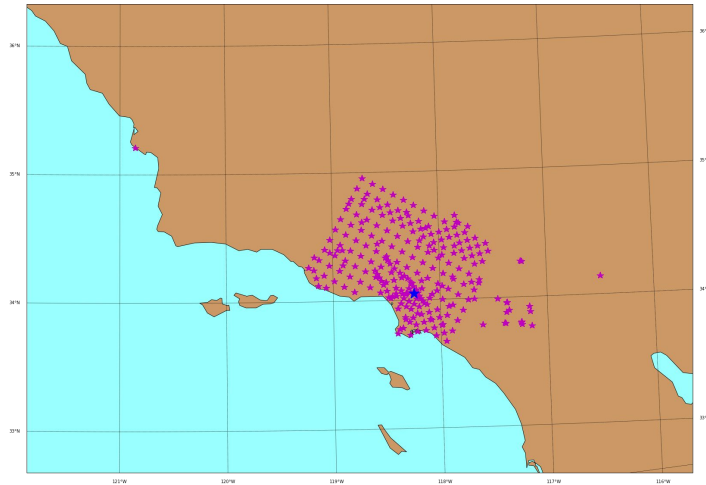
Random Forest → dislib

Neural Network → keras

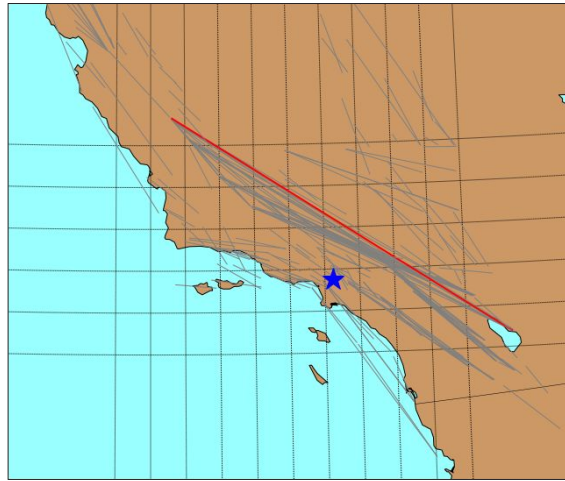
# Physics-based dataset

Los Angeles basin, Southern California (EEUU)

Recording stations (sites)

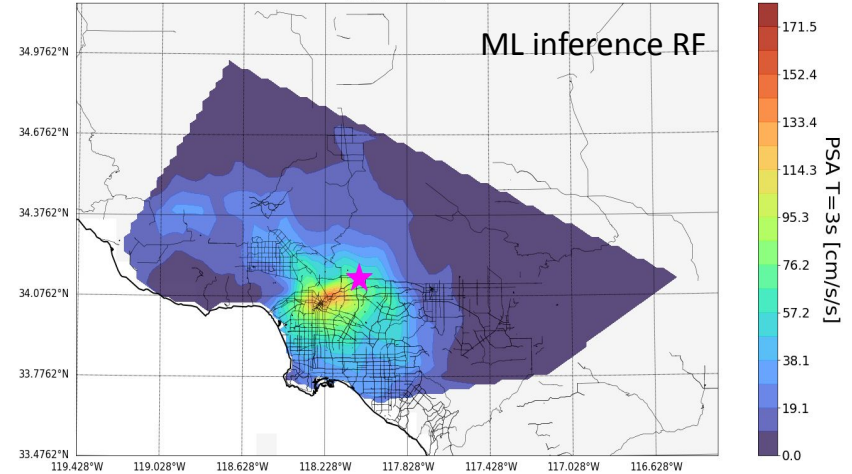
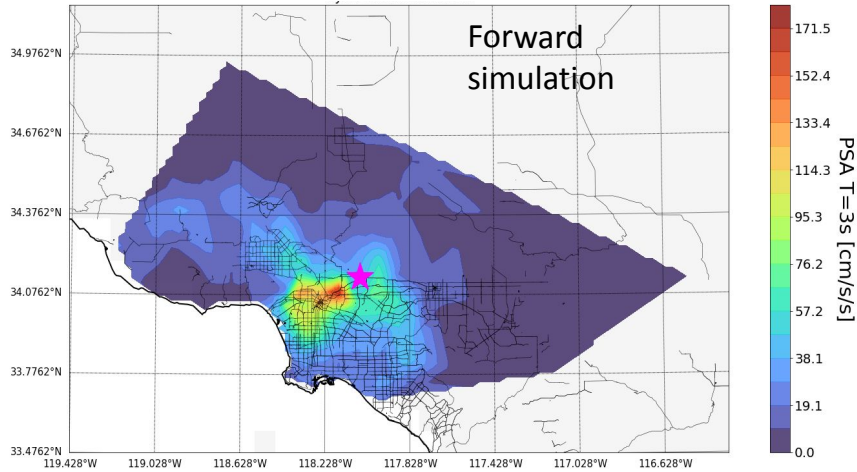


Fault systems



- [CyberShake 15\\_4](#)
- 253 Sites
- 225 Sources (faults or faults segments)
- 2.857.860 observations (seismic scenarios) per site
- Total of **721.687.578** events

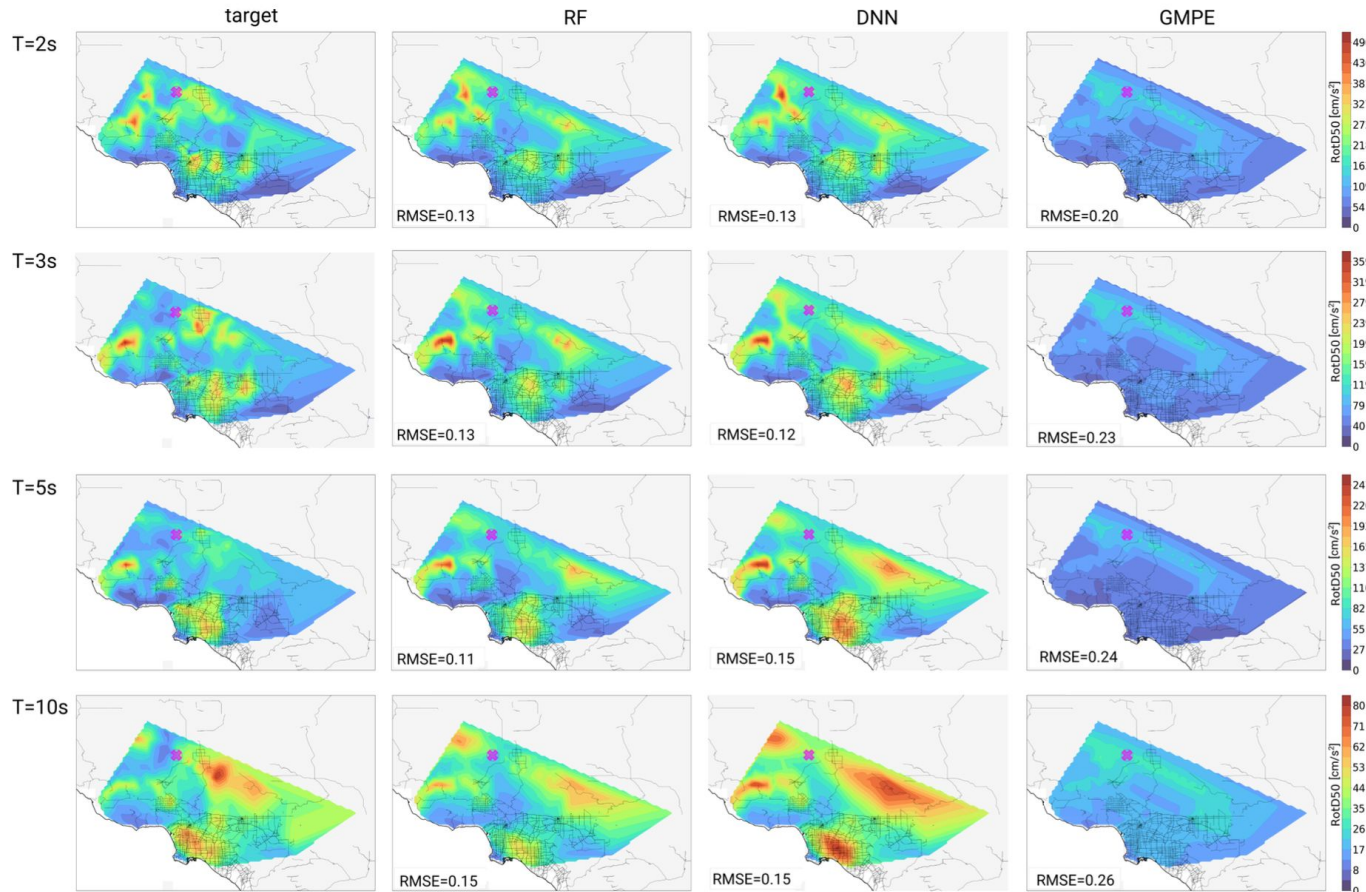
# MLEsmap on synthetic unseen example





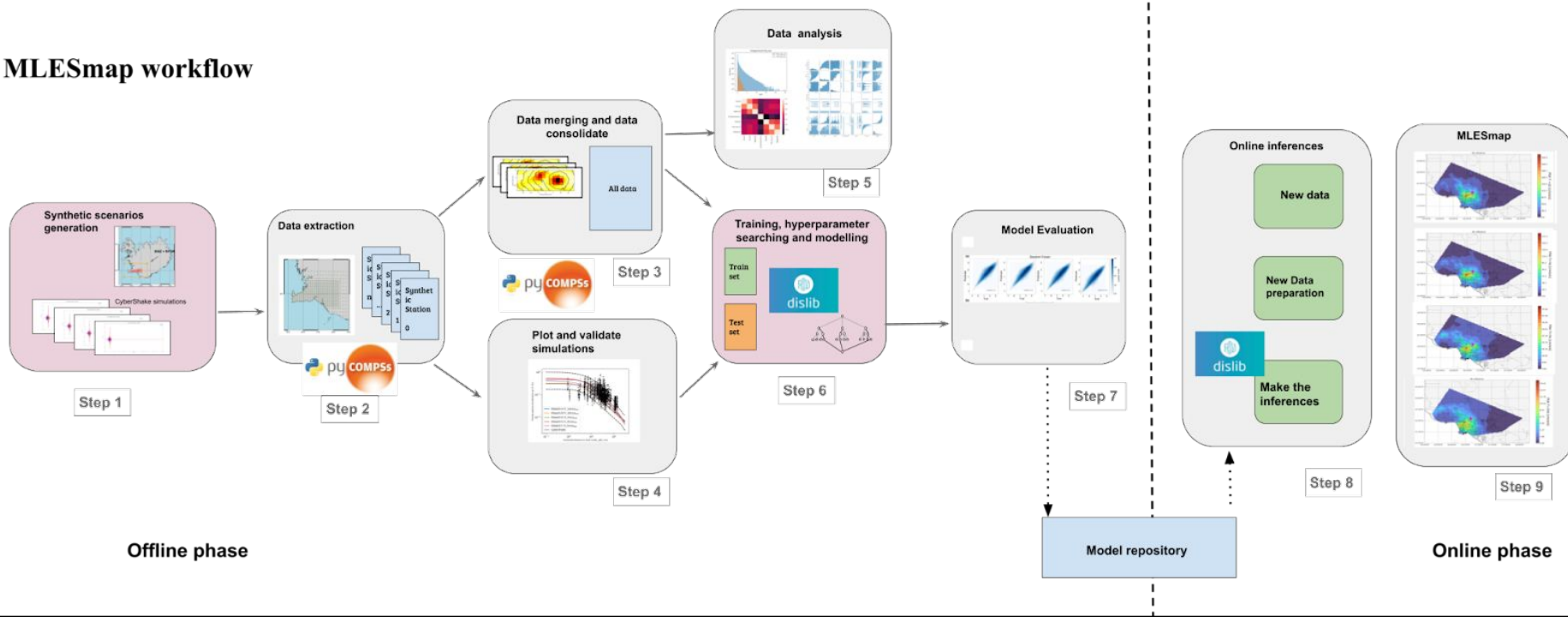
# Test results on synthetic EQ

Synthetic EQ of  
magnitude 8.05

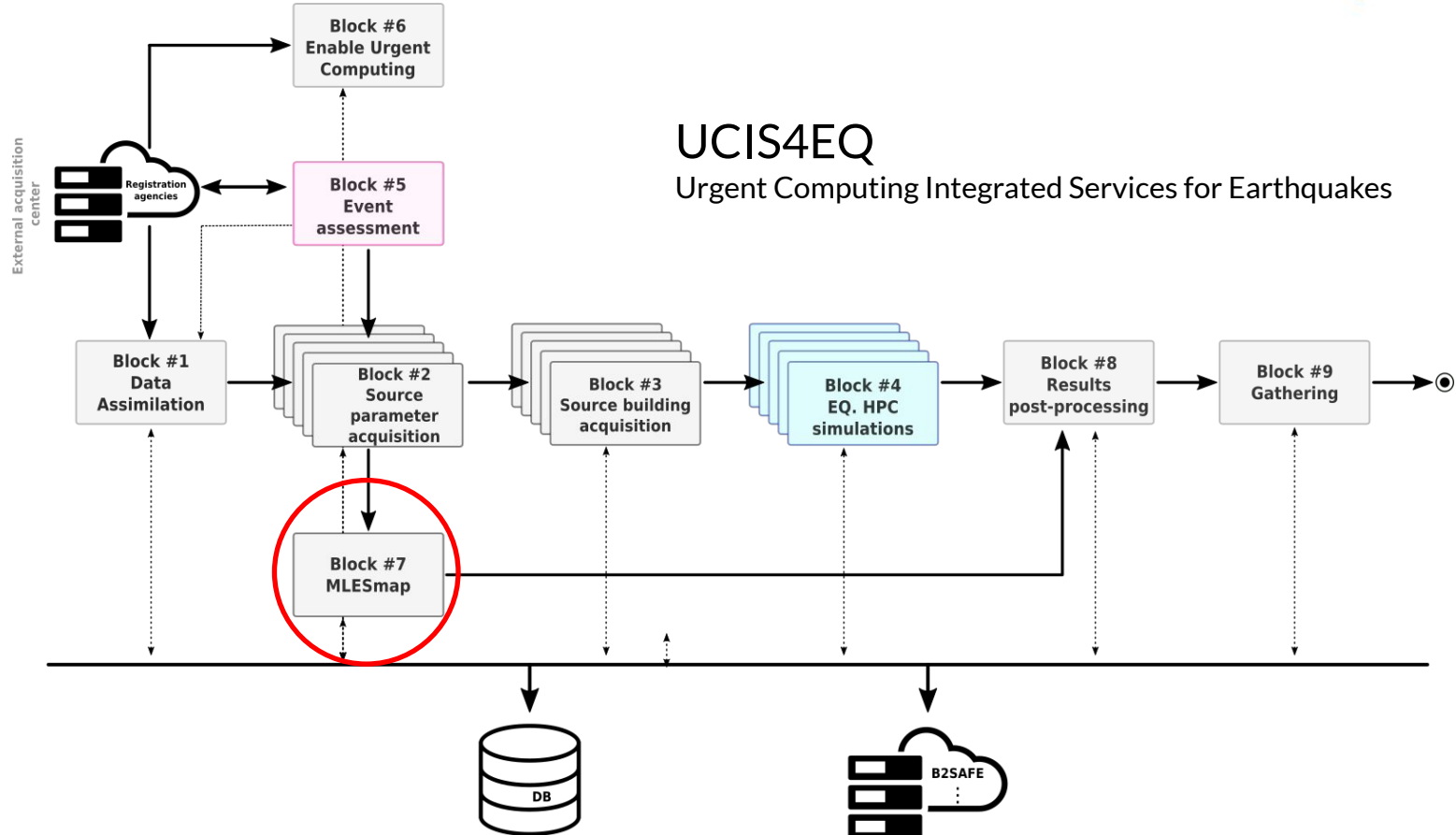


# MLEsmap workflow

## MLEsmap workflow

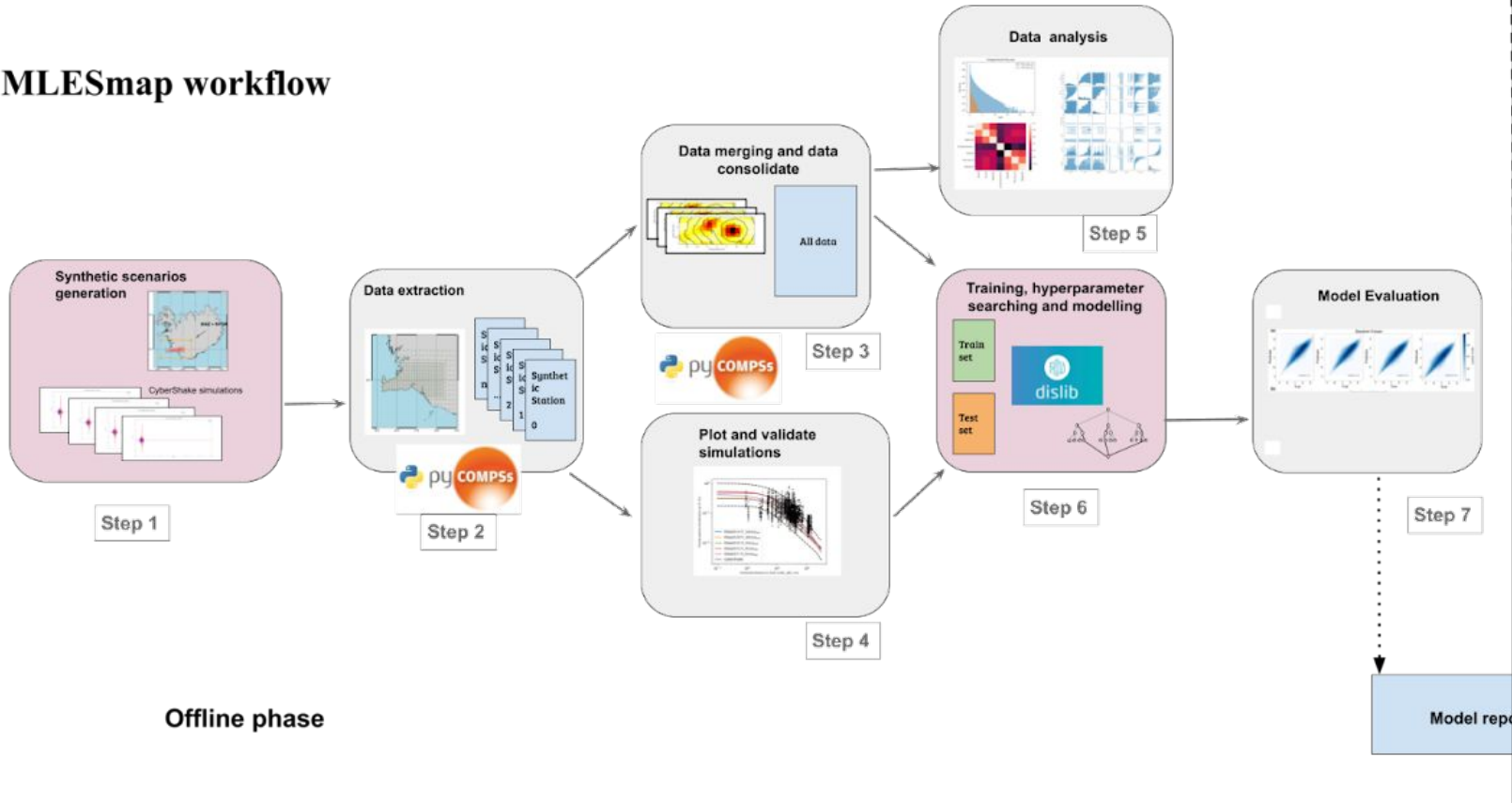


# MLEsmap models integrated into UCIS4EQ



# MLEsmap workflow offline phase

## MLEsmap workflow

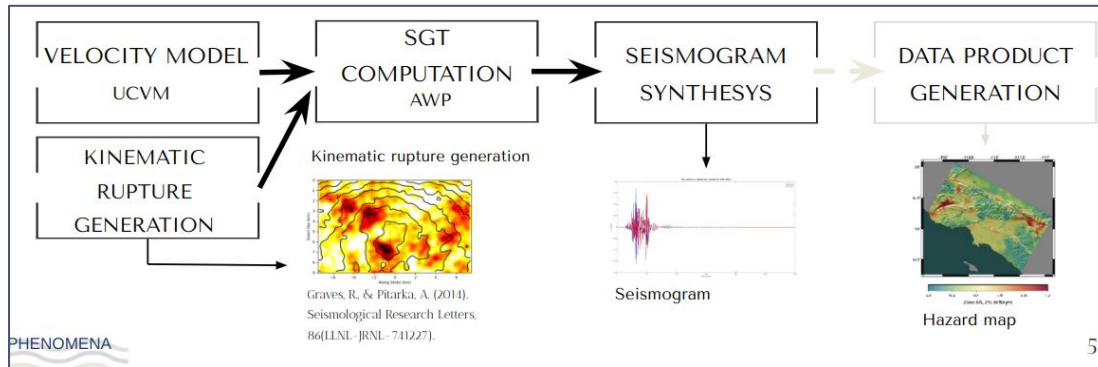


# MLEsmap workflow offline phase

## CyberShake WORKFLOW

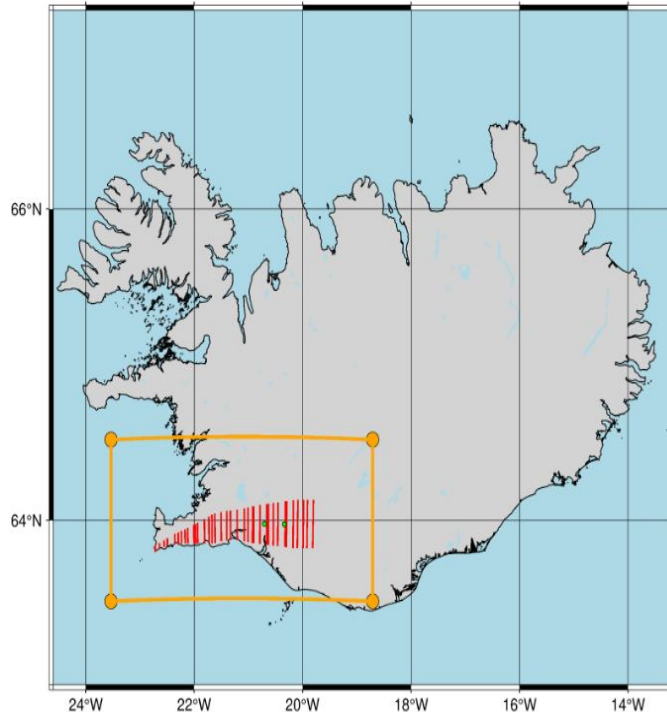
CyberShake generates the database from physics-based seismic scenarios. The number of synthetic seismograms depend on the number of stations and the number of faults to be simulated.

Computer resources per each station



Stages	CPU's	Node	Tasks	Runtime
Pre-SGT	48	1	1	1 min
pre-AWP	48	1	1	15 s
AWP_X	576	12	576	20 min
AWP_Y	576	12	576	20 min
post-X	48	1	1	10 min
post-Y	48	1	1	10 min
run_DS	576	12	288	5 min

# MLEsmap -- Study area

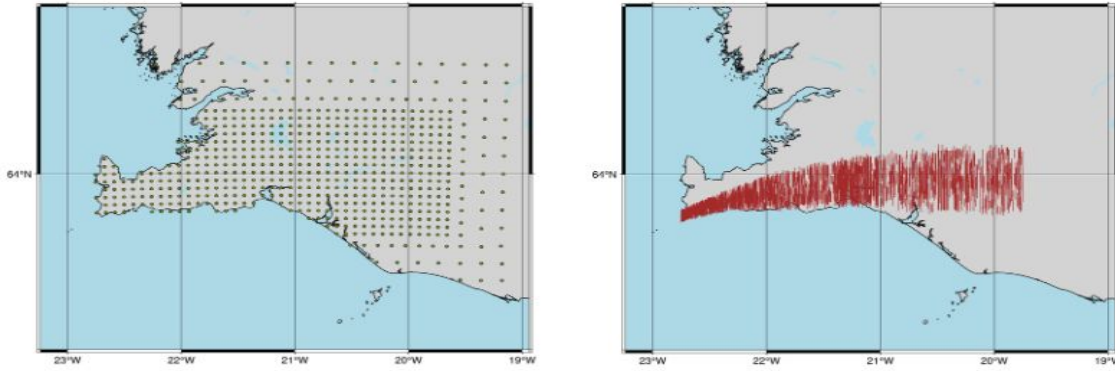


Southwest Iceland bookshelf transform zone

- **Iceland is the most seismically active region in northern Europe**, due to its location on the Mid-Atlantic Ridge, which along with the Icelandic hot spot, is responsible for the tectonics and its active seismicity and volcanism
- **The largest earthquakes** in Iceland occur within the two transform fault zones in the country, the South Iceland Seismic Zone (SISZ) and Reykjanes Peninsula Oblique Rift (RPOR)
- The SISZ is characterized by the bookshelf faulting model containing seismogenic **strike-slip N-S striking faults**

# MLEsmap data generation

CyberShake generates the database from physics-based seismic scenarios. The number of synthetic seismograms depend on the number of stations and the number of faults to be simulated.



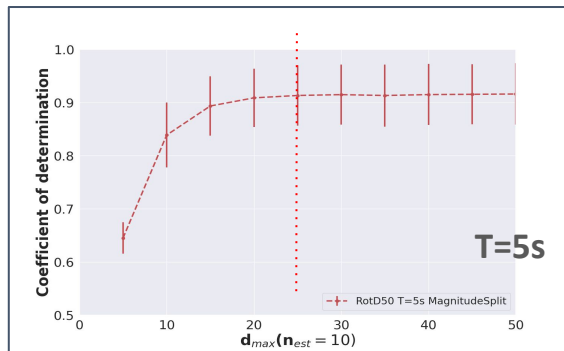
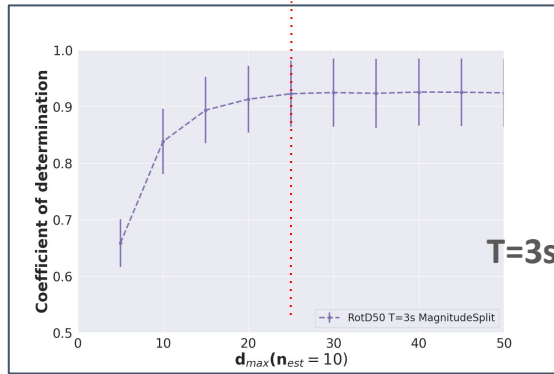
Computer resources per each station

Stages	CPU's	Node	Tasks	Runtime
Pre-SGT	48	1	1	1 min
pre-AWP	48	1	1	15 s
AWP_X	576	12	576	20 min
AWP_Y	576	12	576	20 min
post-X	48	1	1	10 min
post-Y	48	1	1	10 min
run_DS	576	12	288	5 min

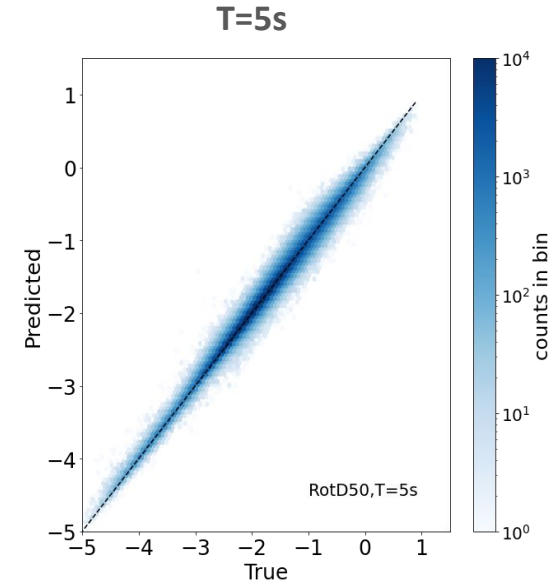
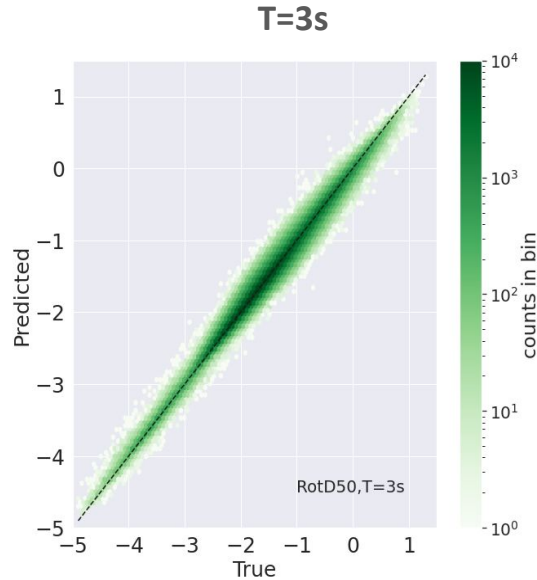
Location map of the synthetic seismic stations and the location of the faults 593 Synthetic Stations and 16633 events

# Preliminary results on SISZ region

## Hyperparameters RF dislib



## Results on validation set





# MLEsmap conclusions

- **MLEsmap: towards the combination of physics-based data and ML engine to fast estimate the ground shaking intensity using EQ information available shortly after the event**



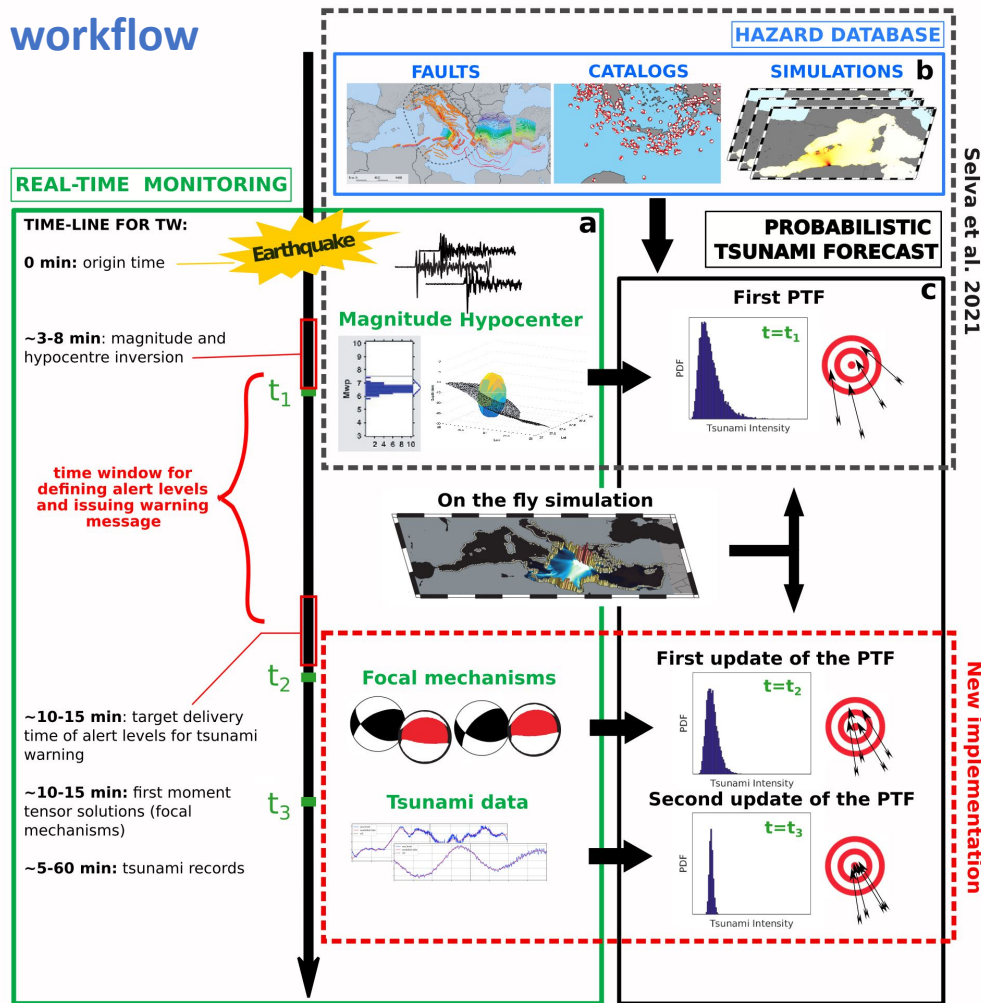
# Tsunami workflow

## PTF (Probabilistic Tsunami Forecast)

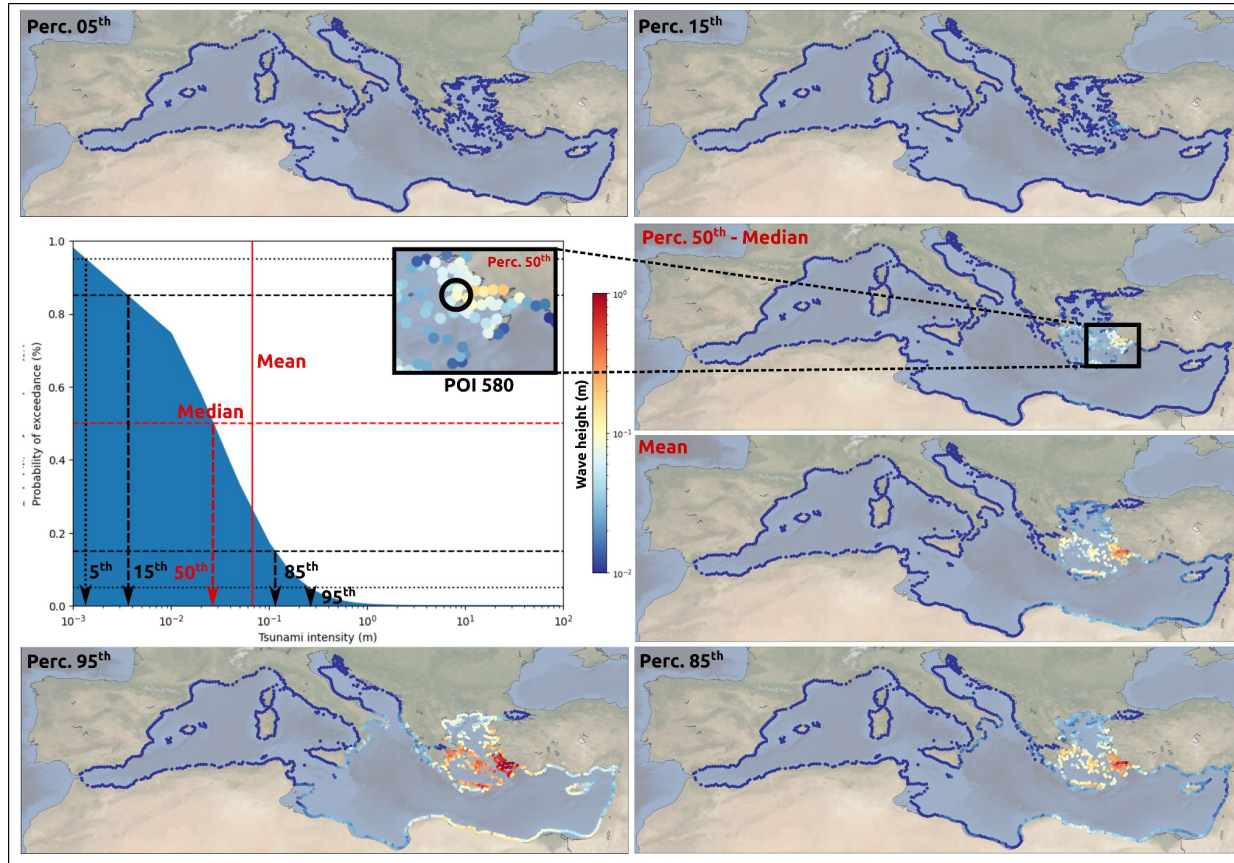
### Content

- introduction and motivation
- workflow description: technical and scientific improvements
- further developments

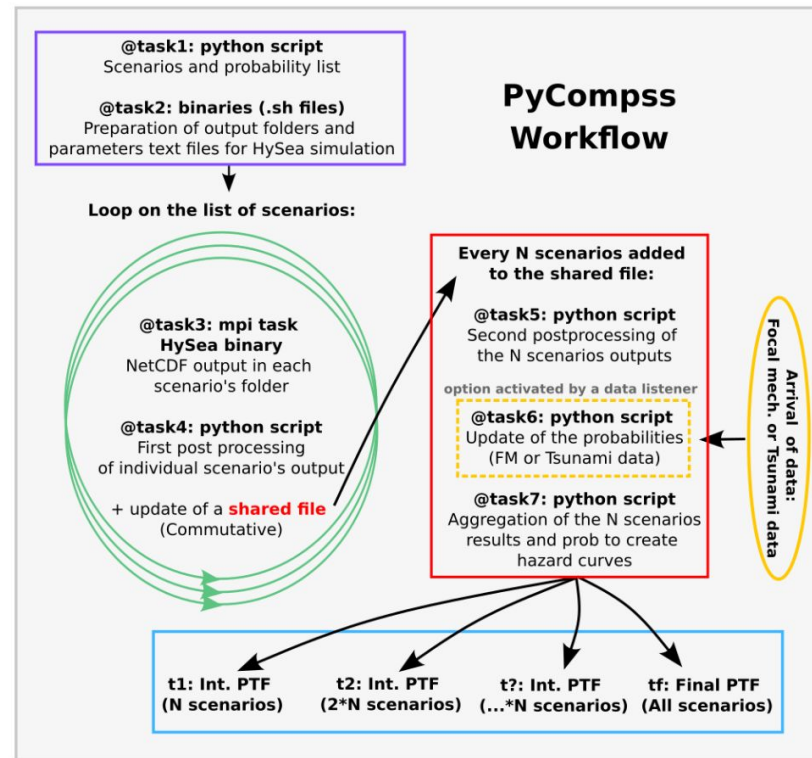
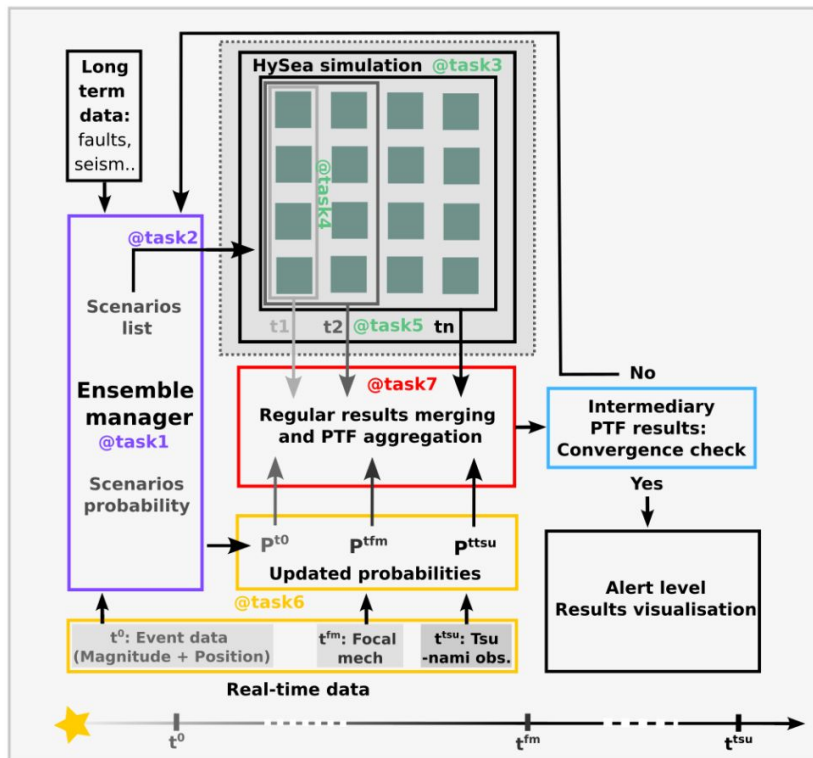
# Introduction of the PTF workflow



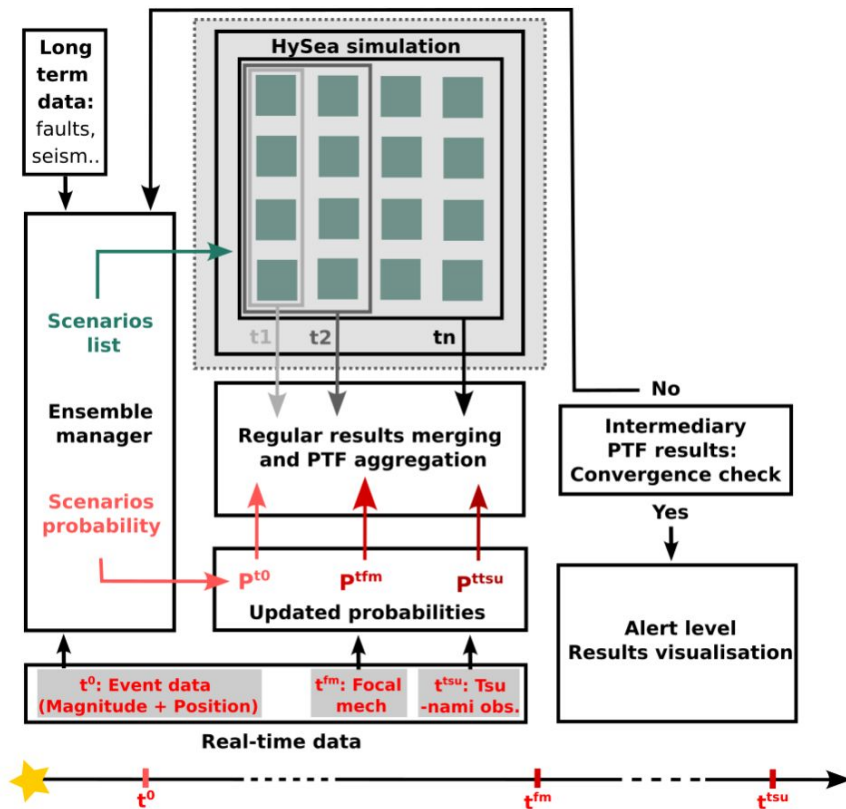
# Introduction of the PTF workflow



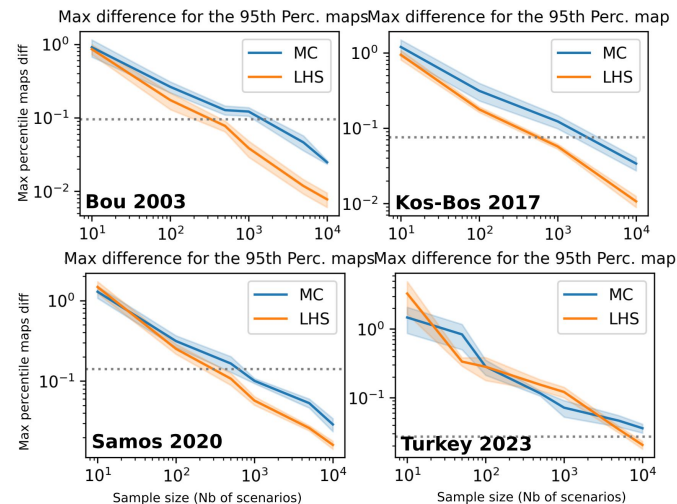
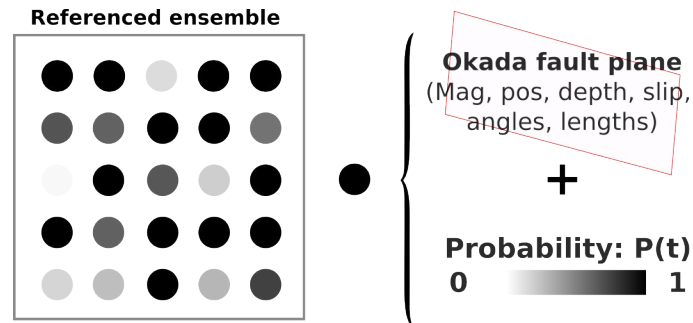
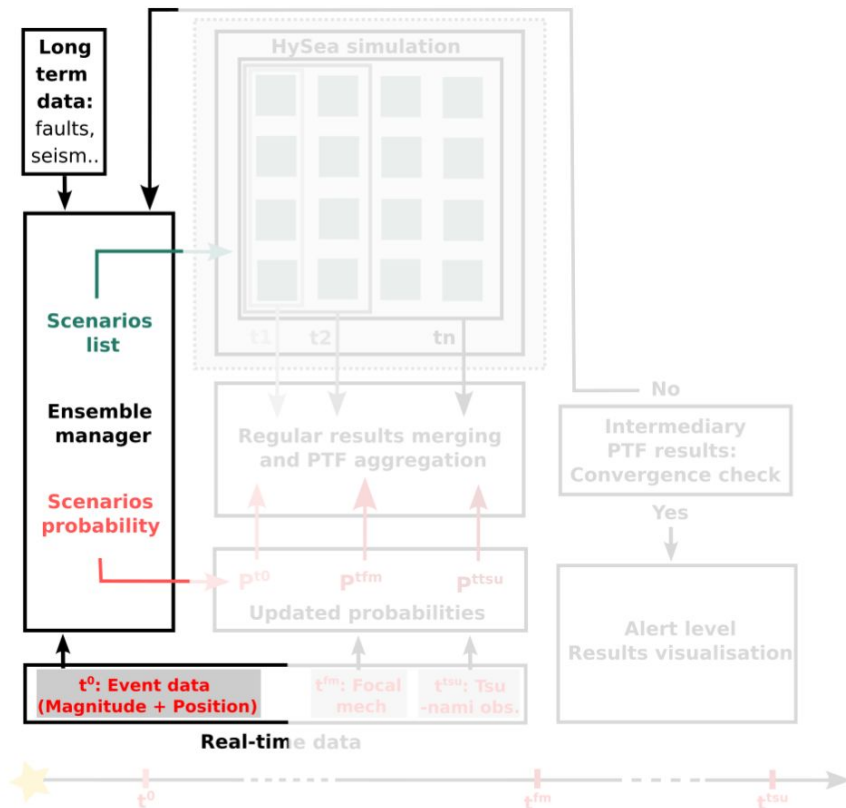
# First end-to-end version of PTF orchestrated with PyCOMPSs



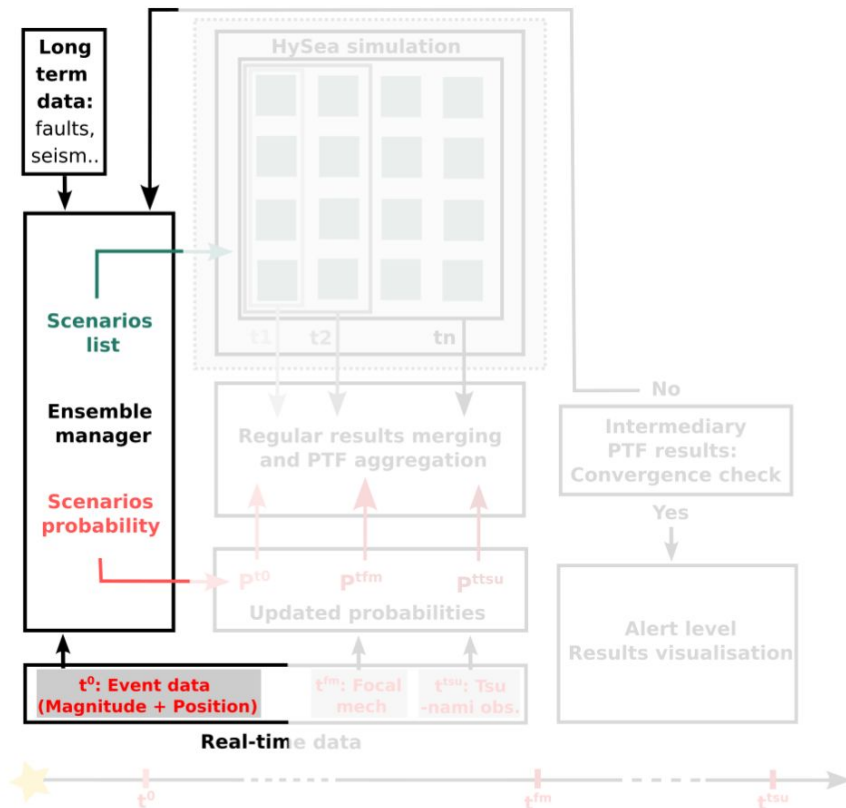
# PyCOMPSs workflow



# PyCOMPSs workflow: Step1, ensemble manager



# PyCOMPSs workflow: Step1, ensemble manager

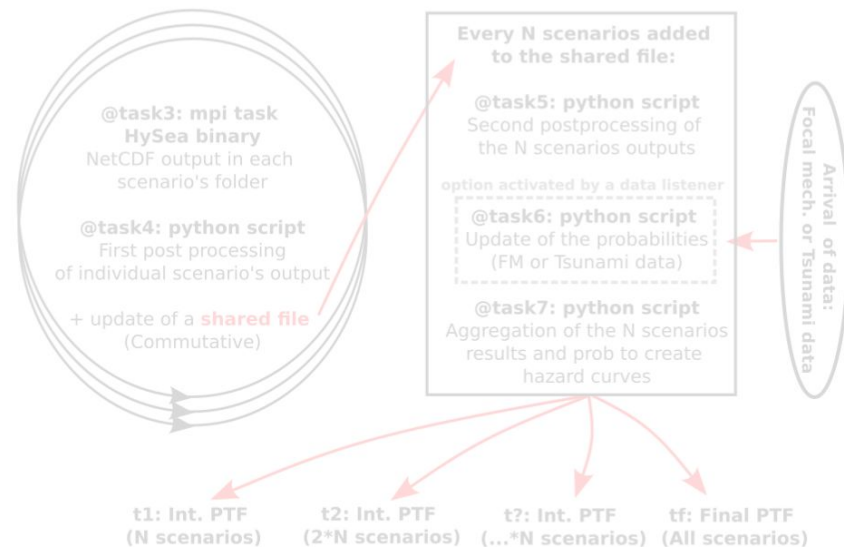


## PyCompss workflow

**@task1: python script**  
Scenarios and probability list

**@task2: binaries (.sh files)**  
Preparation of output folders and parameters text files for HySea simulation

Loop on the list of scenarios:

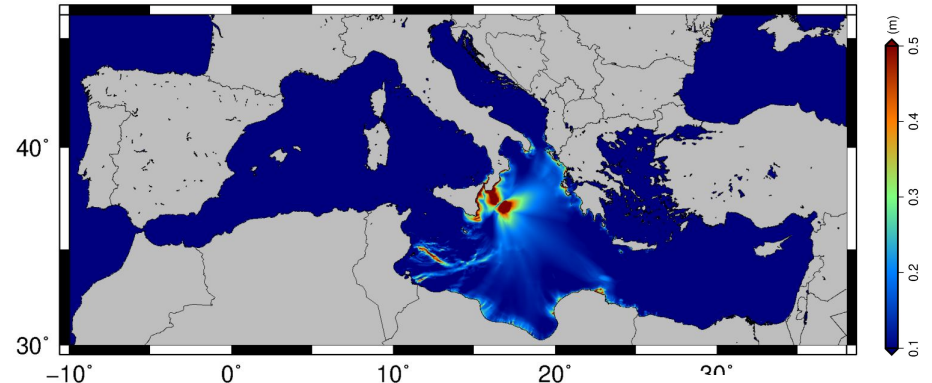
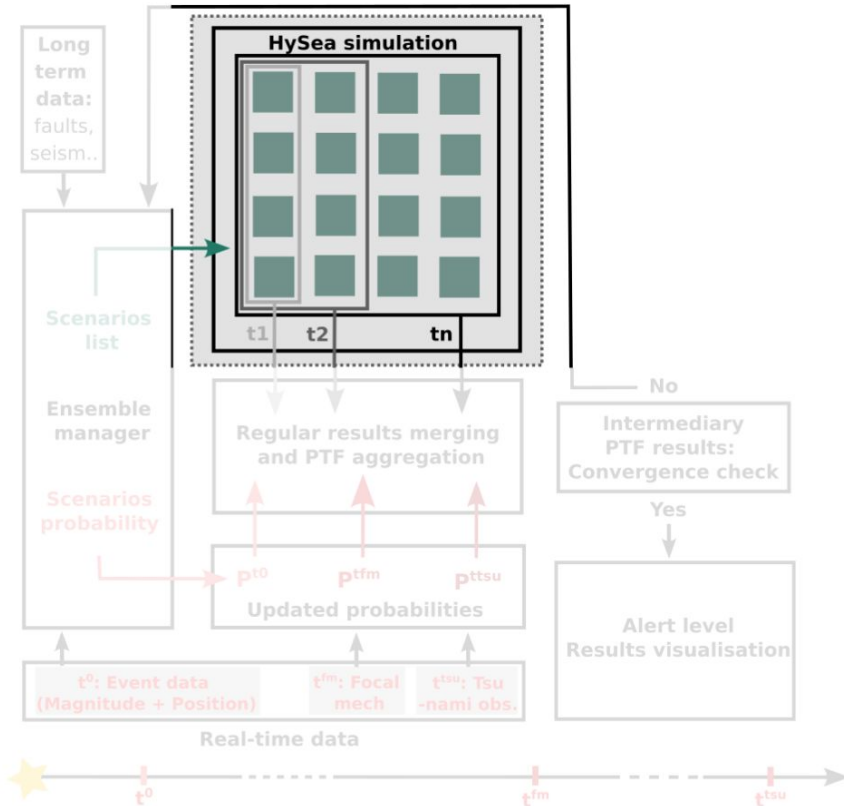
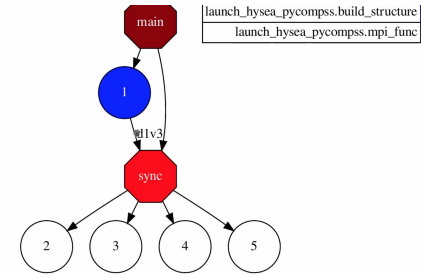




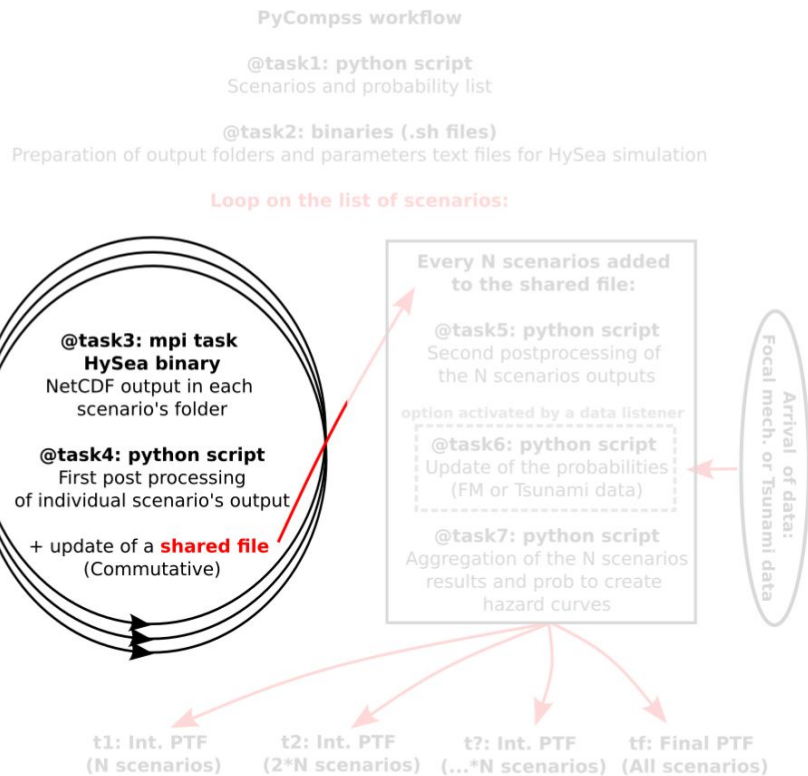
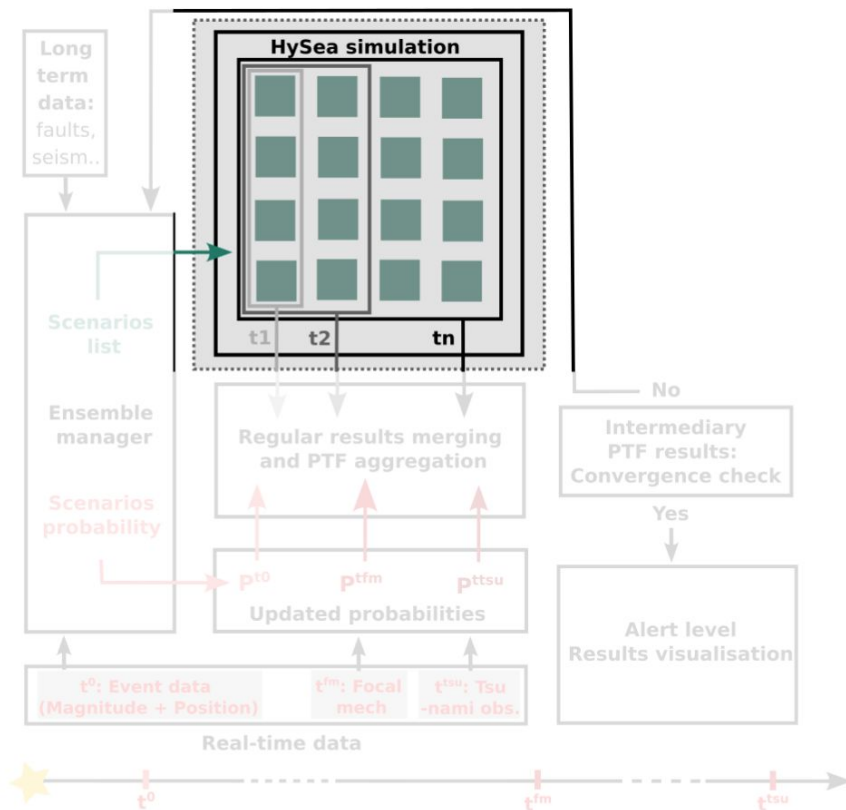
# PyCOMPSs workflow: Step2, HySea simulations

## Integration of HySEA in the workflow and mpi-mc parallelisation

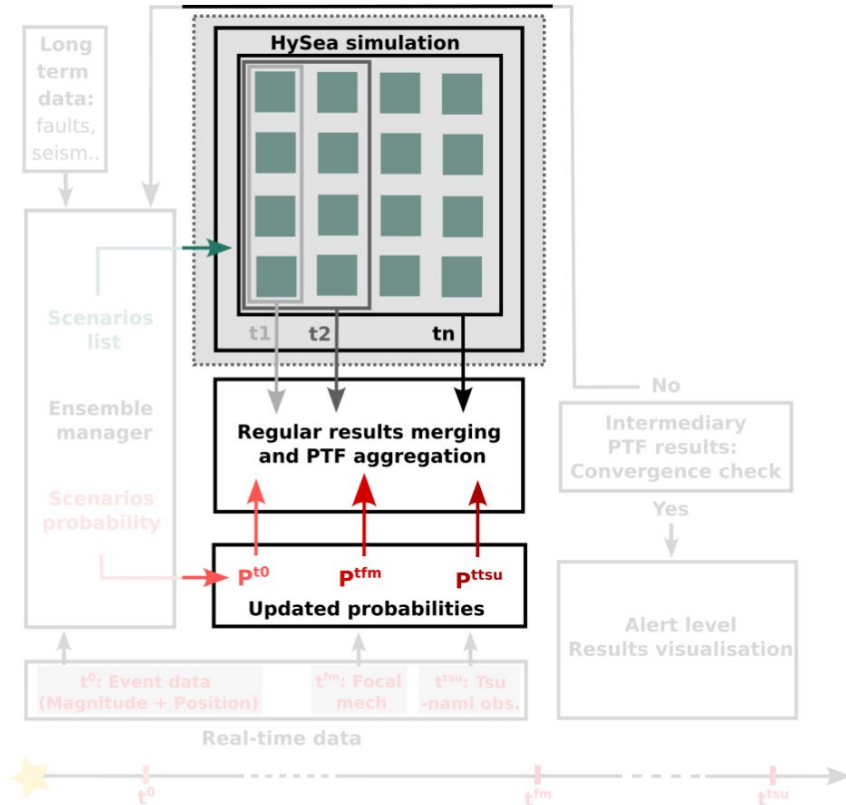
PyComps calls the HySEA binary task in several nodes in parallel. Each task runs a single job to the queue system that implicitly carries out the parallel execution of a predefined number of simulations dividing into internal jobs, and allowing the traceability of each processes involved to be observed.



# PyCOMPSs workflow: Step2, HySea simulations



# PyCOMPSs workflow: Step3, post-processing of the output

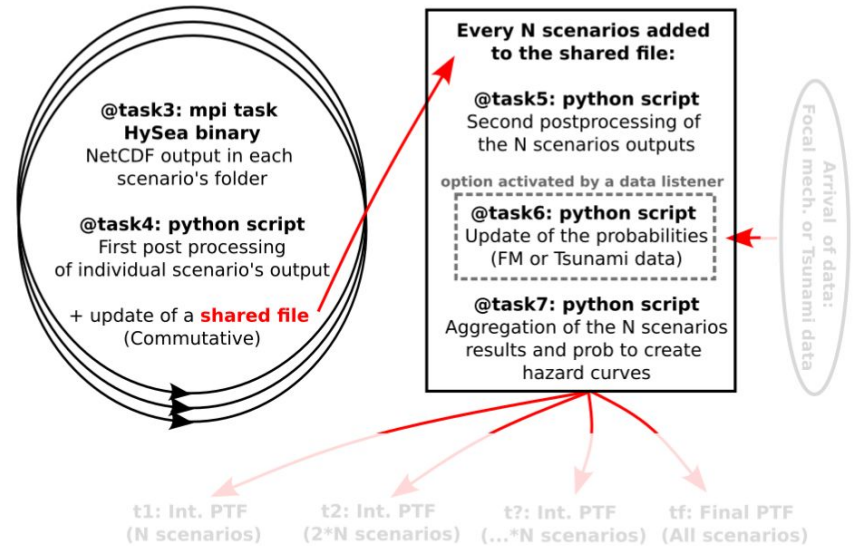


## PyCompss workflow

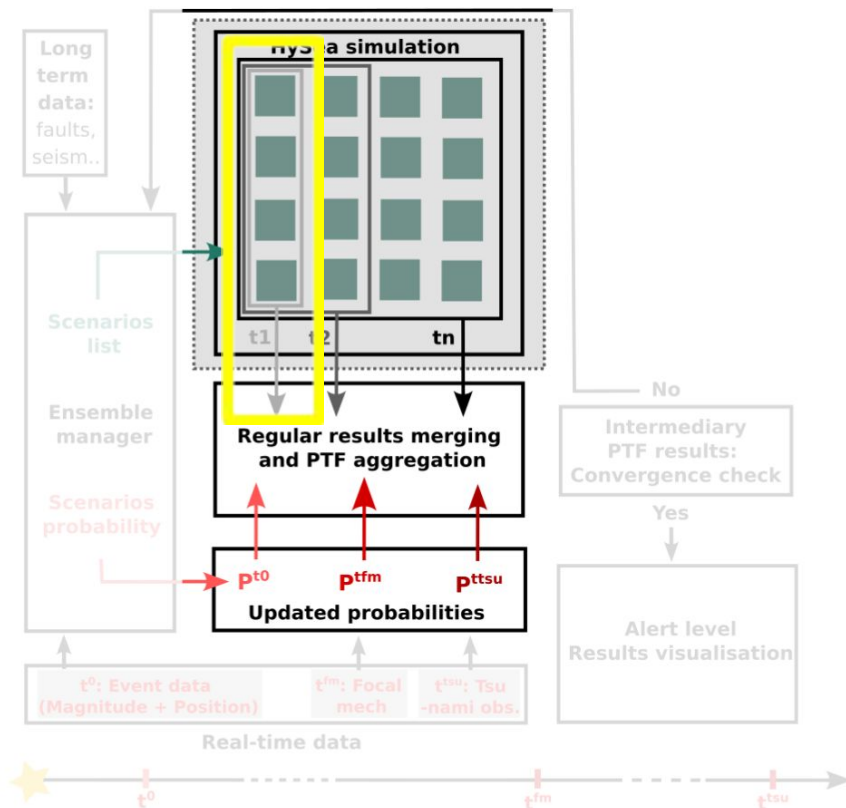
@task1: python script  
Scenarios and probability list

@task2: binaries (.sh files)  
Preparation of output folders and parameters text files for HySea simulation

### Loop on the list of scenarios:



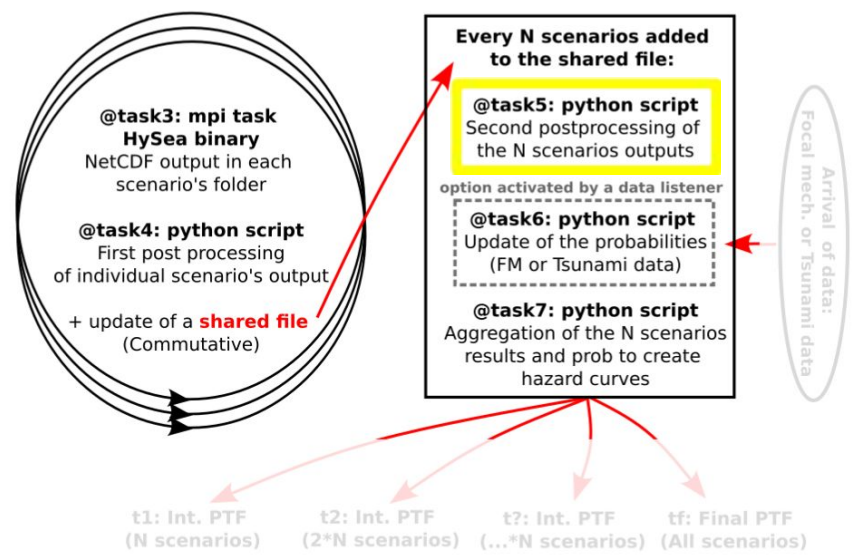
# PyCOMPSs workflow: Step3, post-processing of the output



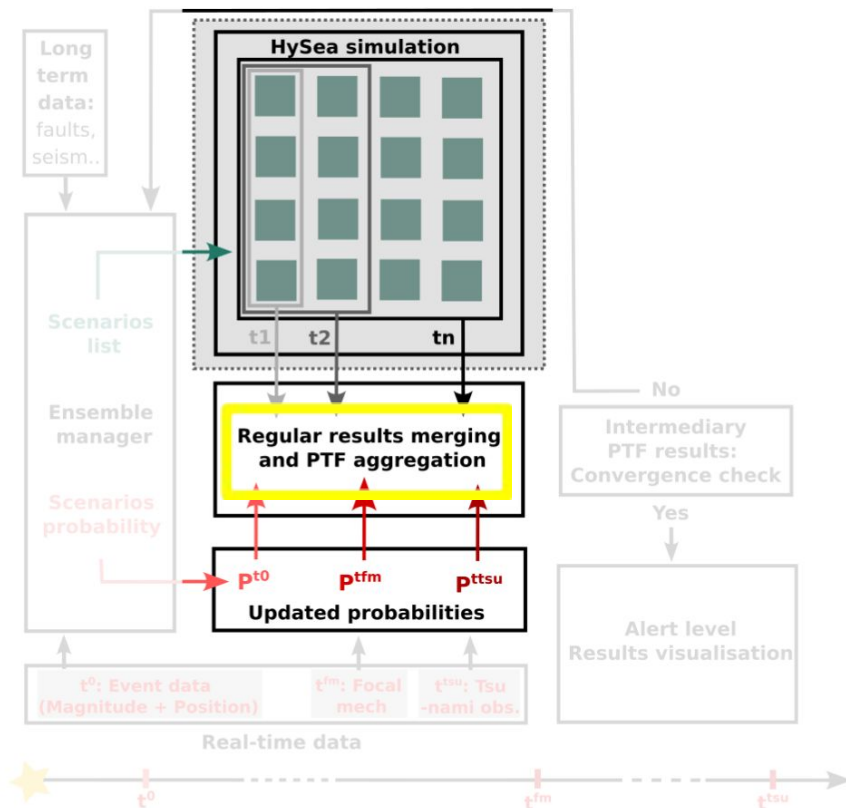
PyCompss workflow

- @task1: python script  
Scenarios and probability list
- @task2: binaries (.sh files)  
Preparation of output folders and parameters text files for HySea simulation

**Loop on the list of scenarios:**



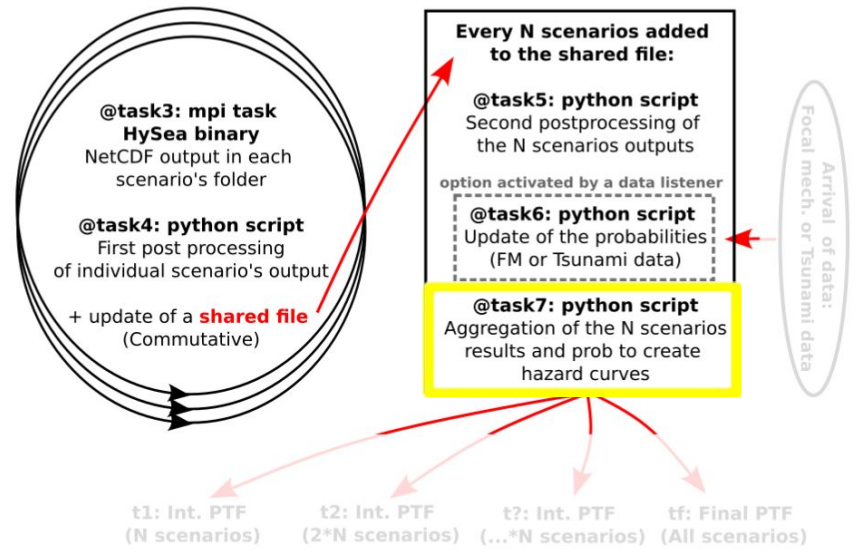
# PyCOMPSs workflow: Step3, post-processing of the output



PyCompss workflow

- @task1: python script  
Scenarios and probability list
- @task2: binaries (.sh files)  
Preparation of output folders and parameters text files for HySea simulation

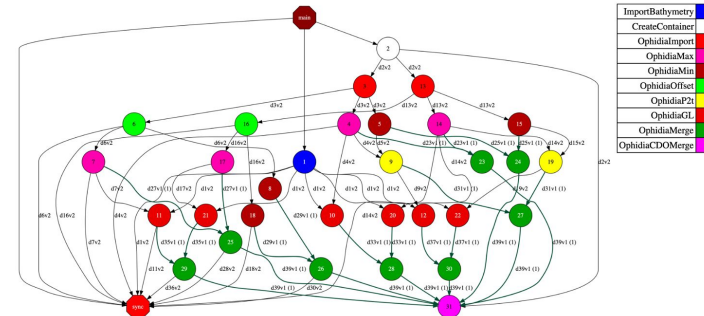
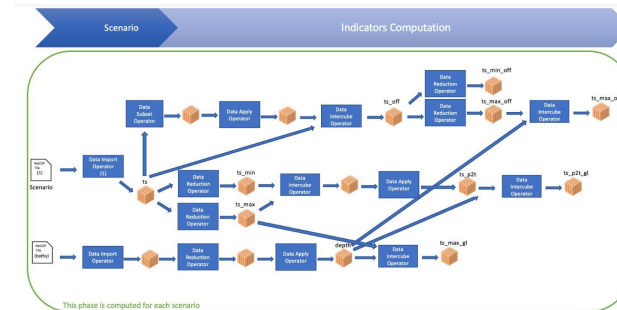
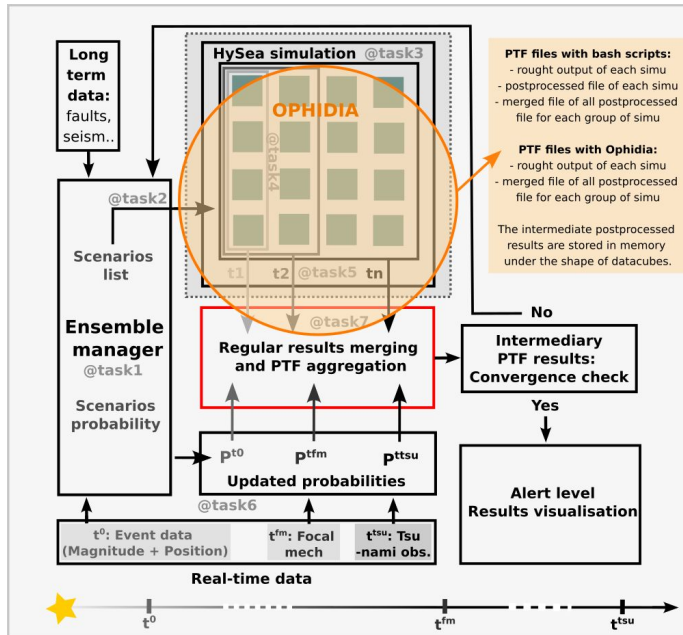
**Loop on the list of scenarios:**



# PyCOMPSs workflow: Step3, post-processing of the output

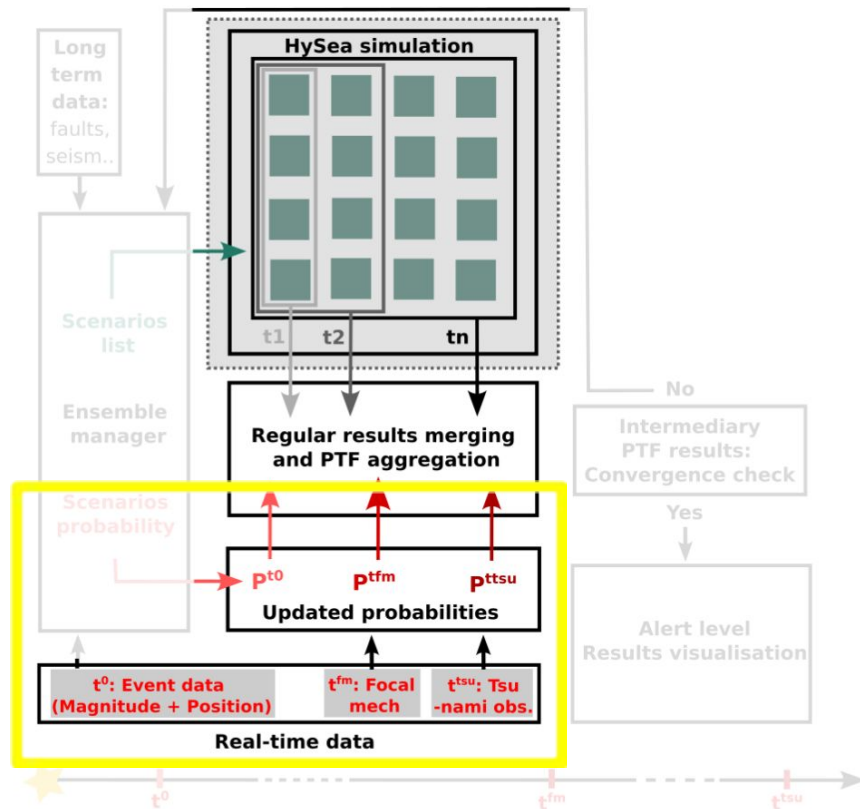
## Post-Processing in 2 steps with python scripts or using Ophidia

- STEP3 is implemented with **2 python scripts**, one running after each simulation, and one running when all simulations are completed. The use of the **Ophidia** framework avoid generating required continuous I/O operations from disk to save and then retrieve the outputs for the final merging phase.



This figure shows the PyCOMPSs tasks graph generated at the end of the workflow.

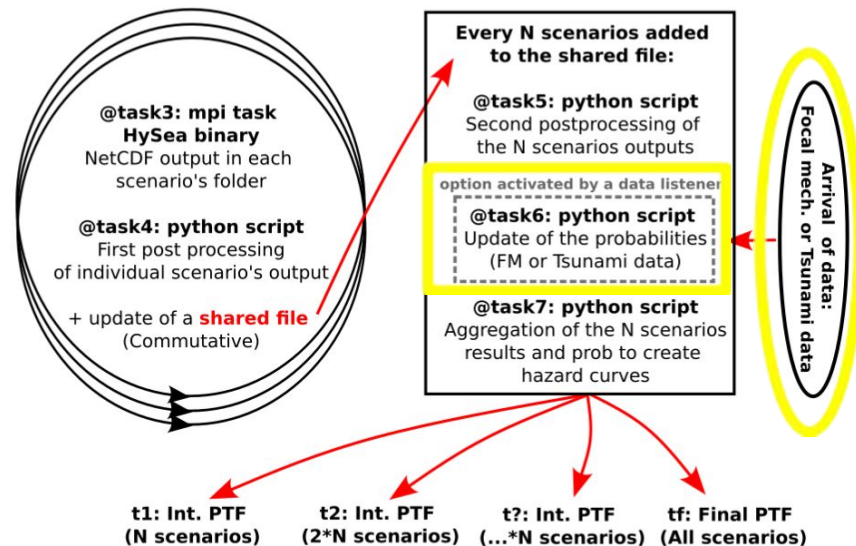
# PyCOMPSs workflow: Data-driven update of the PTF



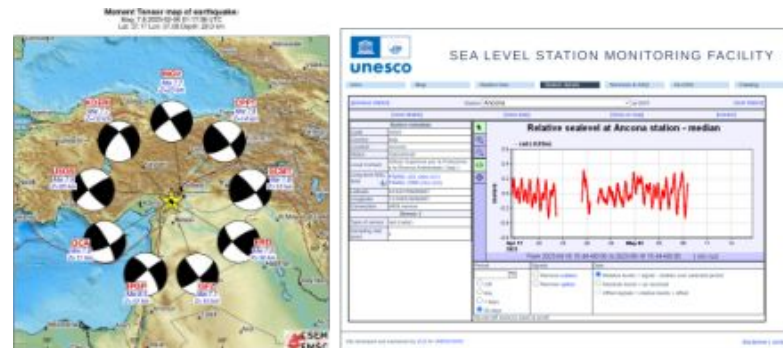
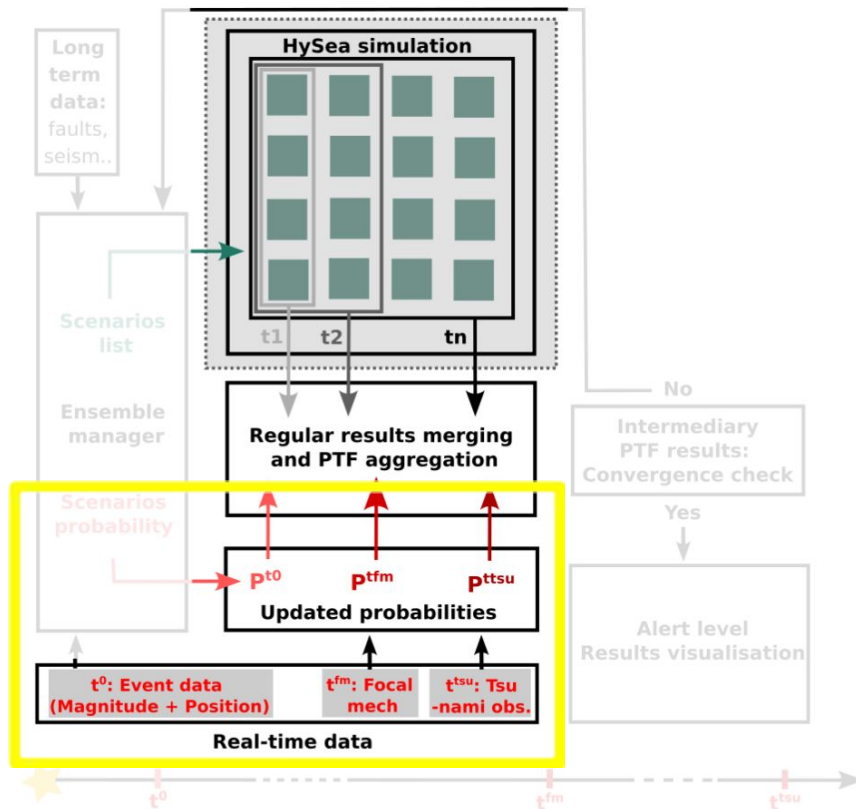
PyCompss workflow

- @task1: python script  
Scenarios and probability list
- @task2: binaries (.sh files)  
Preparation of output folders and parameters text files for HySea simulation

**Loop on the list of scenarios:**



# PyCOMPSs workflow: Data-driven update of the PTF



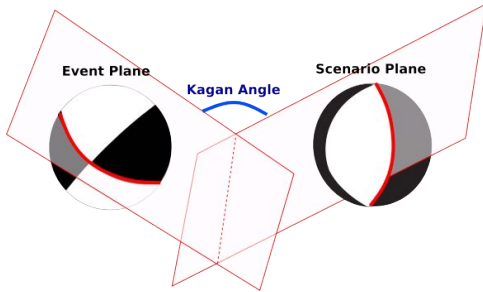


# PyCOMPSs workflow: Data-driven update of the PTF

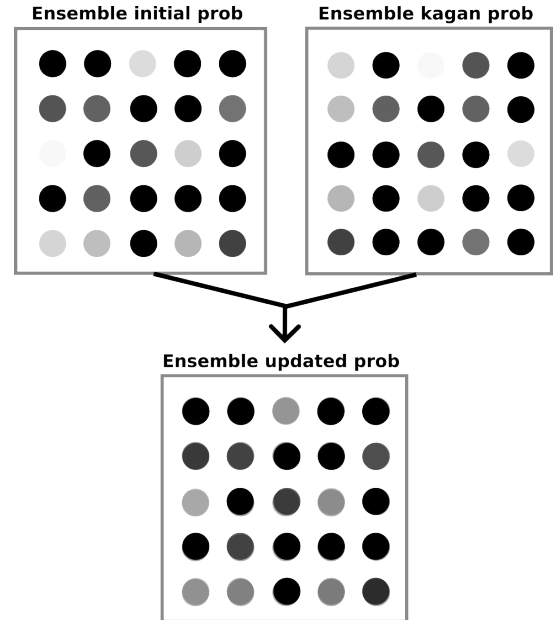
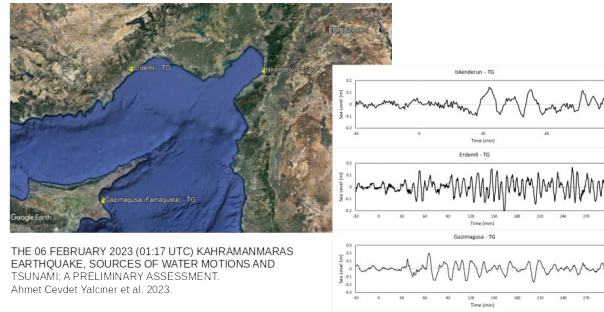
## Use of new incoming information to update the scenarios' probabilities

- After the post-processing step and before the aggregation step, two tasks can be optionally (listener/parameter?) activated and allow a re-weighting of the probabilities based on information on the earthquake or the tsunami
- One task takes into input data on the earthquake focal-mechanism and the second one takes into input the tsunami observations (tide-gage records)

Focal mechanism (Kagan angle)

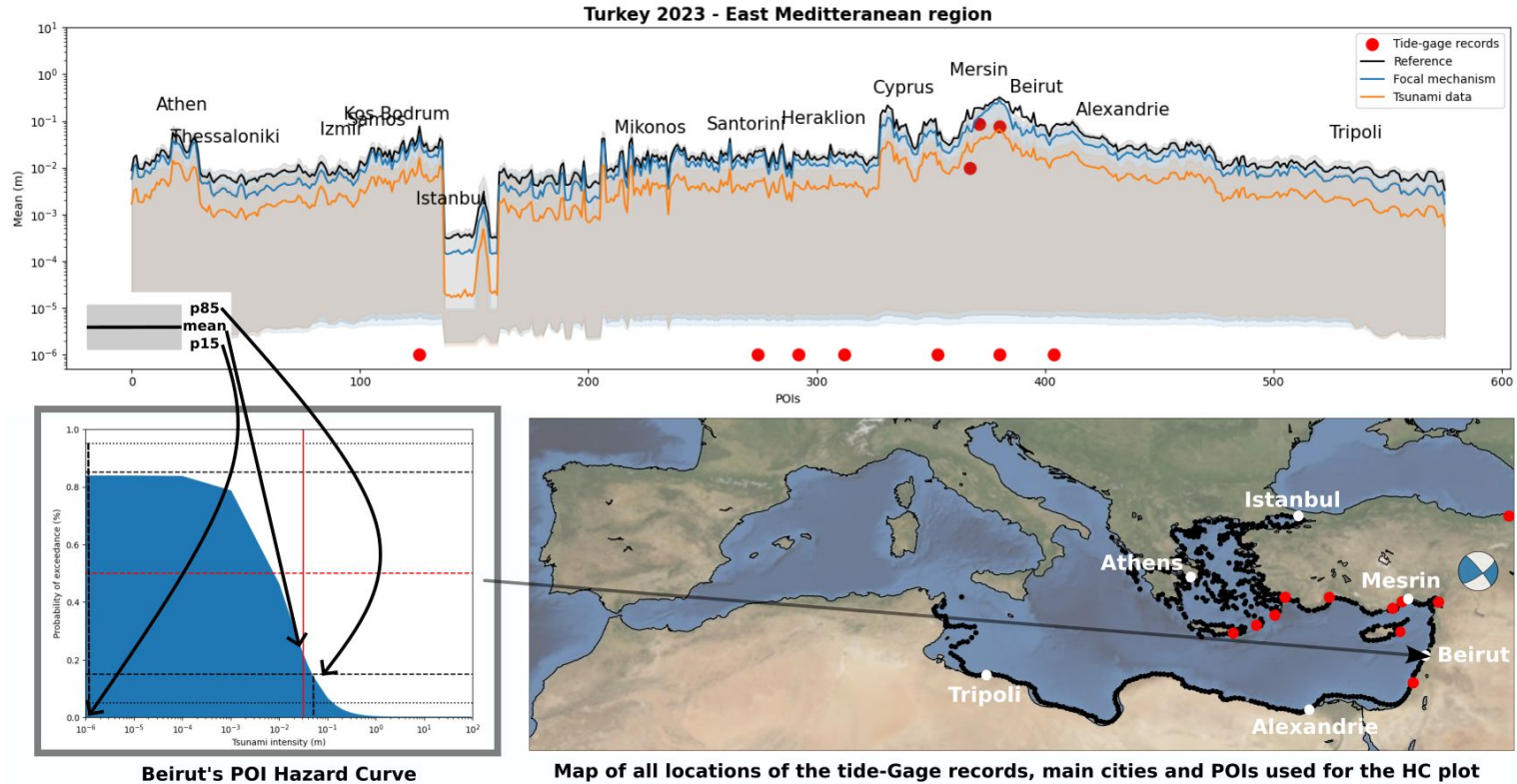


Tsunami data

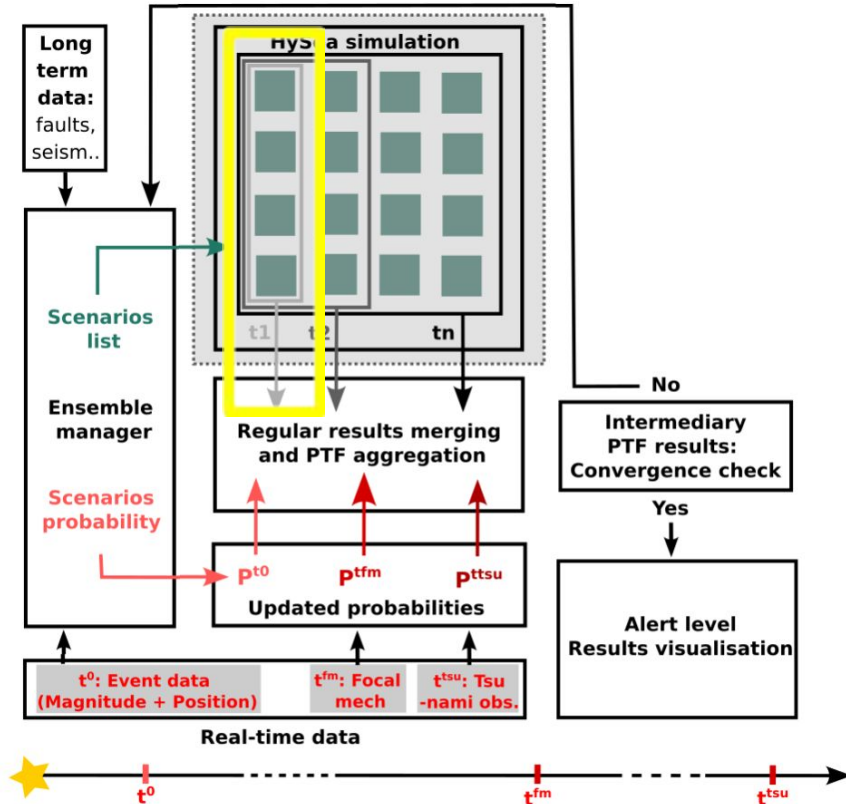


# PyCOMPSs workflow: Data-driven update of the PTF

Use of new incoming information to update the scenarios' probabilities



# PyCOMPSs workflow: Step3, intermediate evaluation of the PTF

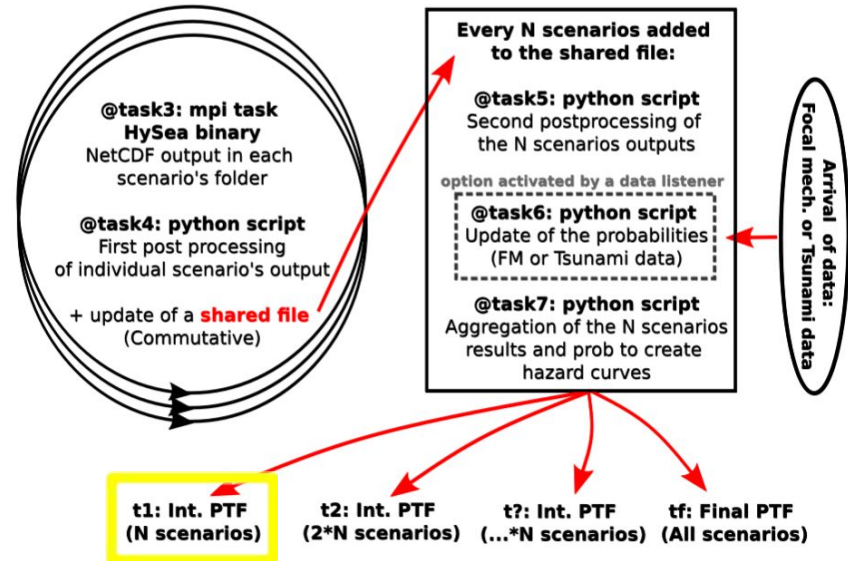


## PyComps workflow

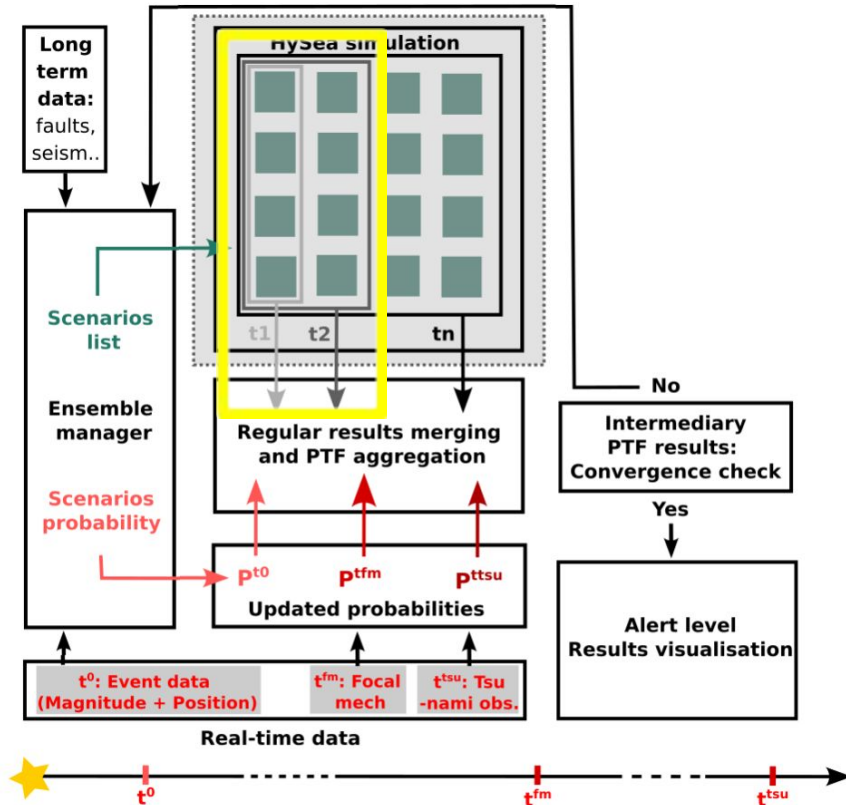
**@task1: python script**  
Scenarios and probability list

**@task2: binaries (.sh files)**  
Preparation of output folders and parameters text files for HySea simulation

### Loop on the list of scenarios:



# PyCOMPSs workflow: Step3, intermediate evaluation of the PTF

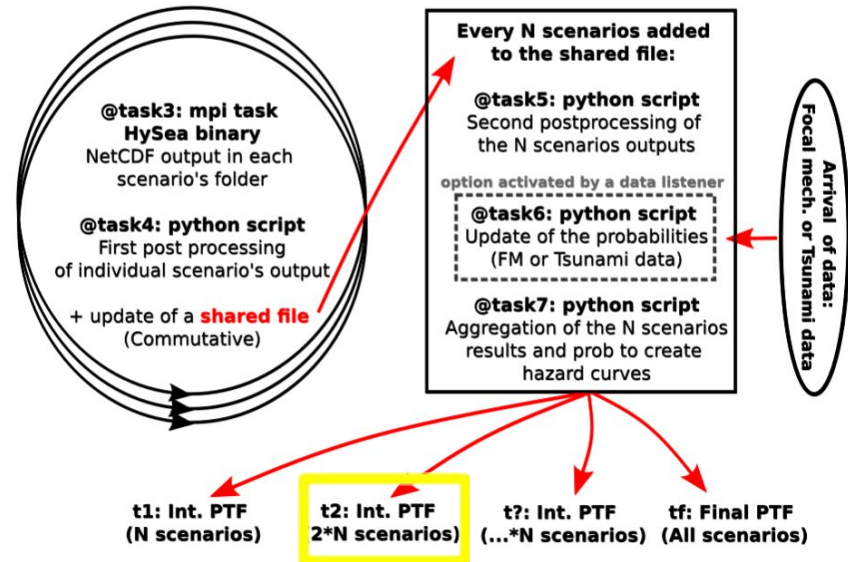


## PyComps workflow

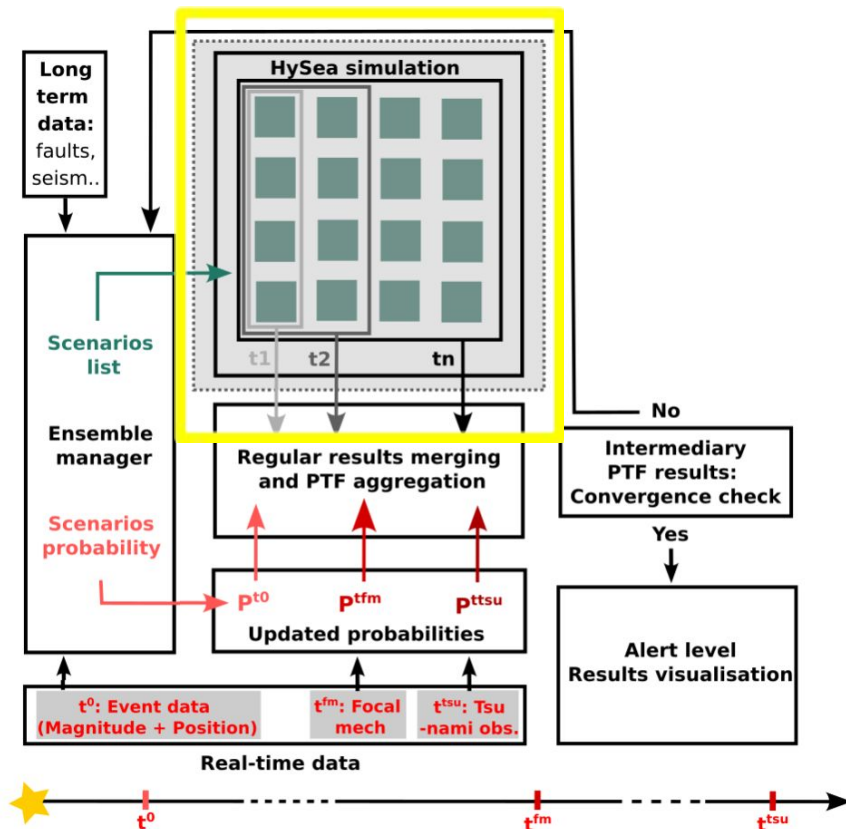
**@task1: python script**  
Scenarios and probability list

**@task2: binaries (.sh files)**  
Preparation of output folders and parameters text files for HySea simulation

### Loop on the list of scenarios:



# PyCOMPSs workflow: Step3, intermediate evaluation of the PTF

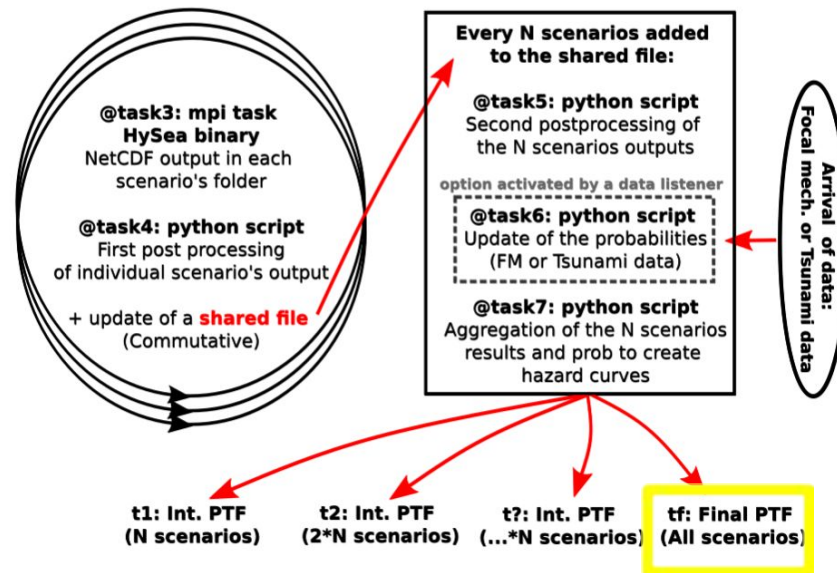


## PyComps workflow

**@task1: python script**  
Scenarios and probability list

**@task2: binaries (.sh files)**  
Preparation of output folders and parameters text files for HySea simulation

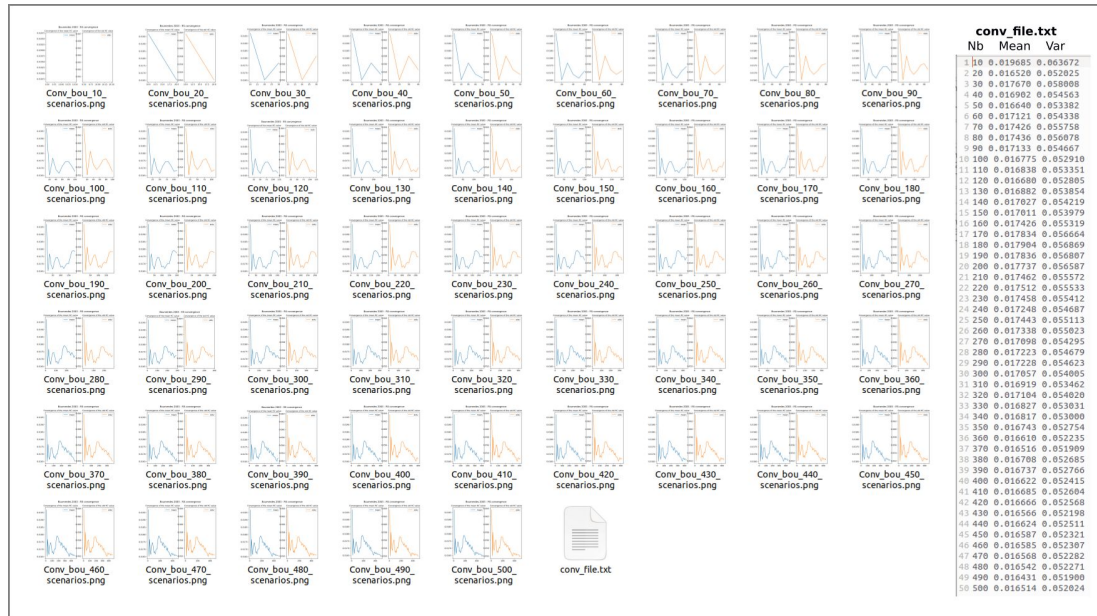
### Loop on the list of scenarios:

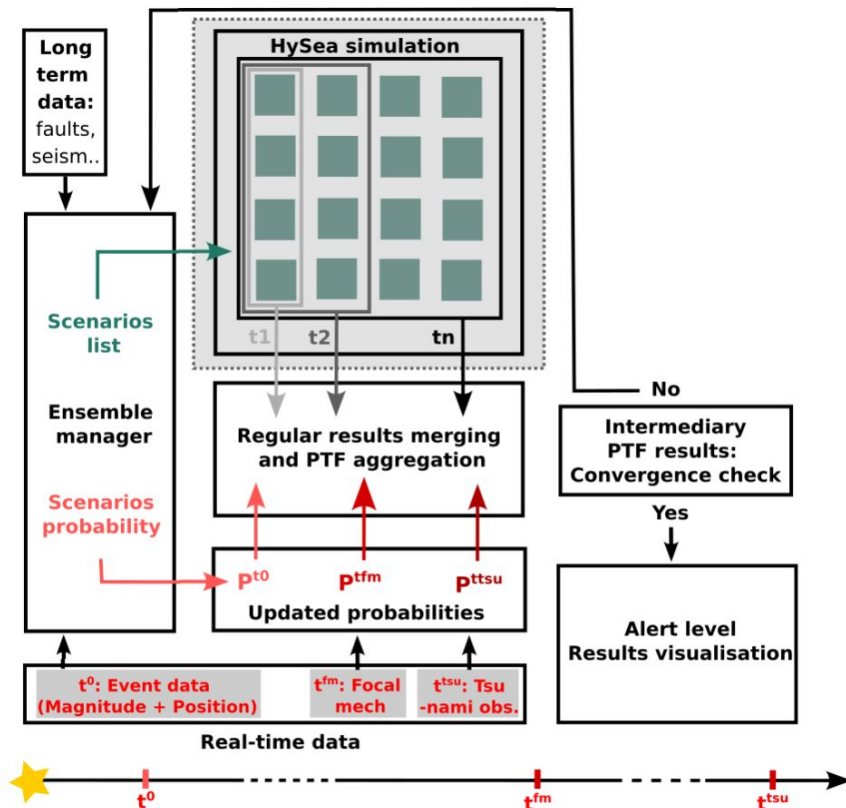


# STEP 4 – Aggregation, calculation of the hazard curves

## Intermediate PTF results delivery

- A PyCompass commutative shared file allows the calculation of the intermediate/partial PTF hazard curves based on the available completed simulations and based on a predefined number N (every 100 scenarios for example)
- Monitoring of the results: the failed simulations and the convergence of the results are monitored through the creation of different files.



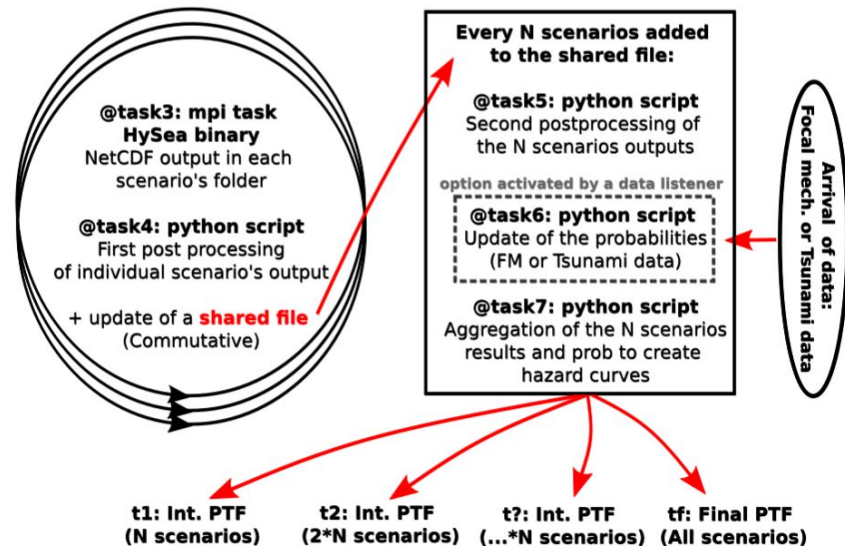


## PyComps workflow

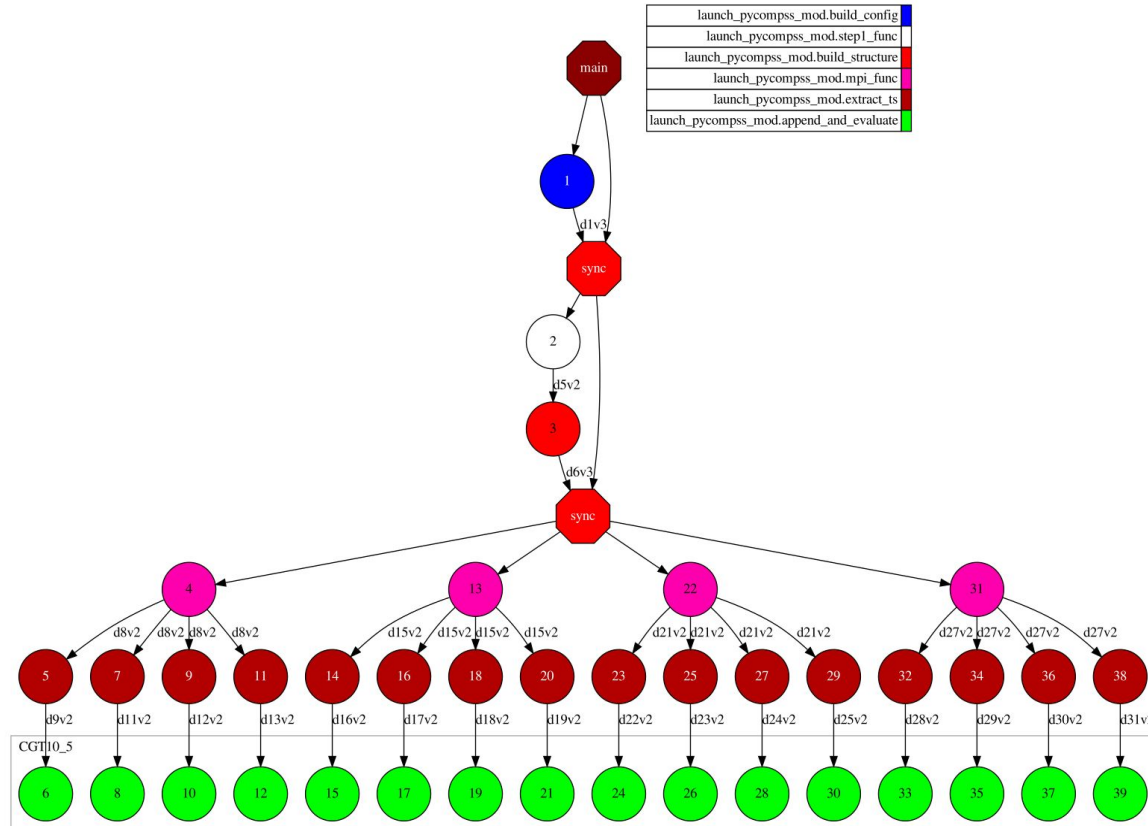
**@task1: python script**  
Scenarios and probability list

**@task2: binaries (.sh files)**  
Preparation of output folders and parameters text files for HySea simulation

### Loop on the list of scenarios:



# First end-to-end version of PTF orchestrated with PyCOMPSs





# Deployment on HPCWaaS (TOSCA - ALIEN4CLOUD)



The screenshot shows the TOSCA editor interface. The top navigation bar includes 'Applications' and 'Catalog'. Below it, there's a search bar and a breadcrumb trail: 'PTF HPCWaaS deployment and execution > Environment > Topology > Editor (0.1.0-SNAPSHOT)'. The main workspace displays a topology diagram with a 'PyCOMPSJob' node connected to an 'AbstractEnvironment' node. The right-hand pane shows the configuration for the selected 'PyCOMPSJob' node.

**Selected node: PyCOMPSJob**

Type: PyCOMPSJob

**Properties**

- environment
- submission\_para...
- application
- keep\_environment

**Capabilities**

- feature: Node

**Attributes**

- tosca\_id
- tosca\_name
- state

**Prerequisites**

- img\_transfer: Node
- environment: ExecutionEnvironment
- dependency: Node

**Relationships**

- dependsOnAbstractEnvi...: DependsOn
- Target: AbstractEnvironment

This screenshot shows the 'Edit submission\_parameters' dialog box. It has two main sections: 'submission\_params' and 'Edit application'.

**submission\_params**

- compes\_modules:
- num\_nodes: 1
- qos: debug
- python\_interpreter: python2
- extra\_compes\_opts: --emc\_script\_dir

**Edit application**

Arguments table:

arguments	value
0	--stage_dir \$1
1	--parameters_dir \$2
2	--data_path \$3
3	--run_path \$4
4	--template_path \$5
5	--hagen_weight \$6
6	--mark_weight \$7

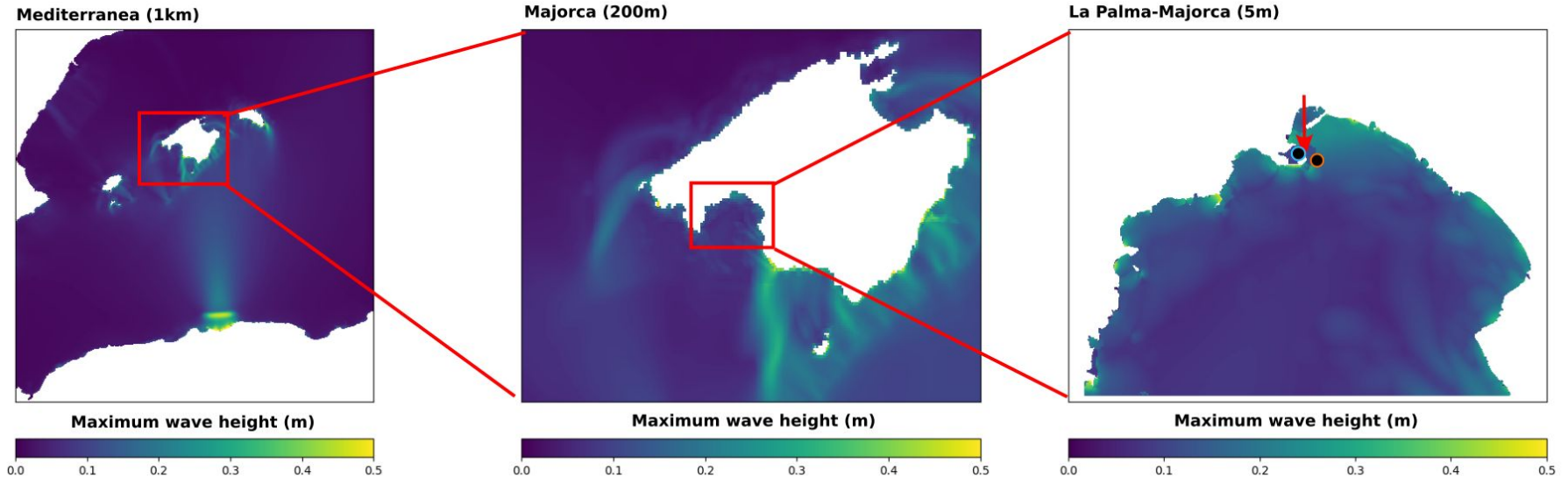
This screenshot shows the 'Matching' view in the TOSCA editor. The breadcrumb trail is 'PTF HPCWaaS deployment and execution > Environment > Matching'. The interface shows a 'Deployed' status and buttons for 'Version', 'Topology', 'Inputs', 'Locations', 'Matching', and 'Review & deploy'. Below this, there are sections for 'Policies matching' and 'Nodes matching'.

**Nodes matching**

Name	Type
<input type="radio"/> bsc_nord3:1.0.0	<input checked="" type="checkbox"/> eflows4hpc:env.nodes:AbstractEnvironment
<input type="radio"/> bsc_amd:1.0.0	<input checked="" type="checkbox"/> eflows4hpc:env.nodes:AbstractEnvironment
<input type="radio"/> CMCC_2eus:1.0.0	<input checked="" type="checkbox"/> eflows4hpc:env.nodes:AbstractEnvironment
<input type="radio"/> bsc_mn4:1.0.0	<input checked="" type="checkbox"/> eflows4hpc:env.nodes:AbstractEnvironment
<input type="radio"/> bsc_p9:1.0.0	<input checked="" type="checkbox"/> eflows4hpc:env.nodes:AbstractEnvironment

## High resolution HySea simulations

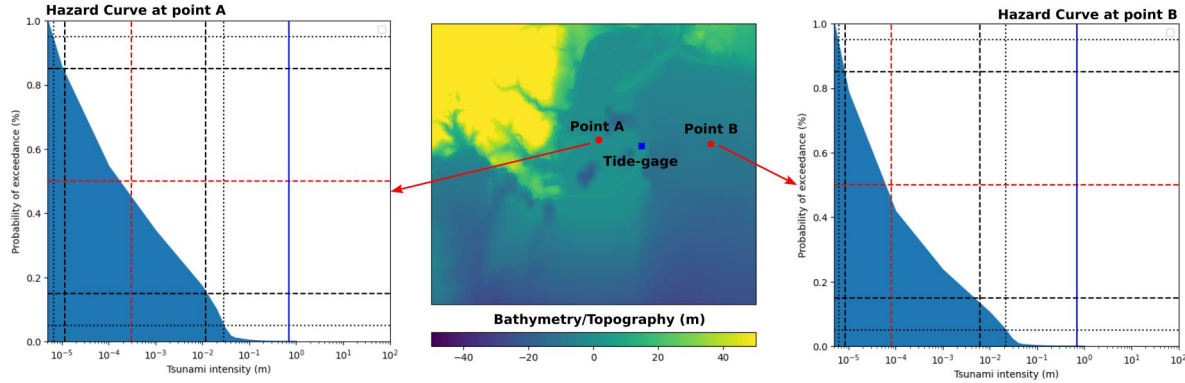
Example of one scenario for the 2003 earthquake and tsunami of Boumerdes



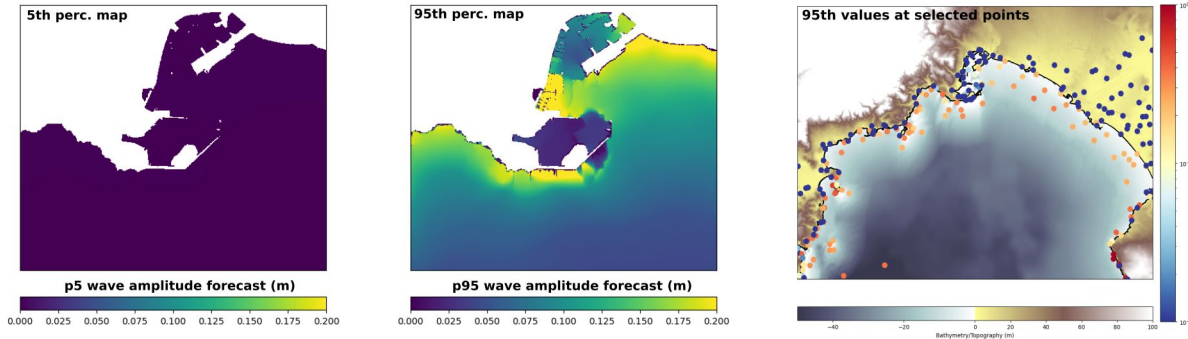
# Further developments: High-Resolution PTF-PyCOMPSs workflow

## Aggregation of the results of 500 simulations for the forecast calculation

Calculation of the hazard curves at each point of the grid

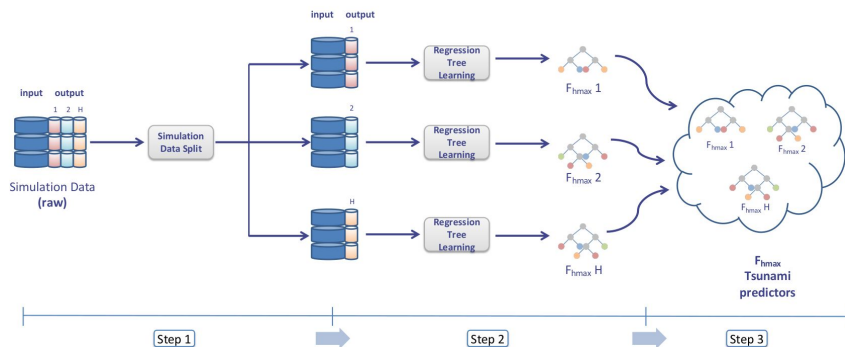


Creation of mean or percentiles maps (mean, p5, p95) - Extraction of the values at specific locations



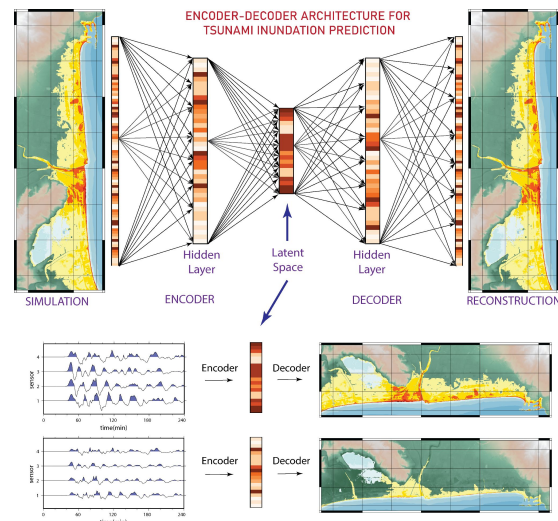
## Tsunami Forecasting exploiting Regression and Classification Trees

This activity is aimed at developing machine learning approaches based on regression and classification trees, to model and forecast tsunami simulation results.



## Inundation Prediction from Offshore Time-Series

To use Machine Learning to Predict High-Resolution inundation (expensive computations) from Offshore Time-Series (far cheaper computations) for Accurate Hazard Prediction in Urgent Tsunami Computations



# Conclusions

- The development of UC workflows for earthquakes and tsunamis has been incorporating the deployment of advanced tools and the development of complex tasks to reach an operational level.
- The sustainability and improvements in the workflows will be done under ChEES-2p and DT-GEO projects

# Thank you



## eFlows4HPC

Enabling dynamic and Intelligent workflows  
in the future EuroHPC ecosystem

[www.eFlows4HPC.eu](http://www.eFlows4HPC.eu)



@eFlows4HPC



eFlows4HPC Project



This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway.

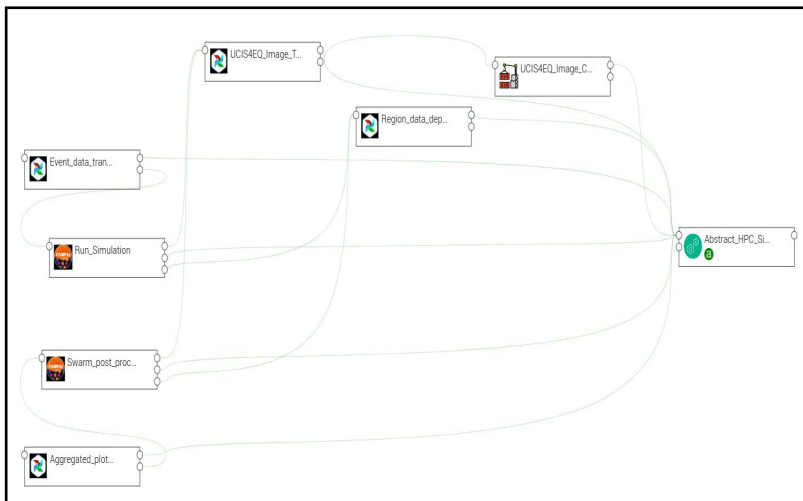
# Requirements & Metrics for Pillar III workflows

ID	Name	Priority
1	Urgent computing access	must
2	Data accessibility	should
3	Data replication	must
4	Execution robustness	must
5	Infrastructure interoperability	must
6	Portability and Reusability	may
7	Streaming Data Source	must
8	Integrated workflow manager	must
9	Integration with permanent storage	must
10	Inference with online/offline ML models	must
11	DA integration	may
12	Workflow malleability	should

Acronym	Name	Description
RT	Response time	End-to-solution time constraints in an urgent computing context. This metric is defined as the clock time measured from the event reception until a first valid solution for the event is delivered to the stakeholders such as civil protection agencies.
UAR	Urgent Assignment of Resources	Time to obtain necessary resources for an urgent computing execution. The inclusion of this metric quantifies the QoS in HPC facilities that provide UC services. Moreover, it is a measure to evaluate if the adopted policies are adequate for an UC execution
RUQ	Results Uncertainty Quantification	High-fidelity and high-accuracy results. This metric is proposed to fulfill the specific UCIS4EQ workflow. RUQ metrics is related to the uncertainty of the service outputs, as it is crucial to constrain and reduce the uncertainty of provided impact estimates.
Conv	Convergence	This metric is proposed to evaluate the specificity of the PTR/FTRT requirements in particular the convergence of the results based on a reference solution

# Deployment with HPCWaaS platform

To facilitate the reusability of these complex workflows in federated HPC infrastructure.



Integration of the UCIS4EQ in the HPCWaaS platform describing the TOSCA components using the Alien4Cloud software.

TOSCA components involved in the deployment and execution of the UCIS4EQ workflow:

## Setup

## phase:

The **Abstract\_HPC\_Site** component defines the properties (login node address, CPU architecture, supported container engine, ...) of the HPC system where we mean to deploy and run the workflow.

## Deployment

## phase:

The **UCIS4EQ\_Image\_Creation** component implements the interaction with the eFlows4HPC Container Image Creation (CIC) service to build a container image including all the software components required for the workflow. The **UCIS4EQ\_Image\_Transfer** component implements the interaction with the Data Logistics Service (DLS). It depends on the **UCIS4EQ\_Image\_Creation** component because it has to know the URL of the generated container image in order to perform the image deployment. The **Region\_Data\_deployment** component interacts with the DLS, but in this case it is configured to download the data of a region (maps, etc.) from the data-set stored in the UCIS4EQ B2DROP repository.

## Execution phase:

**two TOSCA components** (Run\_Simulation and Swarm\_post\_processing ) and **two data pipelines** (the stage-in of the event data to simulate (*Event\_data\_transfers*) and for the stage-out to upload the generated plots at the end of the swarm post-processing workflow (*Aggregated\_plots\_upload*)).