

Delivering easy-to-use frameworks to empower data-driven research

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Background

PhD Computer Science – University Carlos III of Madrid, Spain

- *Dynamic optimization techniques (reducing overhead in I/O and communication systems) to enhance performance of MPI-based applications*
- Compute-Intensive Applications

Research Fellow – EPCC, University of Edinburgh, UK

- Scalability and performance of applications executed on HPC and Cloud
- Workflows, data-frameworks, containers and reproducibility tools, etc.
- Data-Intensive Computing Applications

Big Data Science Era, Data Intensive Computing Applications



Scientific fields

Data-driven

Astronomy, Geosciences,
Meteorology, Bioinformatics



Common points

Big complex data sets

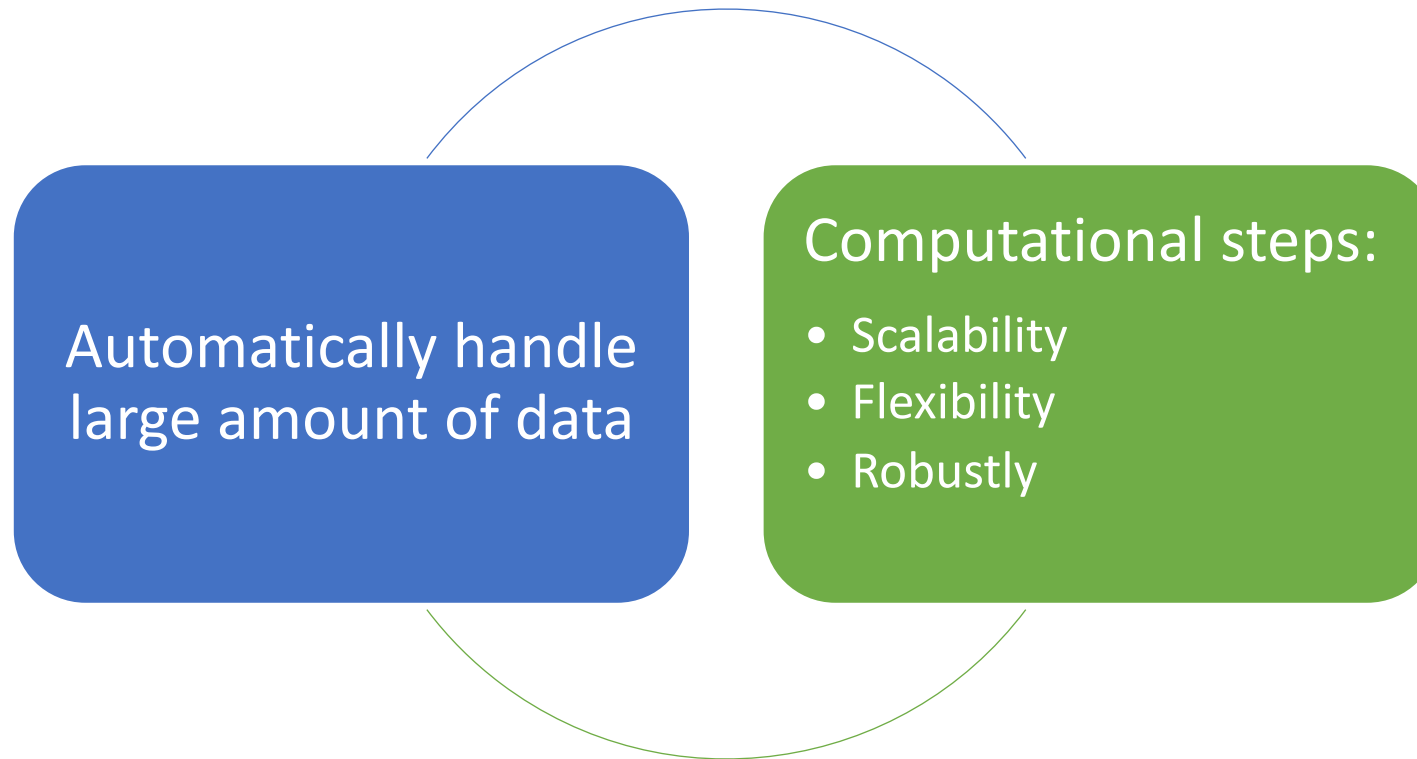
Need to be analysed

Numerous software tools

Data transformation and visualisation

Big Data Science Era, Data Intensive Computing Applications

Scientific Workflows and Computing environments



Big Data Science Era, Data Intensive Computing Applications



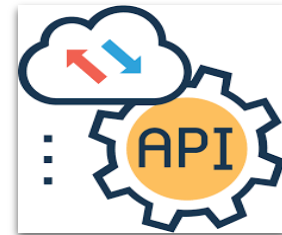
Seismology



Scientific Workflows:
dispel4py
CWL



Computing environments:
Local
Cloud
HPC



API

DARE

Delivering Agile Research Excellence on European e-Infrastructures

Aim: To empower domain experts to invent and improve their methods and models

How: By providing a new platform and working environment

Outcome:

- * Tools/frameworks/APIs for data-driven experiments
- * Rapid prototyping
- * Run applications at scale on heterogenous systems.

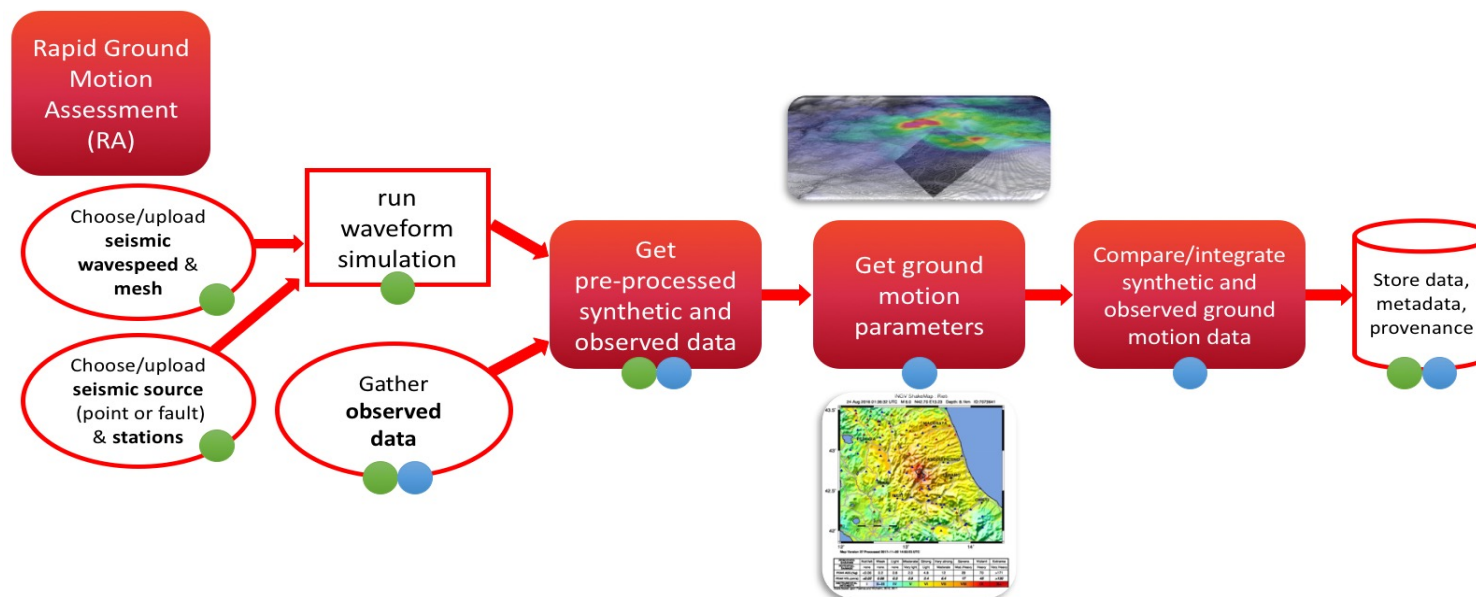
Domains: Seismology (INGV) and Climate (CERFACS)



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Rapid Ground Motion Assessment (RA)

- * Quickly analyse earthquakes
- * Model the ground motion after earthquakes
- * Rapid assessment of earthquakes' impact, and emergency response

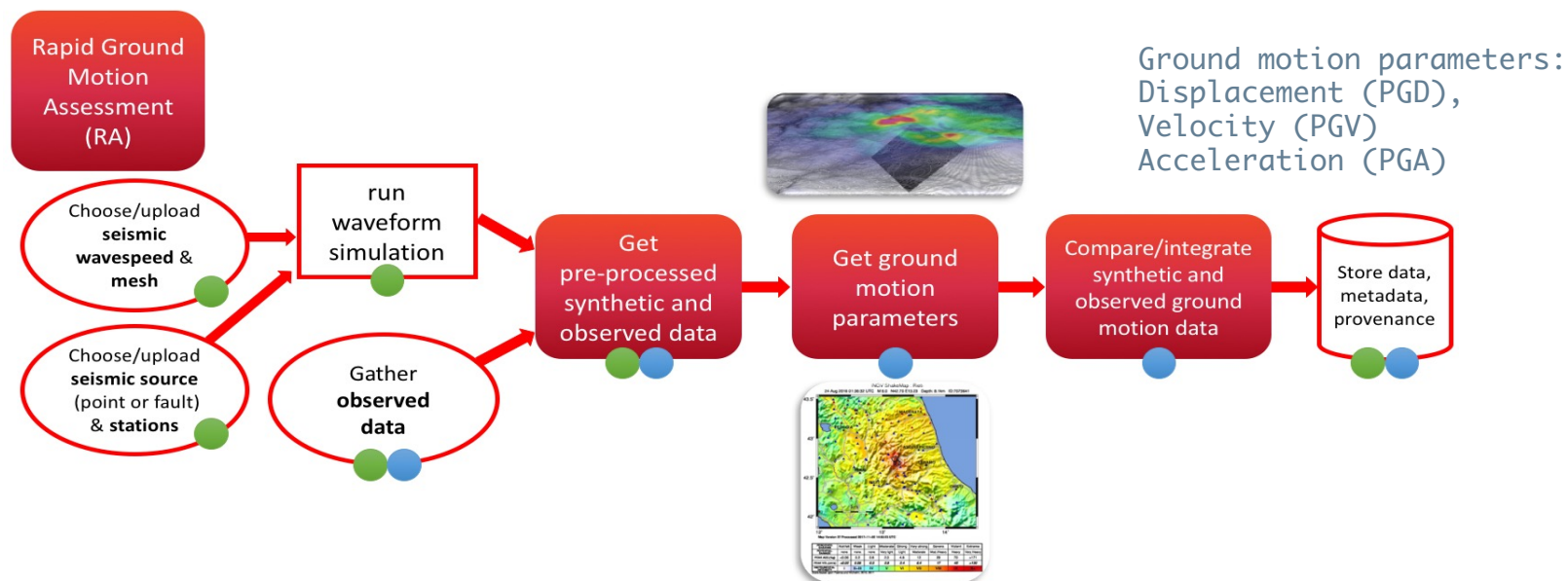


RA – Five main phases



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- (1) Select an earthquake gathering the real **observed** seismic waveforms
- (2) Simulate **synthetic** seismic waveforms corresponding to the same earthquake
- (3) Pre-process both synthetic and real data;
- (4) Calculate the ground motion parameters for synthetic and real data
- (5) Compare them with each other (two types of normalization: mean | max)
 - shake maps and json files



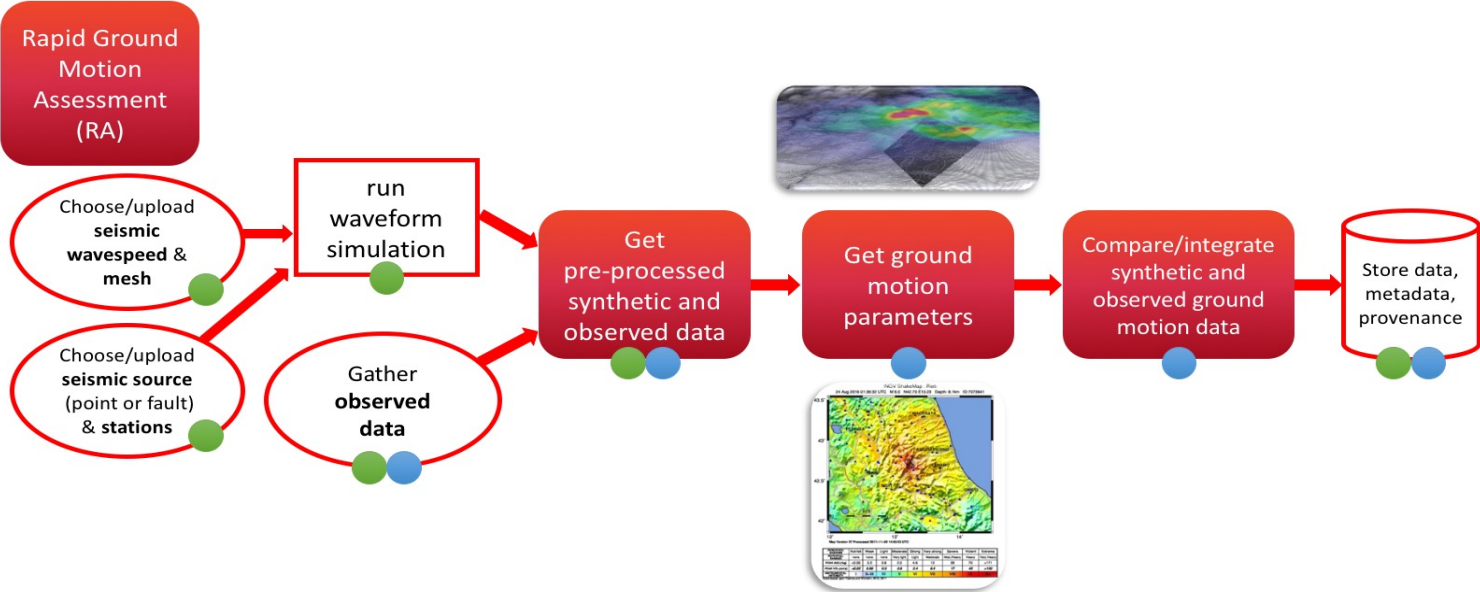
RA – Five main phases

Earthquake Sora: Southern Italy (Lazio - Frosinone) – 16 Feb 2013
 Magnitude : 4.9

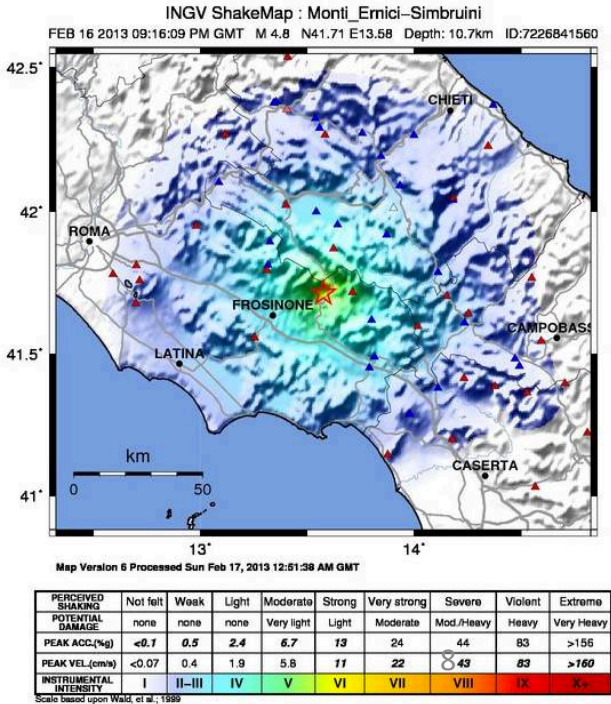
Synthetics:
 43 stations * (3 components) simulated data == 129 synth waveforms

Real – Download from EIDA archive
 31 stations * (3 components) observed data == 93 real waveforms

Outputs: 2 maps – one per normalization type == 62 files



3-Component Seismogram
 Records Seismic-wave Motion

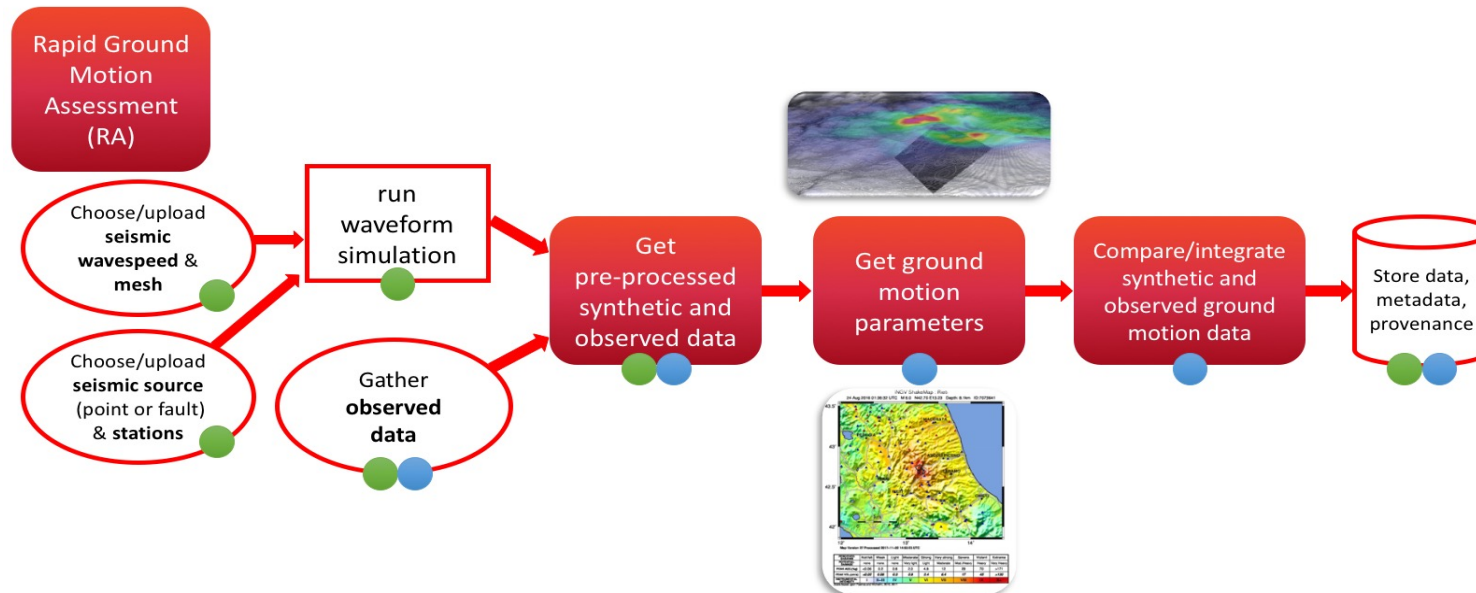


RA – Five main phases



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- * Rapid data analyses and transfer between co-working environments
- * Multiple data formats (ascii, xml, obspy, jpg, binary, geojson)
- * Multiple data sources (public databases)
- * Combination of numerous outputs from multiple workflows/software → Provenance
- * Computing and storage resources on demand
- * Flexibility and abstraction of workflow pipelines



RA – User Stories – Agile Methodology



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Closed
20
0

As a seismologist I want to upload to an archive simulation configuration parameters (waveform model, mesh and seismic source)

C - API C - DataStore T - Rapid Assessment

T - Seismic Source Characterisation

#29

As a seismologist I want to search and select from an archive of configuration parameters (waveform model, mesh and seismic source) to setup my simulation

C - API C - DataStore T - Rapid Assessment

T - Seismic Source Characterisation

#28

As seismologist I want to run a waveform simulator with my selected configuration parameters

C - API C - Provenance C - Workflow Language

C- Processing T - Rapid Assessment

T - Seismic Source Characterisation

#31

Closed
20
0

As a seismologist I want to access observed data from external archives for further processing

C - API C - DataStore C - Provenance

C - Workflow Language C- Processing

T - Ensemble Simulations T - Rapid Assessment

T - Seismic Source Characterisation

#32

As seismologist I want to preprocess waveforms for further analyses

C - API C - PE Catalogue C - Provenance

C - Workflow Language C- Processing

T - Ensemble Simulations T - Rapid Assessment

T - Seismic Source Characterisation

#41

As a seismologist I want extract selected ground motion parameters from waveforms

C - API C - PE Catalogue C - Provenance

C - Workflow Language C- Processing

T - Ensemble Simulations T - Rapid Assessment

#12

Closed
20
0

As a seismologist I want to compare simulation outputs (e.g. ground motion parameters) with observed data

C - API C - PE Catalogue C - Provenance

C - Workflow Language C- Processing

T - Ensemble Simulations T - Rapid Assessment

#5

As a seismology I want to store output data and visual products produced by any workflow with provenance and metadata

C - DataStore C - Provenance

C - Workflow Language T - Ensemble Simulations

T - Rapid Assessment

T - Seismic Source Characterisation

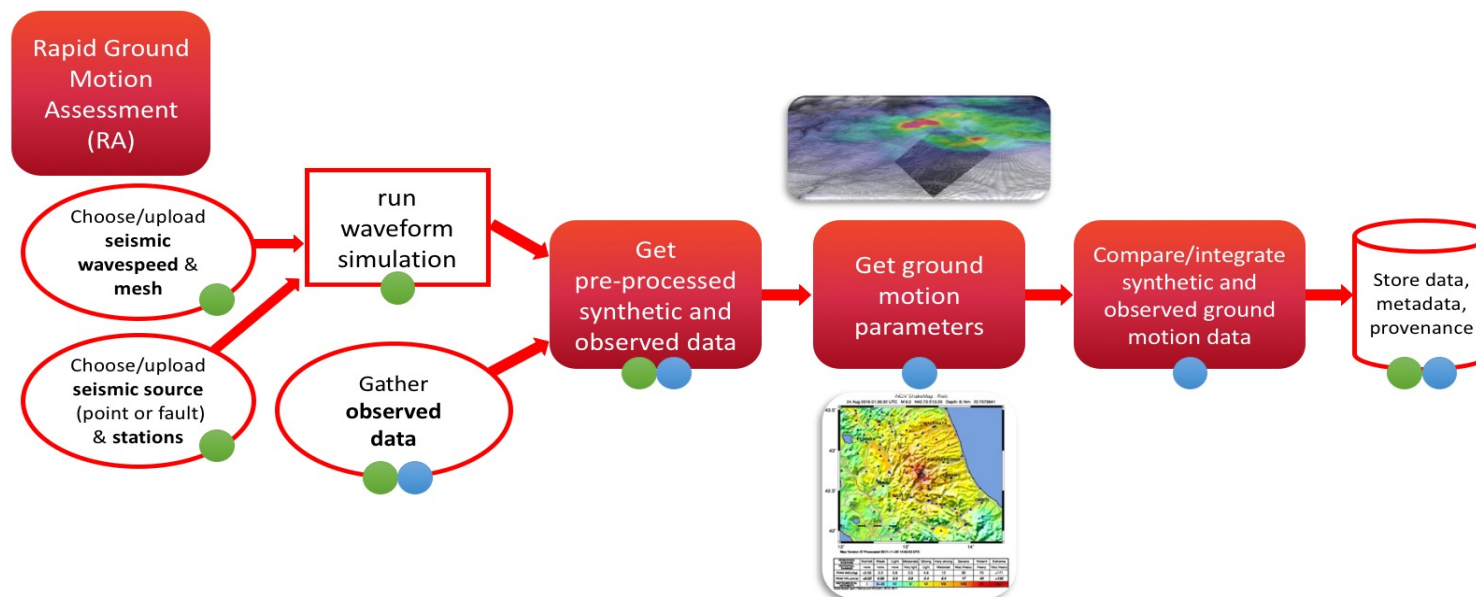
#19

RA – Portable and Reproducible

To run it on different computing environments
- without making any (or little) changes

Technologies:

- * Scientific workflows (CWL), stream-based data-flow systems (dispel4py),
- * Containers (Docker), Infrastructure orchestrations (Kubernetes),
- * Notebooks (Jupyter), and Cloud platforms.



RA – Summary Steps (I)

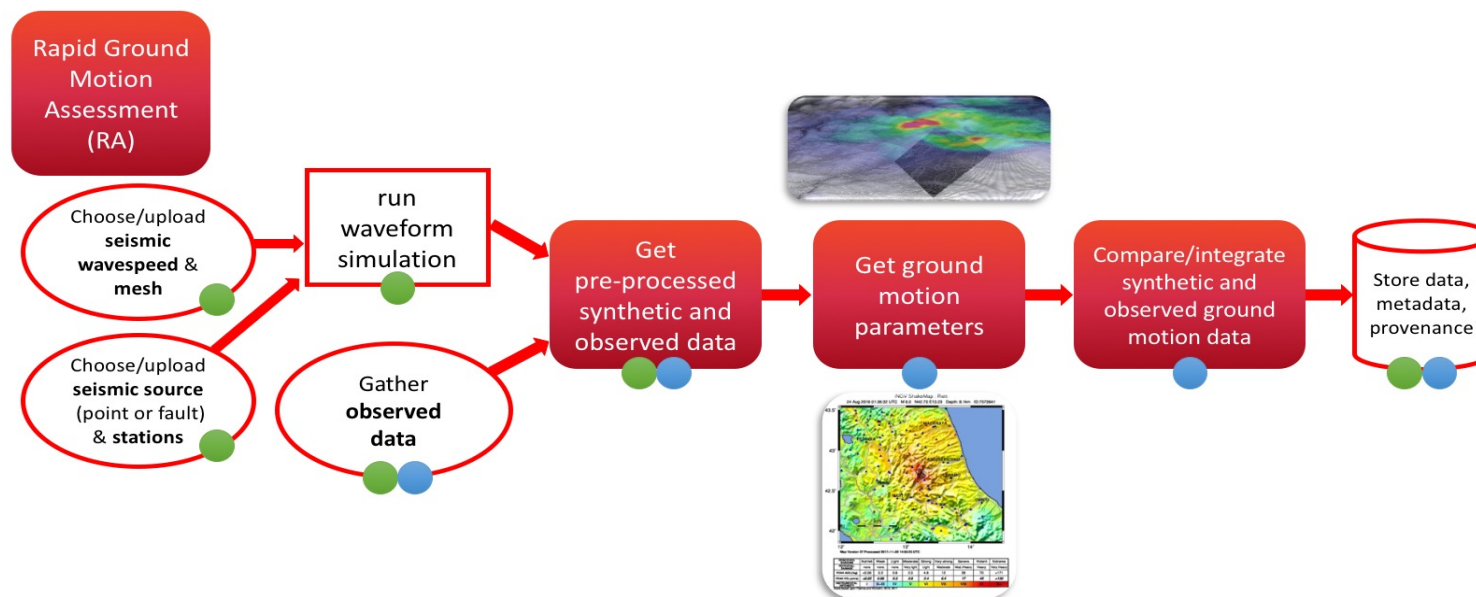
1. Dockerize Specfem3D

Build a CWL workflow for generating synthetic data

2. Build dispel4py workflows to represent each part of the RA (**)

(**) Except for the generation of the synthetic data

3. Use CWL to connect RA dispel4py workflows



RA – Summary Steps (I)

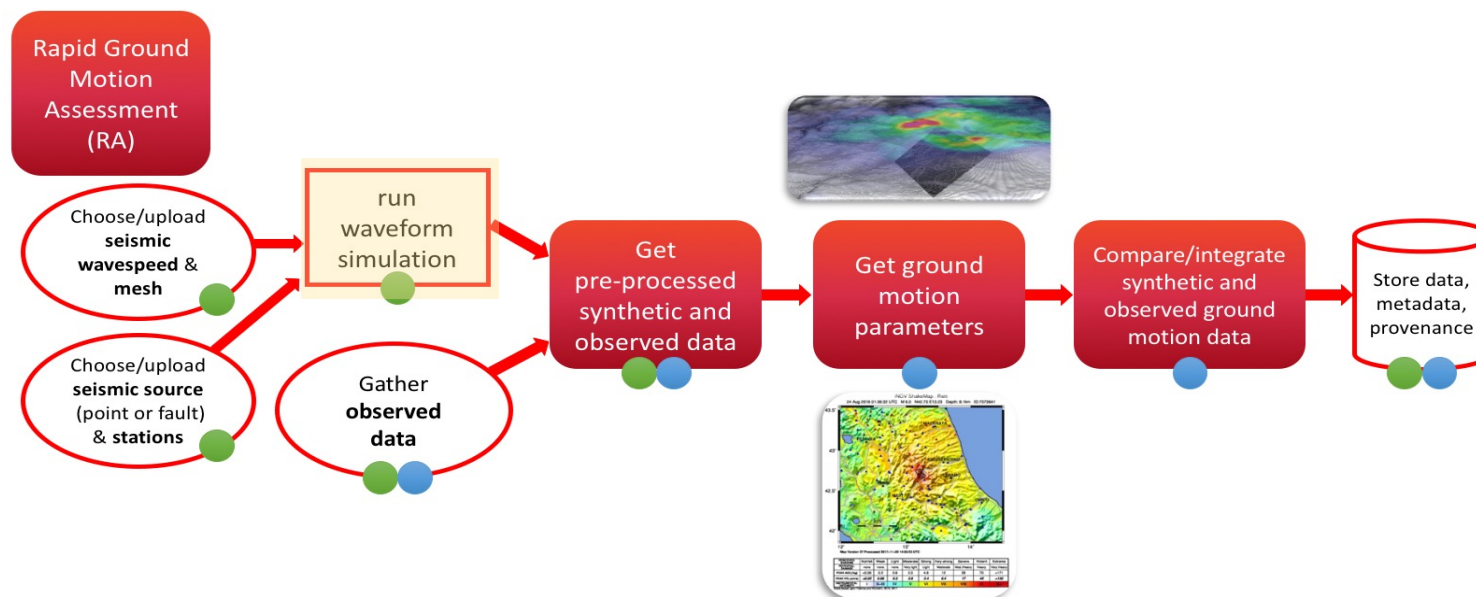
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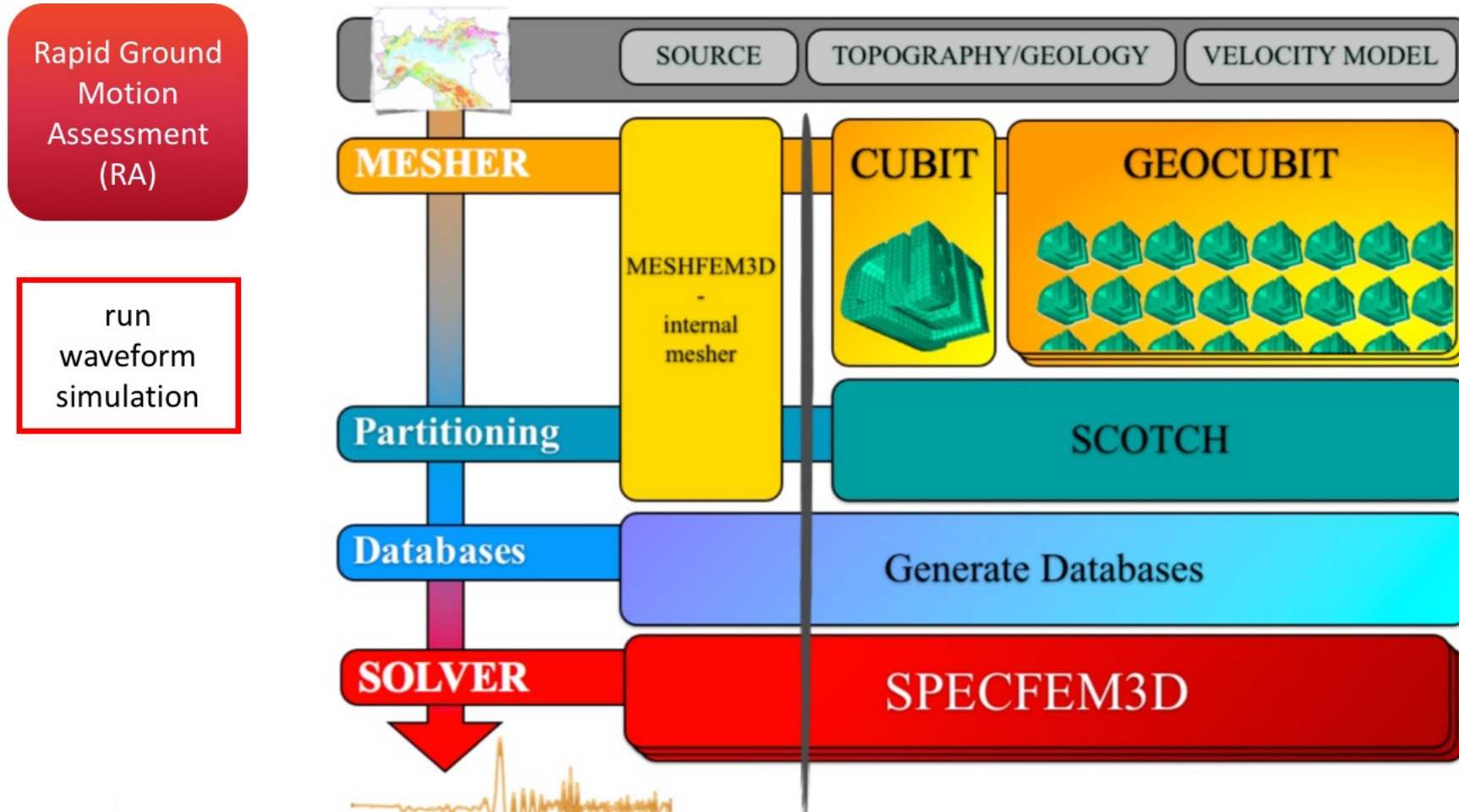
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Seismic Waveform Simulation: SPECFEM3D



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Specfem3d– MPI application that creates the synthetic waveforms

Seismic Waveform Simulation: SPECFEM3D

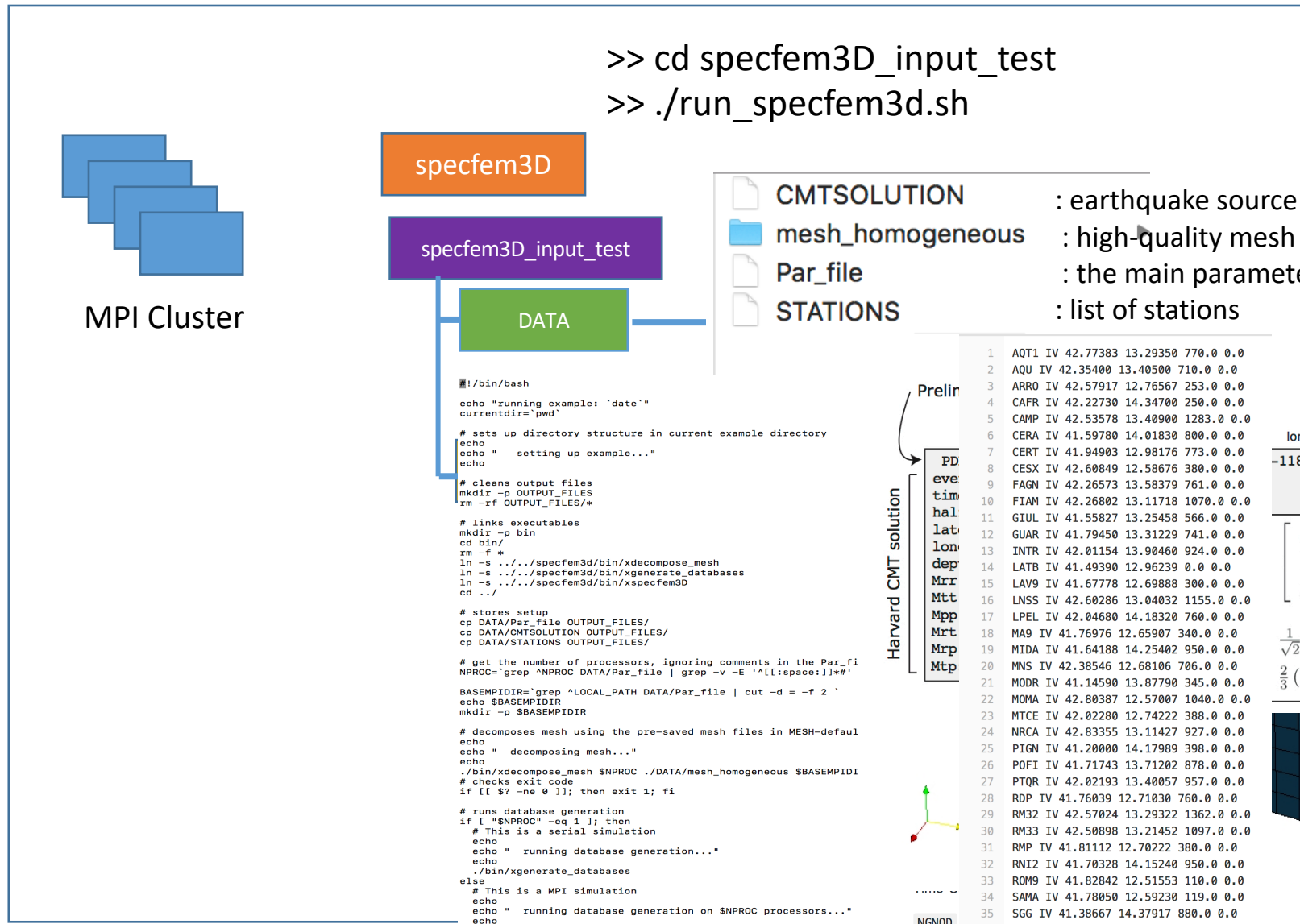


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We run it before
In SuperMUC -
HPC-cluster -
256 cores

Test Case: RA

run waveform
simulation



```
>> cd specfem3D_input_test
>> ./run_specfem3d.sh
```

- CMTSOLUTION : earthquake source parameter file
- mesh_homogeneous : high-quality mesh for the region
- Par_file : the main parameter file
- STATIONS : list of stations

Harvard CMT solution

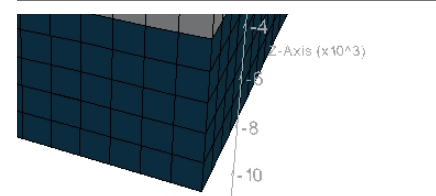
	P	S	Love	Surface	Body
1	AQT1	IV	42.77383	13.29350	770.0 0.0
2	AQU	IV	42.35400	13.40500	710.0 0.0
3	ARRO	IV	42.57917	12.76567	253.0 0.0
4	CAFR	IV	42.22730	14.34700	250.0 0.0
5	CAMP	IV	42.53578	13.40900	1283.0 0.0
6	CERA	IV	41.59780	14.01830	800.0 0.0
7	CERT	IV	41.94903	12.98176	773.0 0.0
8	CESX	IV	42.60849	12.58676	380.0 0.0
9	FAGN	IV	42.26573	13.58379	761.0 0.0
10	FIAM	IV	42.26802	13.11718	1070.0 0.0
11	GIUL	IV	41.55827	13.25458	566.0 0.0
12	GUAR	IV	41.79450	13.31229	741.0 0.0
13	INTR	IV	42.01154	13.90460	924.0 0.0
14	LATB	IV	41.49390	12.96239	0.0 0.0
15	LAV9	IV	41.67778	12.69888	300.0 0.0
16	LNSS	IV	42.60286	13.04032	1155.0 0.0
17	LPEL	IV	42.04680	14.18320	760.0 0.0
18	MA9	IV	41.76976	12.65907	340.0 0.0
19	MIDA	IV	41.64188	14.25402	950.0 0.0
20	MNS	IV	42.38546	12.68106	706.0 0.0
21	MODR	IV	41.14590	13.87790	345.0 0.0
22	MOMA	IV	42.80387	12.57007	1040.0 0.0
23	MTCE	IV	42.02280	12.74222	388.0 0.0
24	NRCA	IV	42.83355	13.11427	927.0 0.0
25	PIGN	IV	41.20000	14.17989	398.0 0.0
26	POFI	IV	41.71743	13.71202	878.0 0.0
27	PTQR	IV	42.02193	13.40057	957.0 0.0
28	RDP	IV	41.76039	12.71030	760.0 0.0
29	RM32	IV	42.57024	13.29322	1362.0 0.0
30	RM33	IV	42.50898	13.21452	1097.0 0.0
31	RMP	IV	41.81112	12.70222	380.0 0.0
32	RNI2	IV	41.70328	14.15240	950.0 0.0
33	ROM9	IV	41.82842	12.51553	110.0 0.0
34	SAMA	IV	41.78050	12.59230	119.0 0.0
35	SGG	IV	41.38667	14.37917	880.0 0.0
36	SMA1	IV	42.63050	13.33530	1150.0 0.0
37	SRES	IV	42.23696	12.50993	410.0 0.0
38	T0104	IV	42.35990	13.33820	754.0 0.0

longitude	depth	mb	Ms	PDE event name
-118.3792	6.4	4.2	4.2	HOLLYWOOD

$$\begin{bmatrix} M_{rr} & M_{r\theta} & M_{r\phi} \\ M_{r\theta} & M_{\theta\theta} & M_{\theta\phi} \\ M_{r\phi} & M_{\theta\phi} & M_{\phi\phi} \end{bmatrix}$$

$$\frac{1}{\sqrt{2}} (M : M)^{1/2} \approx 2.18 \times 10^{22} \text{ dyne cm}$$

$$\frac{2}{3} (\log_{10} M_0 - 16.1) \approx 4.19$$



exahedra. We use either 8-node mesh
rnal mesher. the only option is 8-node

Seismic Waveform Simulation: SPECfem3D

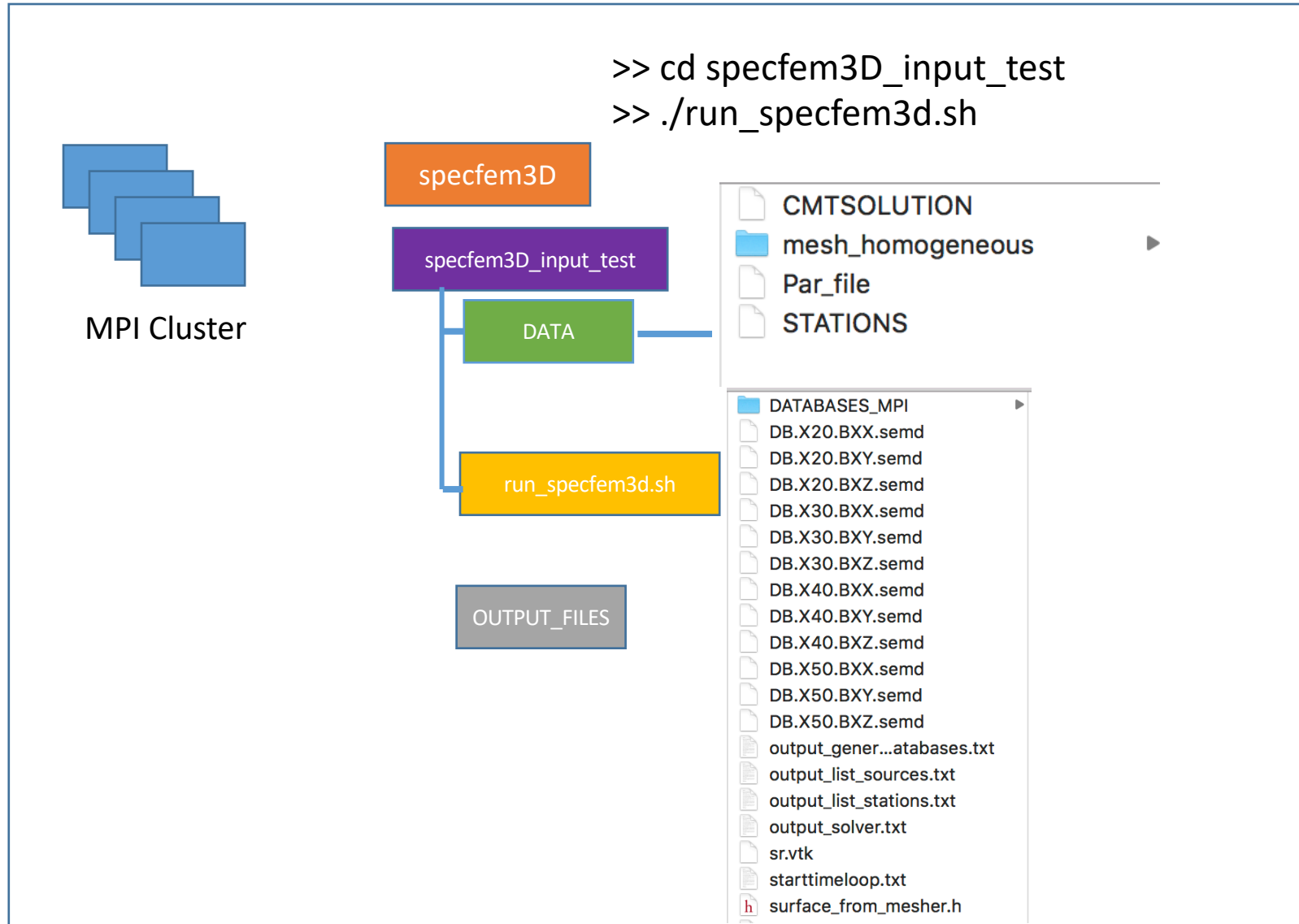


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We run it before
In SuperMUC -
HPC-cluster -
256 cores

Test Case: RA

run waveform
simulation



Common Workflow Language - CWL



Open standard for describing

- workflows and tools
- platform-independent

} Designed to meet the needs of data-intensive science

1st-tool.cwl

```
#!/usr/bin/env cwl-runner

cwlVersion: v1.0
class: CommandLineTool
baseCommand: echo
inputs:
  message:
    type: string
    inputBinding:
      position: 1
outputs: []
```

```
$ cwl-runner 1st-tool.cwl echo-job.yml
[job 1st-tool.cwl] /tmp/tmpmM5S_1$ echo \
  'Hello world!'
Hello world!
[job 1st-tool.cwl] completed success
{}
Final process status is success
```

Next, create a file called `echo-job.yml`, containing the following boxed text, which will describe the input of a run:

echo-job.yml

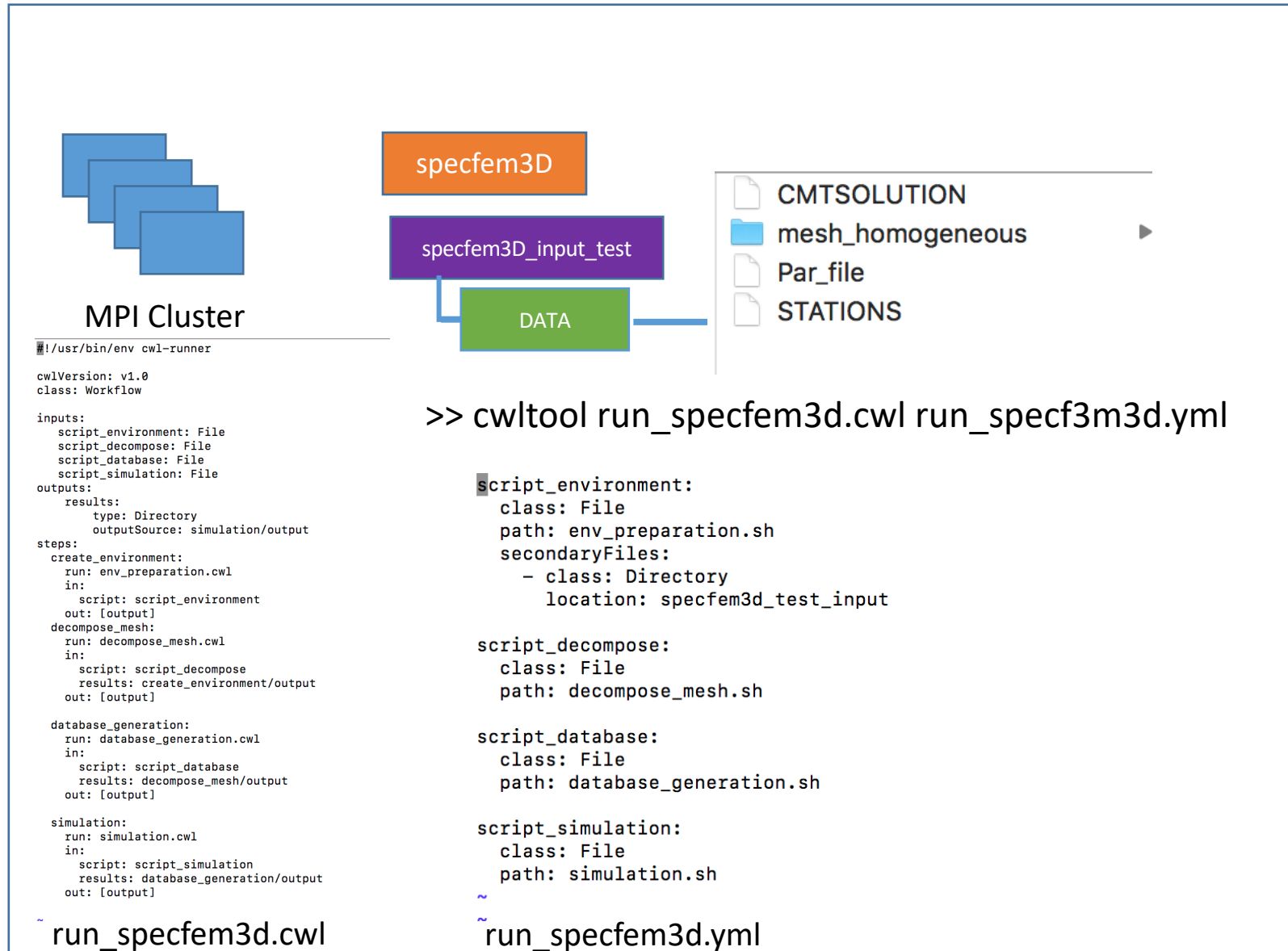
```
message: Hello world!
```

Rules to describe each command line tool and its parameters

Seismic Waveform Simulation: SPECFEM3D



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Test Case: RA

run waveform
simulation



RA – Summary Steps (I)



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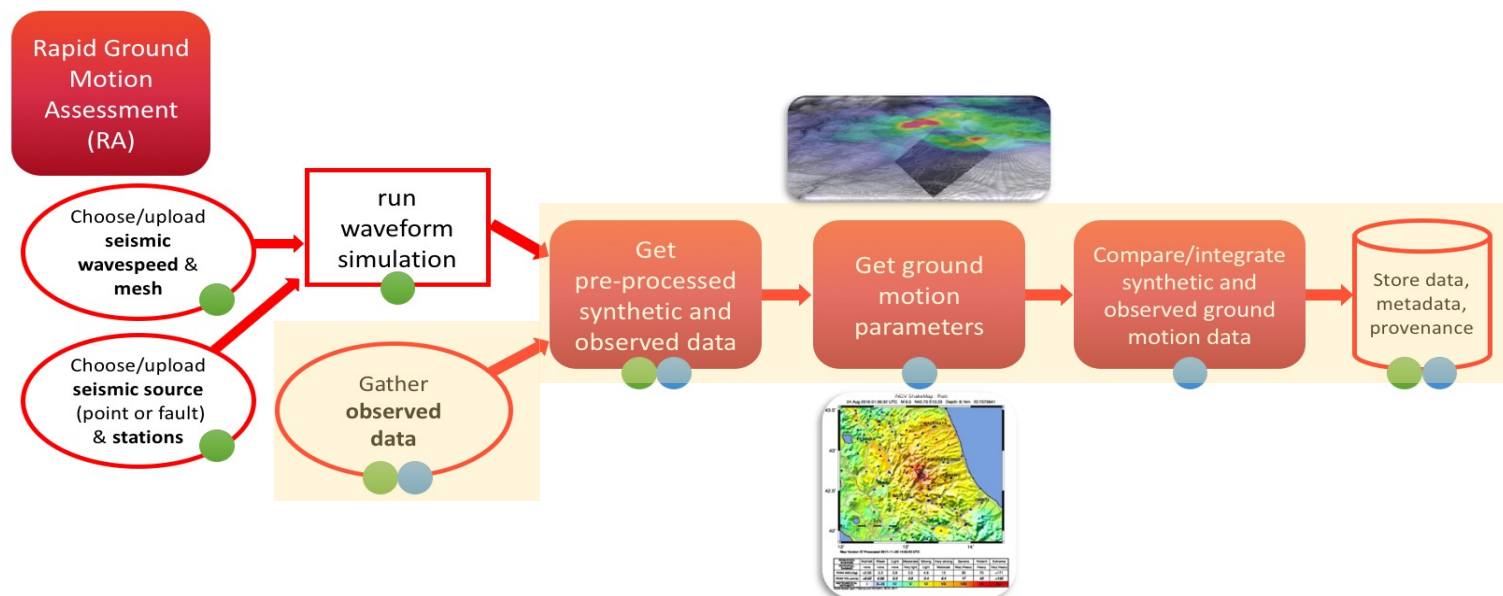
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Build a CWL workflow for generating synthetic data

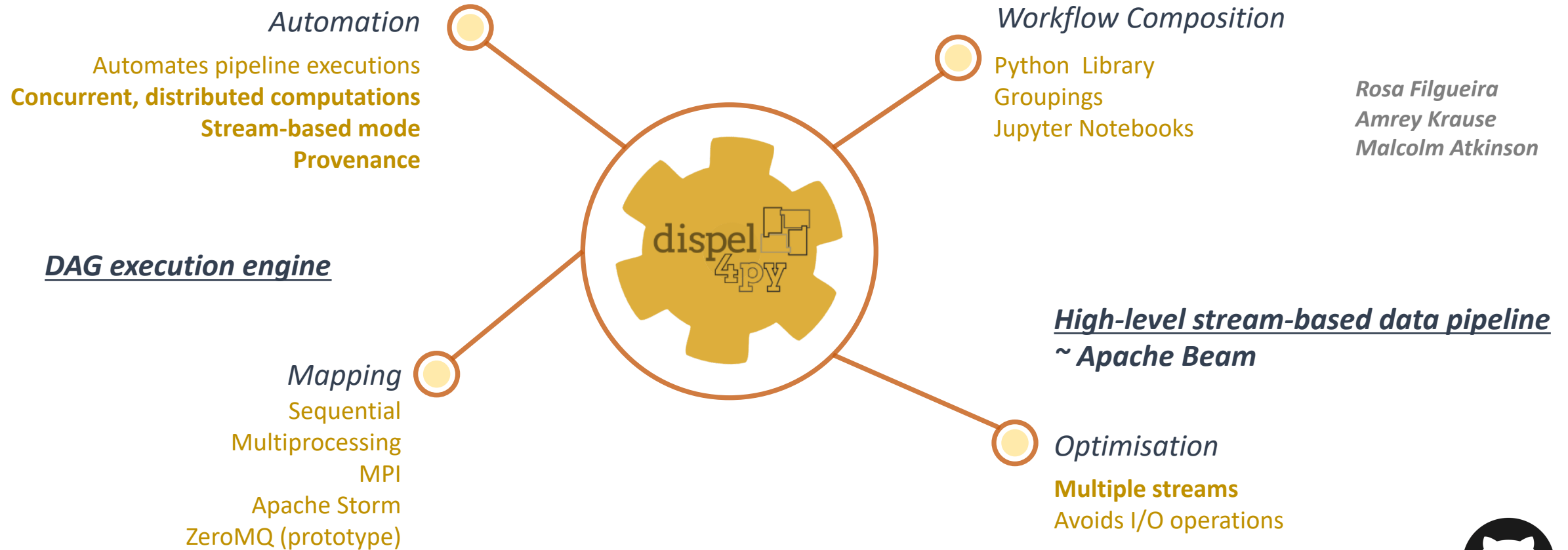
2. Build dispel4py workflows to represent each part of the RA (**)

(**) Except for the generation of the synthetic data

3. Use CWL to connect RA dispel4py workflows



dispel4py parallel stream-based dataflow system



Rosa Filgueira
Amrey Krause
Malcolm Atkinson

Key-features: Automatic mappings to different engines, concurrent & stream-based
Embarrassing parallel data-intensive applications

<https://github.com/dispel4py/dispel4py>



dispel4py parallel stream-based dataflow system

Graph

- Connections among PES
- Abstract workflow

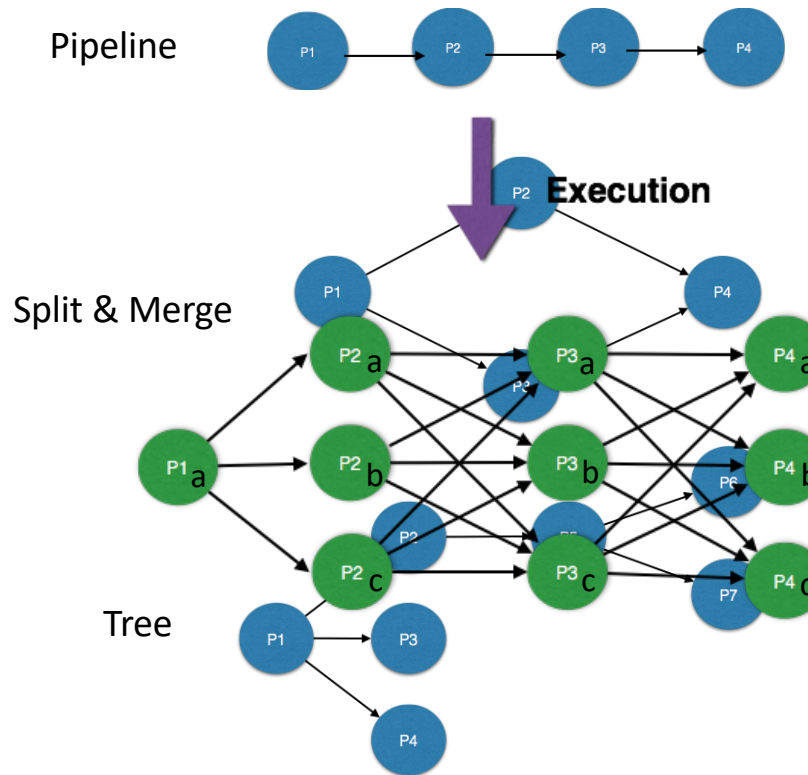
Instance

- Each PE is translated into one or more instances in run-time
- Each instance runs in a process
- dispel4py does it for you
- Concrete workflow

Mappings

- Sequential, multiprocessing, MPI

+ Example of graphs

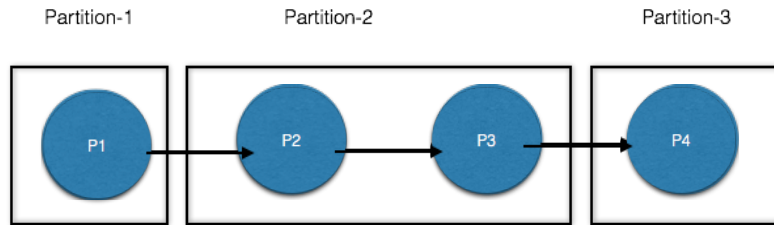


4 PEs & 10 processes



dispel4py parallel stream-based dataflow system

+ Example of Partition



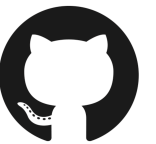
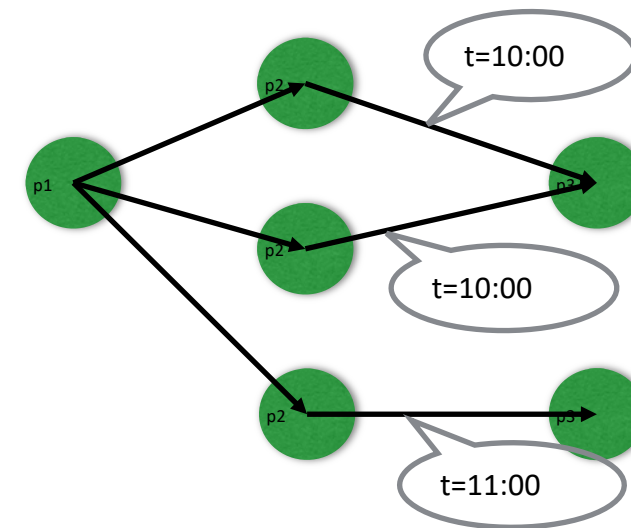
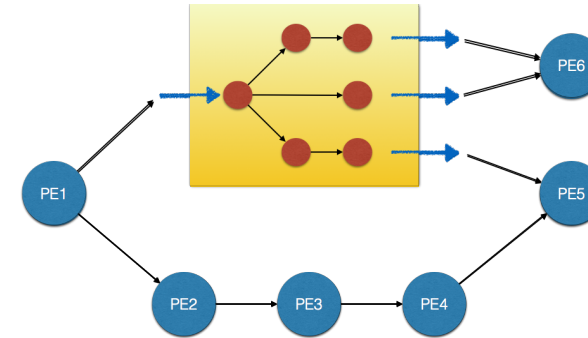
+ Example of Grouping By a feature (MapReduce)



- + All data items that satisfy the same feature are guaranteed to be delivered to the same instance of a PE



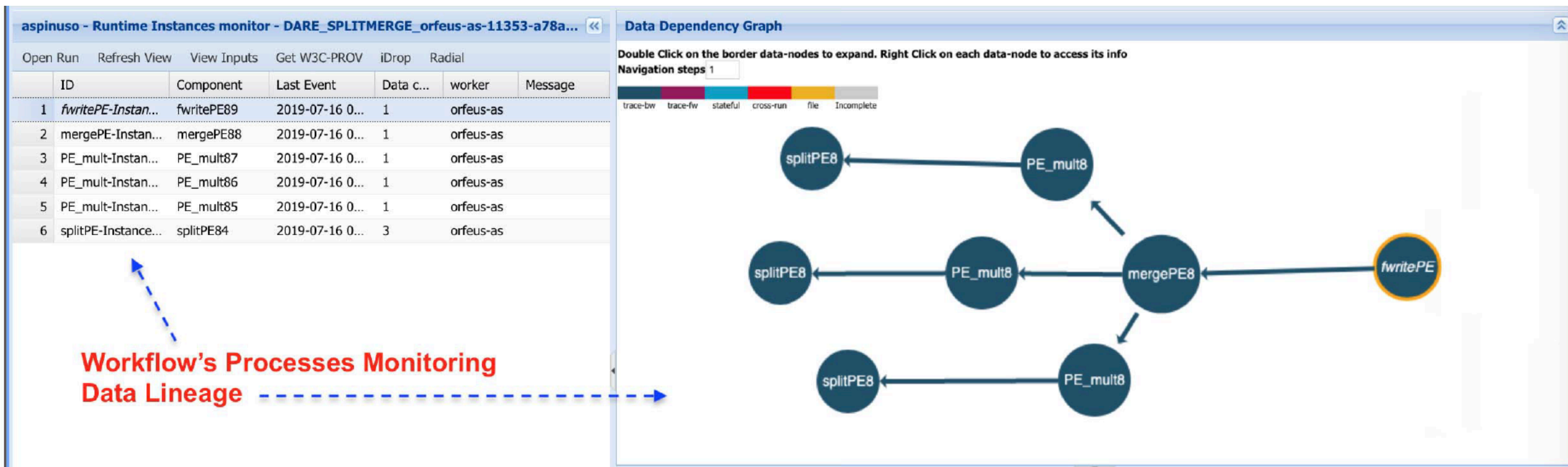
+ Example of Composite PE



dispel4py parallel stream-based dataflow system

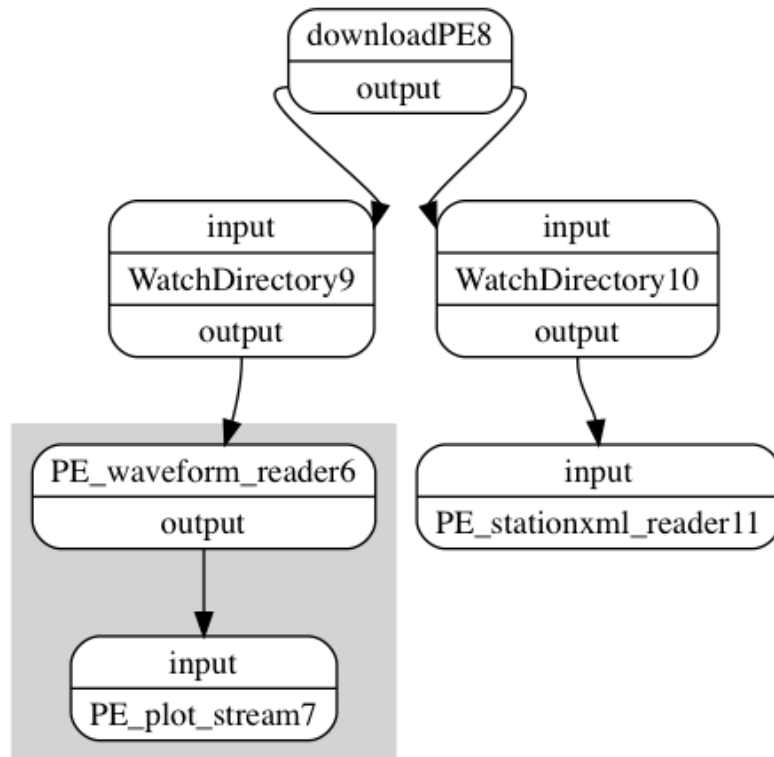


Provenance *Alessandro Spinuso*



Runtime provenance collection with selective paths and user-defined domain information.





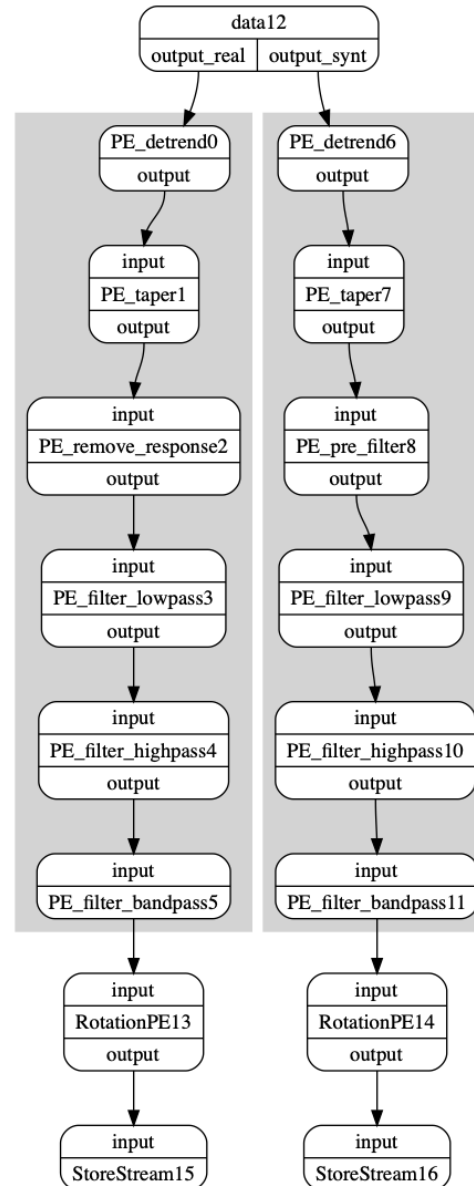
The workflow downloads real waveforms corresponding to the same earthquake.

```
▼ downloadPE:
  ▼ 0:
    ▼ input:
      minimum_interstation_distance_in_m: 100
    ▼ channel_priorities:
      0: "BH[E,N,Z]"
      1: "EH[E,N,Z]"
    ▼ location_priorities:
      0: ""
      1: "00"
      2: "10"
    mseed_path: "./data"
    stationxml_path: "./stations"
    RECORD_LENGTH_IN_MINUTES: 1
    ORIGIN_TIME: "2013-02-16T21:16:09.29"
    minlatitude: 41.10007459633125
    maxlatitude: 42.89777970948071
    minlongitude: 12.041644551237324
    maxlongitude: 14.439665626790928
```

Test Case: RA



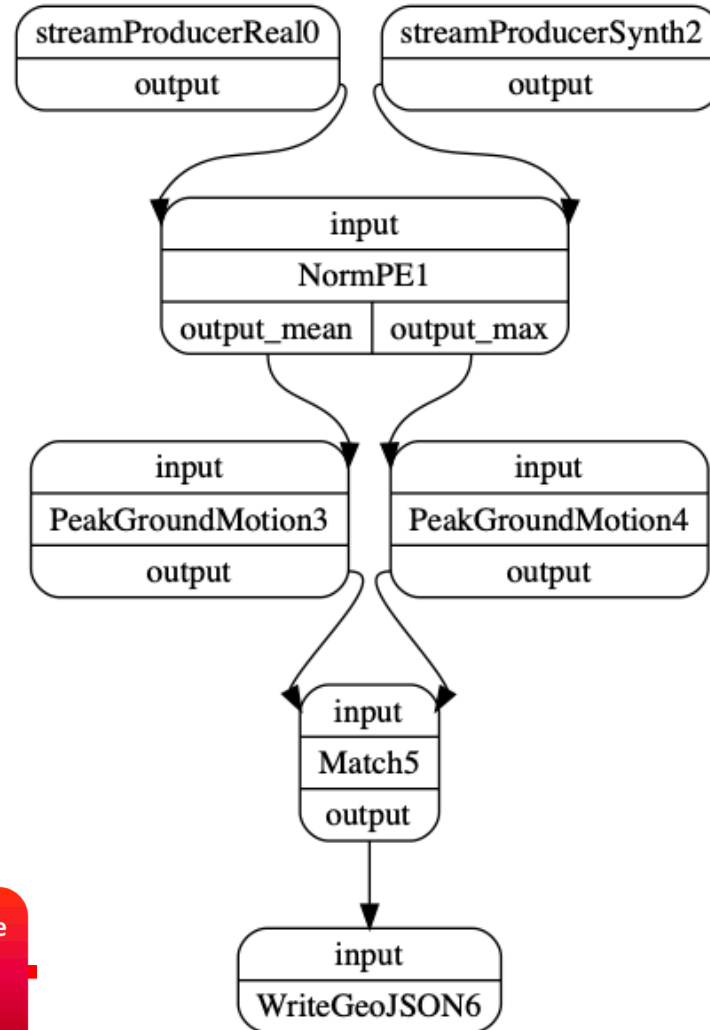
RA – Pre-processing observed and synthetic data



Similar preprocessing steps
in synthetic and observed data

Test Case: RA

Get
pre-processed
synt and data

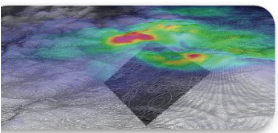


Ground motion parameters:

Peak ground values of displacement, velocity and acceleration.

Two types of normalisation – Mean & Max
Two set of PGM outputs – Max & Mean

Test Case: RA



Get ground
motion
parameters

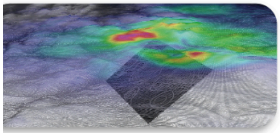
Compare/integrate
synthetic and
observed ground
motion data

RA – Ground motion parameters

Peak ground values of
Displacement (PGD),
Velocity (PGV)
Acceleration (PGA)

output

Test Case: RA



Get ground
motion
parameters

Compare/integrate
synthetic and
observed ground
motion data

```
type: "Feature"
▼ properties:
  station: "ARRO"
  ▼ data:
    PGD: 0.00003058970011915515
    PGV: 0.00015387362683992627
    PGA: 0.0008035731527687157
    p_norm: "max"
    PSA_0.3Hz: 0.000171880777011629
    PSA_1.0Hz: 0.0020140831084336057
    PSA_3.0Hz: 0.0009812436987400703
  ▼ synt:
    PGD: 0.000038899272805005096
    PGV: 0.00011736045694475592
    PGA: 0.00035493665398226155
    p_norm: "max"
    PSA_0.3Hz: 0.0003942182089108563
    PSA_1.0Hz: 0.0007176179285863899
    PSA_3.0Hz: 0.0003707452407479844
  ▼ difference:
    PGD: -0.000008309572685849946
    PGV: 0.000036513169895170355
    PGA: 0.0004486364987864541
    PSA_0.3Hz: -0.0002223374318992273
    PSA_1.0Hz: 0.0012964651798472158
    PSA_3.0Hz: 0.0006104984579920859
  ▼ relative_difference:
    PGD: -0.2716460983102781
    PGV: 0.23729322980834633
    PGA: 0.5583020005592205
    PSA_0.3Hz: -1.2935561251517065
    PSA_1.0Hz: 0.6436999418834826
    PSA_3.0Hz: 0.6221680289778919
  ▼ geometry:
    type: "Point"
    coordinates: []
```

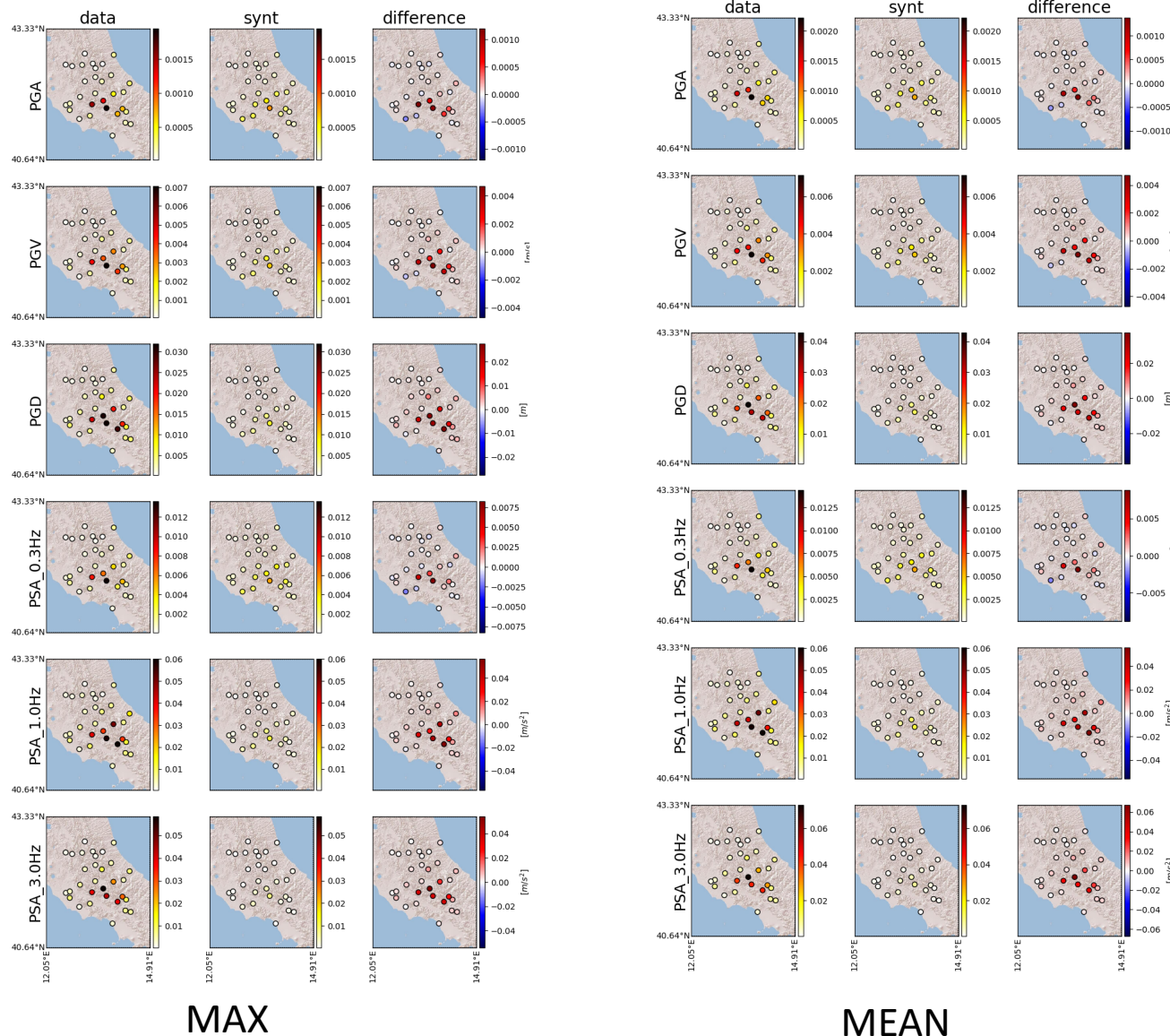
```
type: "Feature"
▼ properties:
  station: "ARRO"
  ▼ data:
    PGD: 0.00003058970011915515
    PGV: 0.00015387362683992627
    PGA: 0.0008035731527687157
    p_norm: "mean"
    PSA_0.3Hz: 0.000171880777011629
    PSA_1.0Hz: 0.0020140831084336057
    PSA_3.0Hz: 0.0009812436987400703
  ▼ synt:
    PGD: 0.000038899272805005096
    PGV: 0.00011736045694475592
    PGA: 0.00035493665398226155
    p_norm: "mean"
    PSA_0.3Hz: 0.0003942182089108563
    PSA_1.0Hz: 0.0007176179285863899
    PSA_3.0Hz: 0.0003707452407479844
  ▼ difference:
    PGD: -0.000008309572685849946
    PGV: 0.000036513169895170355
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    PSA_0.3Hz: -0.0002223374318992273
    PSA_1.0Hz: 0.0012964651798472158
    PSA_3.0Hz: 0.0006104984579920859
  ▼ relative_difference:
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  ▼ geometry:
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    coordinates: []
```

RA – Ground motion parameters maps



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Waveform propagation
snapshots and maps of
ground motion parameters
are fundamental for a
visual representation
of the earthquake



RA – Summary Steps (I)

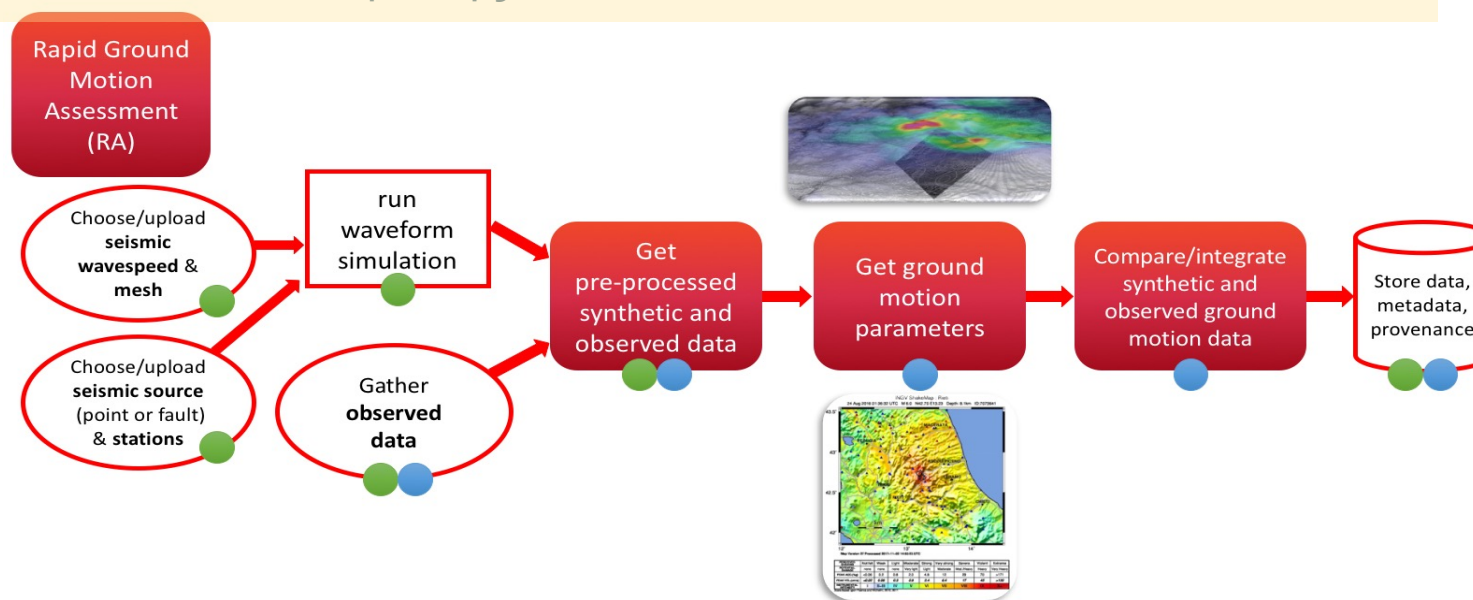
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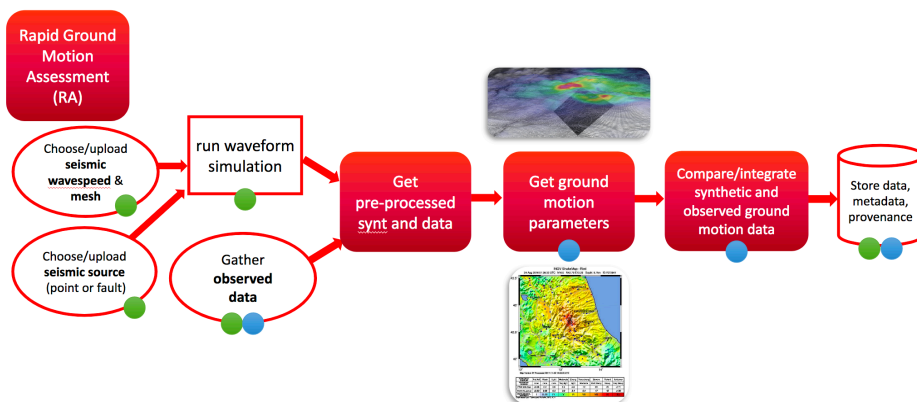
3. Use CWL to connect RA dispel4py workflows



RA – dispel4py + CWL



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dispel4py +  COMMON WORKFLOW LANGUAGE → semantics and descriptions

```
>> cwltool --provenance run-ra/ --full-name "Rosa Filgueira"
run_ra.cwl run_ra.yml
```

```
>> cwlprov --directory run-ra/ validate
Valid CWLProv RO: run-ra
```

```
>> cd run-ra/
>> cwlprov info
Research Object of CWL workflow run
Research Object ID: arcp://uuid:7b810637-40bb-467a-9c0a-a89865bf3c09/
Profile: https://w3id.org/cwl/prov/0.6.0
Workflow run ID: urn:uuid:7b810637-40bb-467a-9c0a-a89865bf3c09
Packaged: 2019-09-17
```

```
>> cwlprov who
Packaged By: cwltool 1.0.20190228155703 <urn:uuid:bbfe3471-2b87-4b11-975a-b96b2f24f4f8>
Executed By: Rosa Filgueira <urn:uuid:7d32cf62-d9c8-467e-8f58-5a74b70091e5>
```

```
#!/usr/bin/env cwl-runner
```

```
cwlVersion: v1.0
class: Workflow
```

```
inputs:
  create_env_script: File
  download_workflow: File
  download_argument_f: File
  preprocess_workflow: File
  ra_workflow: File
  ra_argument_d: string

outputs:
  misfit_data:
    type: Directory
    outputSource: preprocess_data/output
  pgm_data:
    type: Directory
    outputSource: rapid_assessment/output

steps:
  create_env:
    run: create_env.cwl
    in:
      script: create_env_script
    out: [output]
  download_data:
    run: dispel4py_download.cwl
    in:
      workflow: download_workflow
      argument_f: download_argument_f
      misfit_data: create_env/output
    out: [output]
  preprocess_data:
    run: dispel4py_preprocess.cwl
    in:
      workflow: preprocess_workflow
      misfit_data: download_data/output
    out: [output]
  rapid_assessment:
    run: dispel4py-RA-pgm_story.cwl
    in:
      workflow: ra_workflow
      argument_d: ra_argument_d
      misfit_data: preprocess_data/output
    out: [output]
```

RA – Summary Steps (I)

1. Dockerize Specfem3D + CWL
2. RA dispel4py workflows
3. CWL to connect RA dispel4py workflows

Experiment I:

- Run all the steps of the RA in our laptops, small dataset, sequential mapping

Experiment II:

- Run the same codes using NSF-Chameleon cloud, MPI docker cluster, larger dataset, MPI mapping

CWL is in charge to execute and connect each part of the RA application.

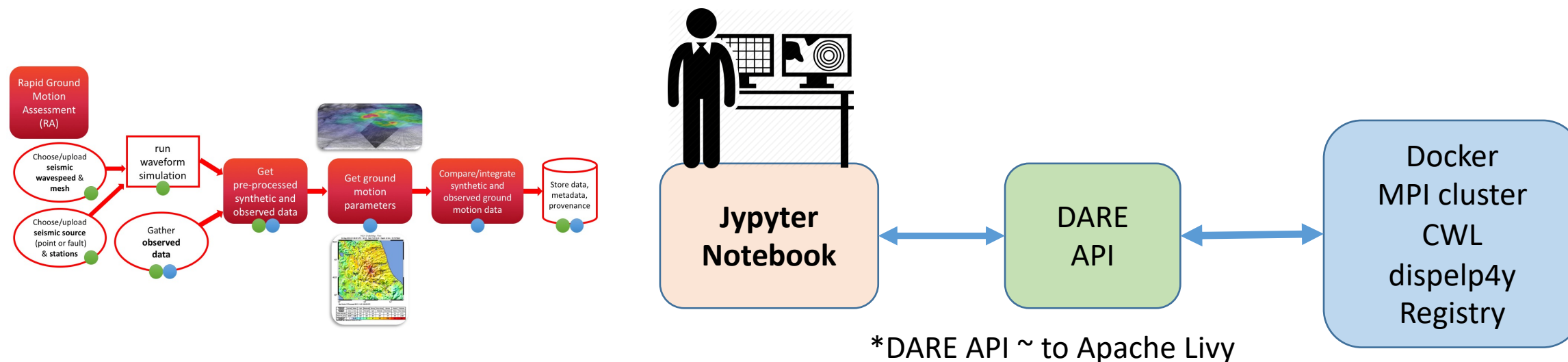
RA – Summary Steps (II)

4. DARE API – Workflows as a Services

5. Orchestration with Kubernetes: MPI cluster, dispel4py, CWL, SPECFEM3D, Registry

6. Jupyter Notebooks to submit applications/workflows to the working environment:

* Talk with the DARE API



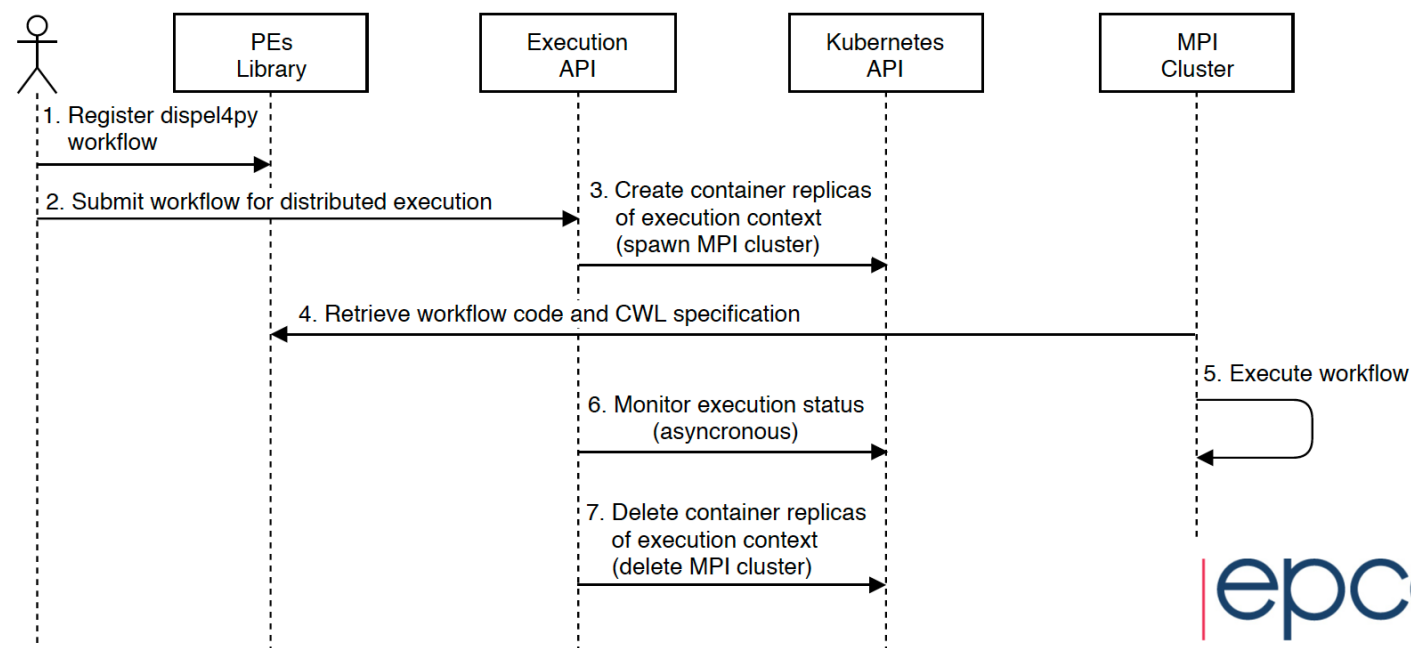
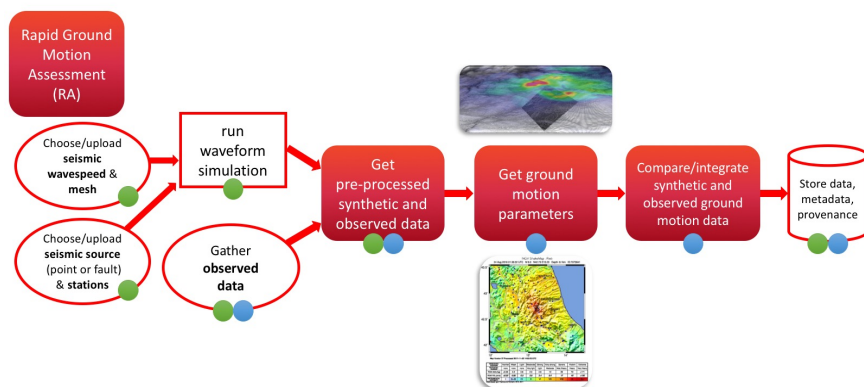
RA – Summary Steps (II)

4. DARE API – Workflows as a Services

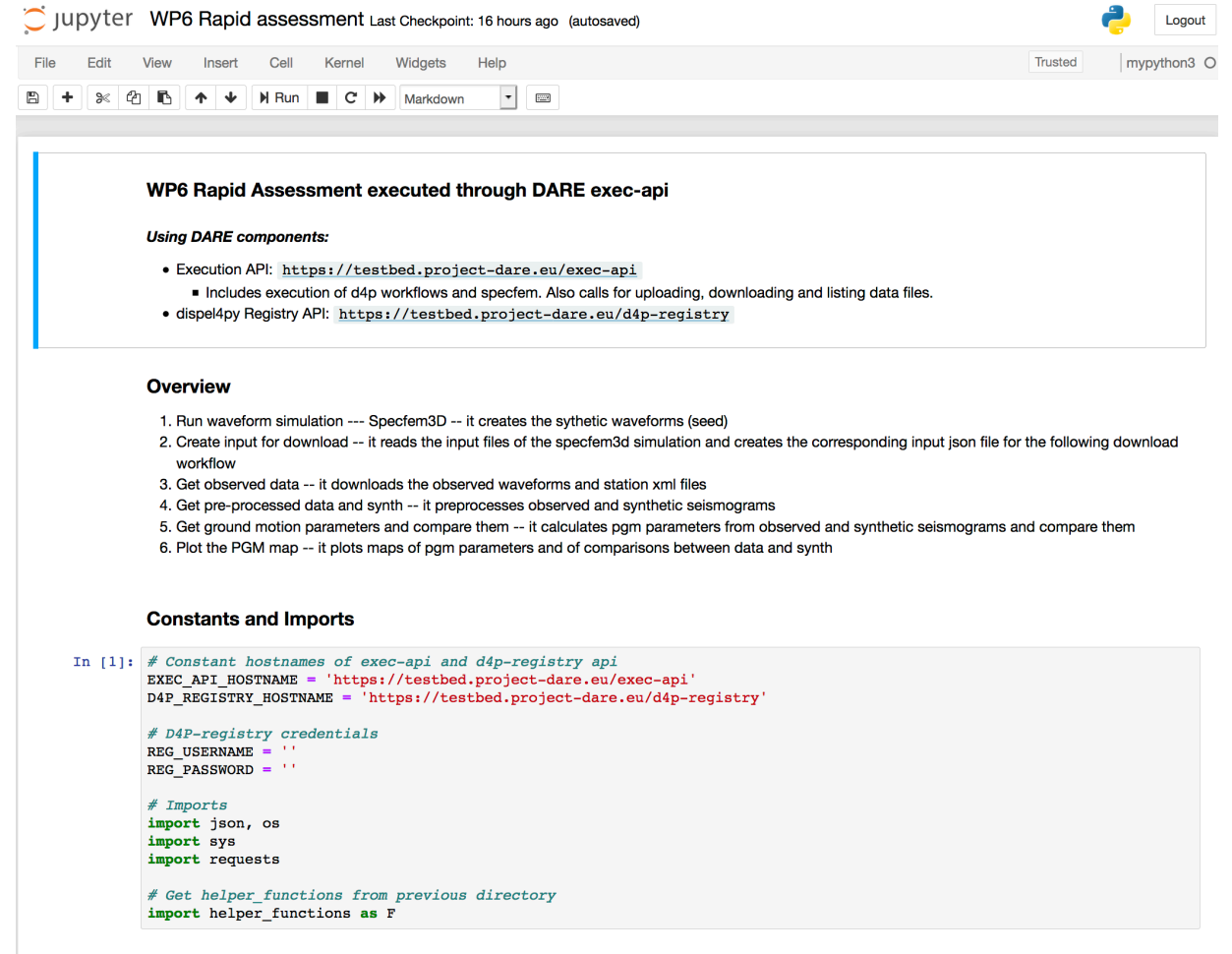
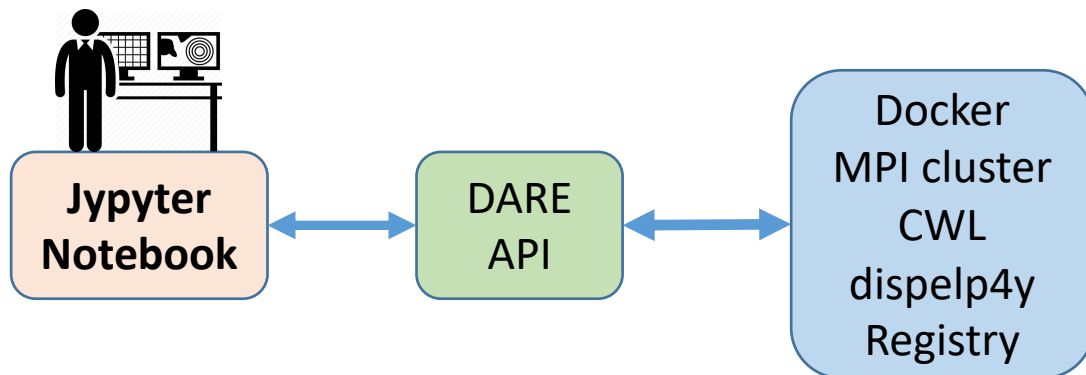
5. Orchestration with Kubernetes: MPI cluster, dispel4py, CWL, SPECFEM3D, Registry

6. Jupyter Notebooks to submit applications/workflows to the working environment:

* Talk with the DARE API



- Web service
- Acts as an intermediary between:
 - users' applications
 - the underlying computing resources
- Provisions a computing environment
 - Docker MPI cluster spawned on demand / Kubernetes
- Runs and monitors an application
- Collect its provenance and results



The screenshot shows a Jupyter Notebook titled "WP6 Rapid assessment" with a "Last Checkpoint: 16 hours ago (autosaved)" status. The interface includes a menu bar (File, Edit, View, Insert, Cell, Kernel, Widgets, Help) and a toolbar with icons for file operations, zooming, and running cells. The notebook content is displayed in a light blue box and includes the following sections:

- WP6 Rapid Assessment executed through DARE exec-api**
- Using DARE components:**
 - Execution API: <https://testbed.project-dare.eu/exec-api>
 - Includes execution of d4p workflows and specfem. Also calls for uploading, downloading and listing data files.
 - dispelp4y Registry API: <https://testbed.project-dare.eu/d4p-registry>
- Overview**
 1. Run waveform simulation --- Specfem3D -- it creates the sythetic waveforms (seed)
 2. Create input for download -- it reads the input files of the specfem3d simulation and creates the corresponding input json file for the following download workflow
 3. Get observed data -- it downloads the observed waveforms and station xml files
 4. Get pre-processed data and synth -- it preprocesses observed and synthetic seismograms
 5. Get ground motion parameters and compare them -- it calculates pgm parameters from observed and synthetic seismograms and compare them
 6. Plot the PGM map -- it plots maps of pgm parameters and of comparisons between data and synth
- Constants and Imports**

```
In [1]: # Constant hostnames of exec-api and d4p-registry api
EXEC_API_HOSTNAME = 'https://testbed.project-dare.eu/exec-api'
D4P_REGISTRY_HOSTNAME = 'https://testbed.project-dare.eu/d4p-registry'

# D4P-registry credentials
REG_USERNAME = ''
REG_PASSWORD = ''

# Imports
import json, os
import sys
import requests

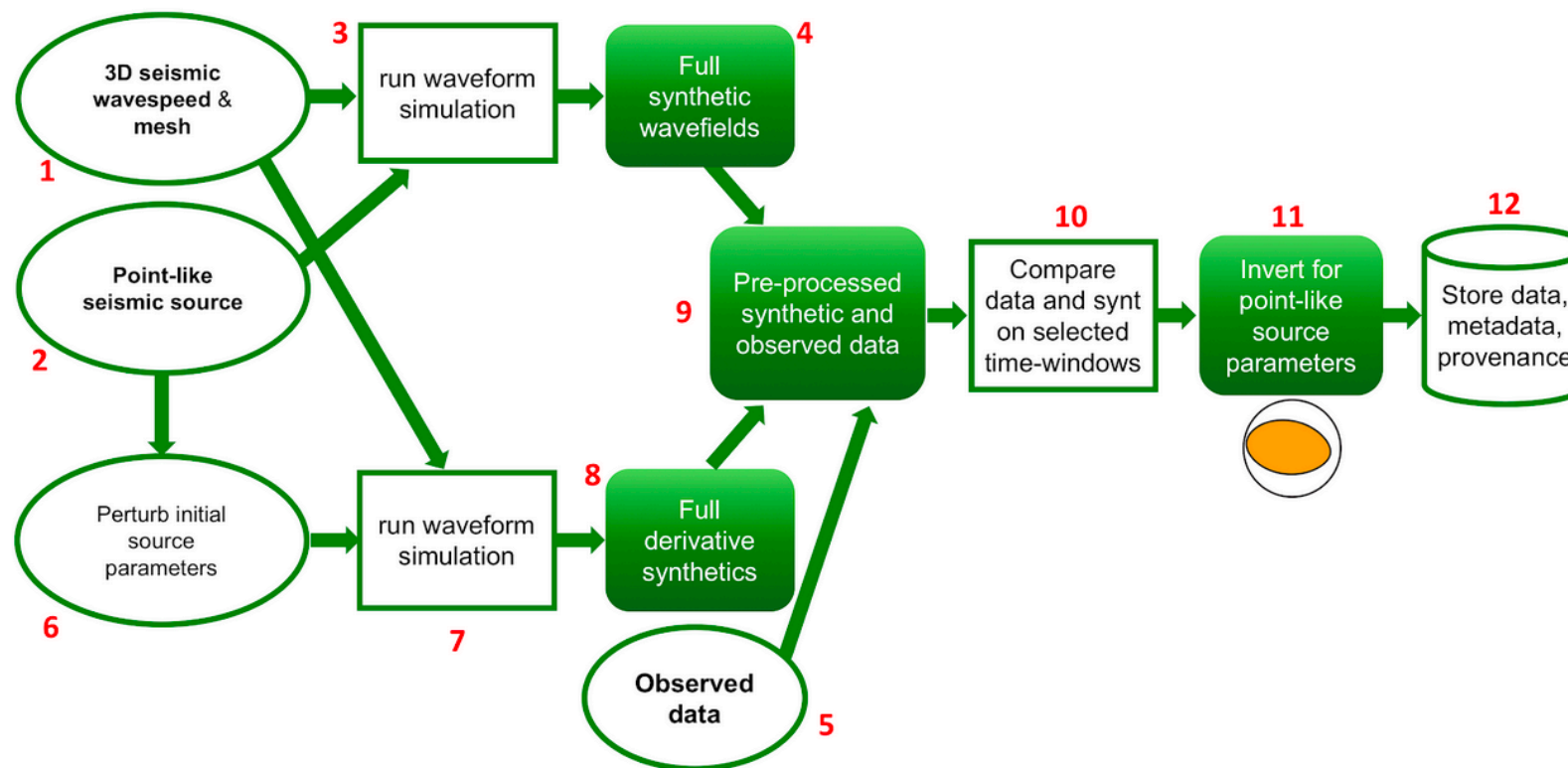
# Get helper_functions from previous directory
import helper_functions as F
```

Seismic Source Analysis (SS) – New Use Case



ISTITUTO NAZIONALE
DI GEOFISICA E VULCANOLOGIA

Characterises the source parameters of an earthquake: **location**, **magnitude** and **rupture mechanism**.



Many simulations by perturbing the source parameters.
Analysis of the impact caused by each simulation on the ground motion.

Conclusions

New interfaces provide a fluent path from prototyping to production.

Data-intensive applications are not locked to platforms

- * can be moved to suitable new platforms
- * without human intervention

Abstract and semantic descriptions to allow reproducibility and portability.

Workflows-as-a-services (Waas): End-users do not need to set up any environment

Future Work

Workflows can be optimised intelligently without the user needing to do that

- New dispel4py mappings – dynamic deployment – *ZeroMQ*
- Handling errors – Recovery from failure(s)
- Automatic optimizations – exploiting data parallelism

CWLProv + dispel4py Provenance – integrate different levels of provenance

Delivering easy-to-use frameworks to empower data-driven research

Questions ?

DARE: A Reflective Platform Designed to Enable Agile Data-Driven Research on the Cloud, IEEE eScience 2019
Comprehensible control for researchers and developers facing data challenges, IEEE eScience 2019

Thanks!

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CCS-EPCC Workshop Tsukuba 2019

