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

Dr. Rosa Filgueira, University of Edinburgh, EPCC

Background

- PhD Computer Science – Madrid/Carlos III
  - *Dynamic optimization techniques to enhance scalability and performance of MPI-based application*
- 5 years as a Postdoc – University of Edinburgh/DIR group
- 2 years as a Senior Data scientist at BGS

Currently – EPCC at the University of Edinburgh

- Data Architect activities across different domains/ Projects/
  - Scalability and performance of applications executed on HPC and Cloud resources
  - Scientific workflows, data-frameworks, containers and reproducibility tools, etc
  - Research activities

https://www.rosafilgueira.com/

Introduction

Big Data Sciences 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

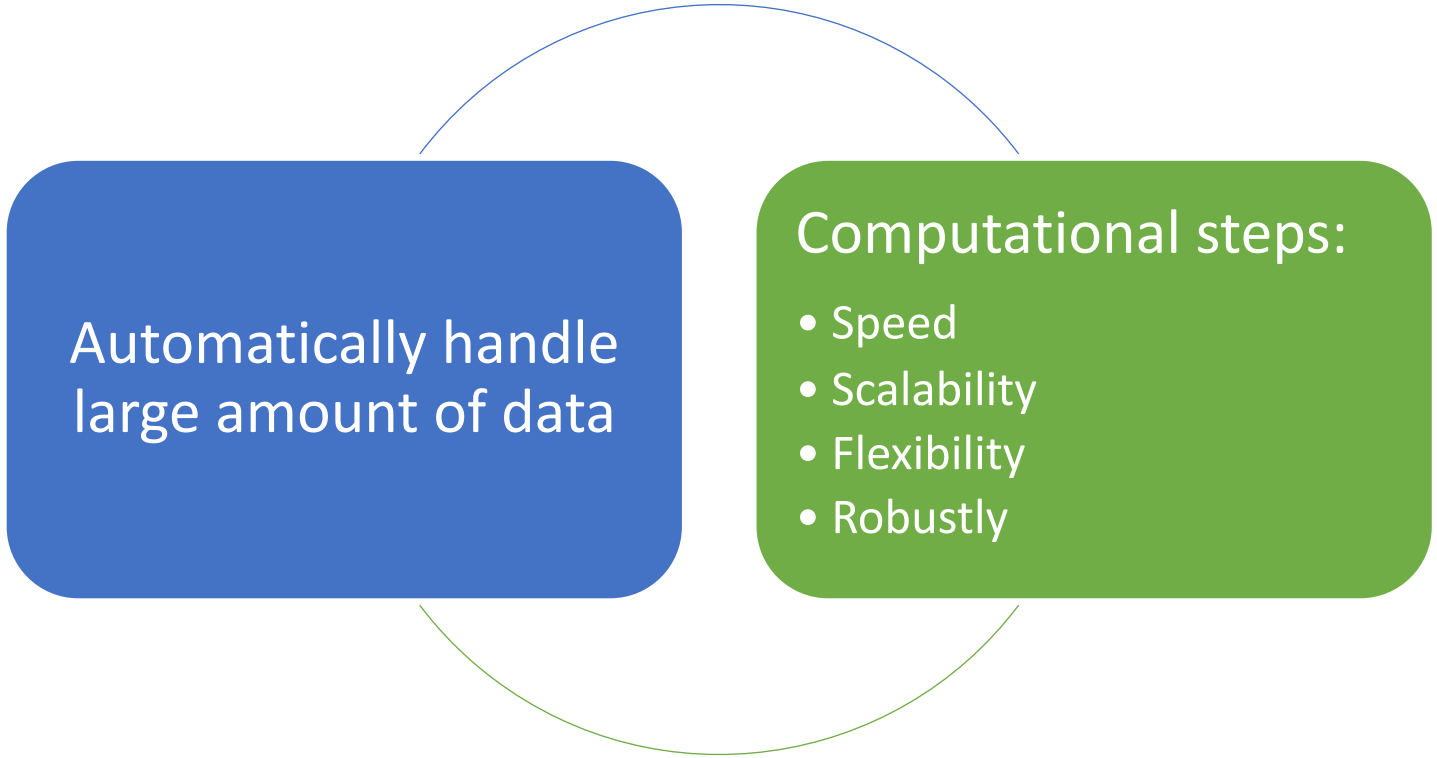
Data transformation and visualisation

epcc

Introduction

Big Data Sciences Era, Data Intensive Computing applications

Data analytic frameworks and Computing environments



epcc

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

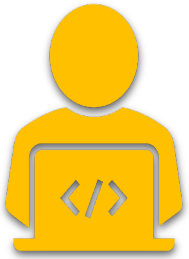
Seismology

Scientific Workflows:

dispel4py

Pegasus

CWL



Computing environments:

HPC Clusters

Cloud

epcc

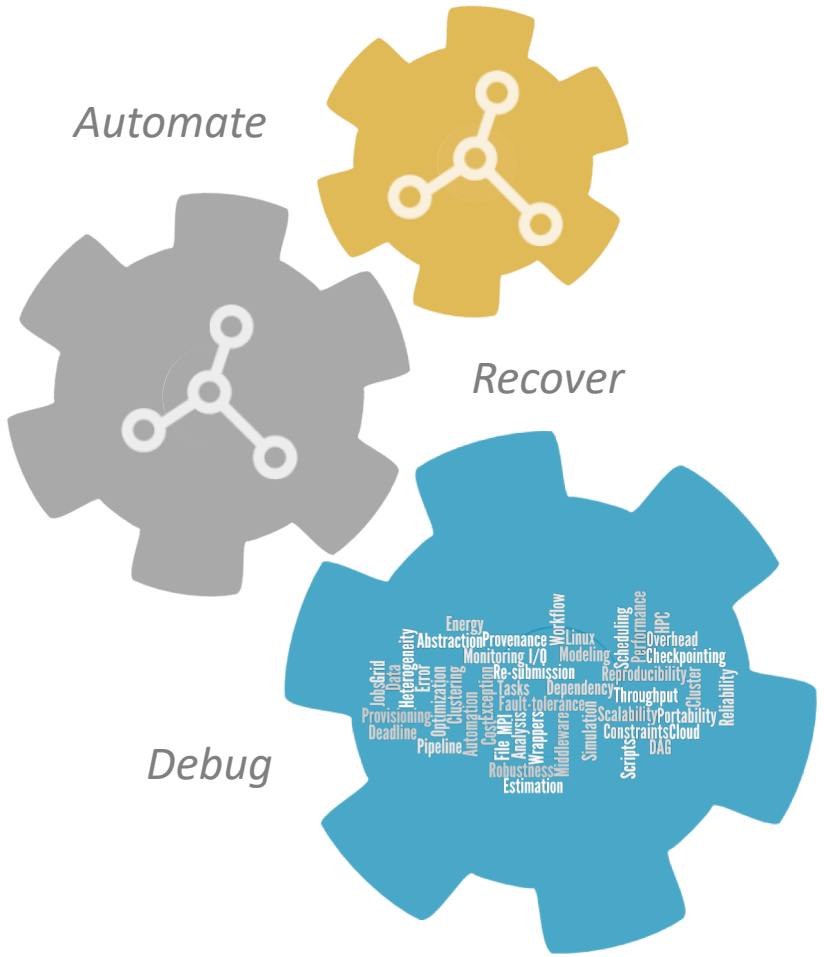
Why Scientific Workflows ?

General Features

Abstraction, scientists can focus on their research and not computation management

Easy composition and execution

Enables parallel, distributed computations



Different types

abstract vs. concrete

task-flow vs. data-flow

files vs. stream-based

Workflow Management Systems (WMS)

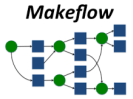
Provide tools to generate the scientific workflow

epcc

WORKFLOW MANAGEMENT SYSTEMS

Taverna
https://taverna.incubator.apache.org

Kepler
https://kepler-project.org



Makeflow
http://ccl.cse.nd.edu/software/makeflow

dispel4py
http://dispel4py.org

Nextflow
https://www.nextflow.io

KNIME
https://www.knime.org

VisTrails
http://vistrails.org

FireWorks
https://pythonhosted.org/FireWorks

Swift
http://swift-lang.org

Pegasus
http://pegasus.isi.edu

epcc

Asterism Framework

Easy to understood, platform-independent, open-source

Simplifies the development applications running across multiple heterogeneous

How ?

Combining the strengths of

Traditional WMS
Pegasus

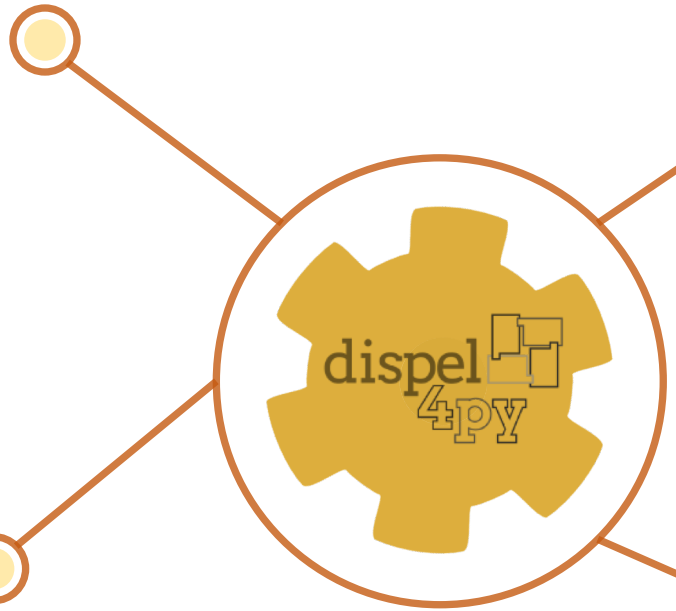
Ewa Deelman, ISI-USC,US
Rafael Ferreira da Silva, ISI-USC, US

New stream-based data-flow systems
dispel4py

Rosa Filgueira, BGS-NERC, UK
Amrey Krause, EPCC-UoE, UK
Malcolm Atkinson, Informatics-UoE, UK

epcc

dispel4py parallel stream-based dataflow system

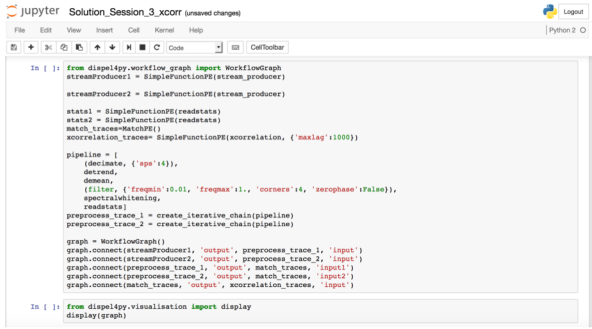


Automation

Automates pipeline executions
Concurrent, distributed computations
Stream-based model

Workflow Composition

Python Library
Groupings
Jupyter



High-level stream-based data pipeline
~ Apache Beam

Mapping

Sequential
Multiprocessing
MPI
Apache Storm
Apache Spark (Prototype)

Optimisation

Multiple streams
Avoids I/O operations

Key-features: Automatic parallelization/mappings, concurrent & stream-based

epcc

https://github.com/dispel4py/dispel4py

dispel4py parallel stream-based dataflow system

Graph

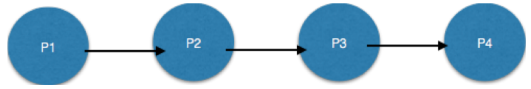
- Connections among PES
- Abstract workflow

Instance

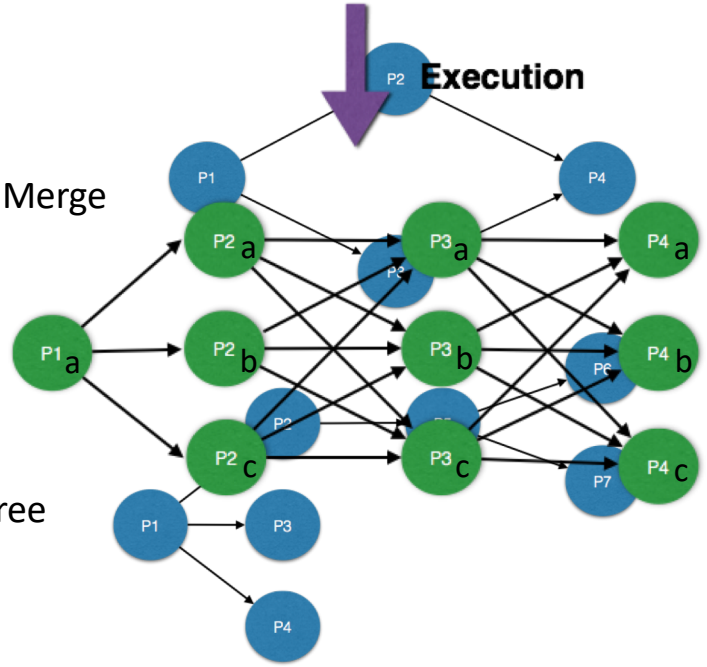
- Executable copy of a PE that runs in a process
- Each PE is translated into one or more instances in run-time
- dispel4py does it for you
- Concrete workflow

+ Example of graphs

Pipeline



Split & Merge

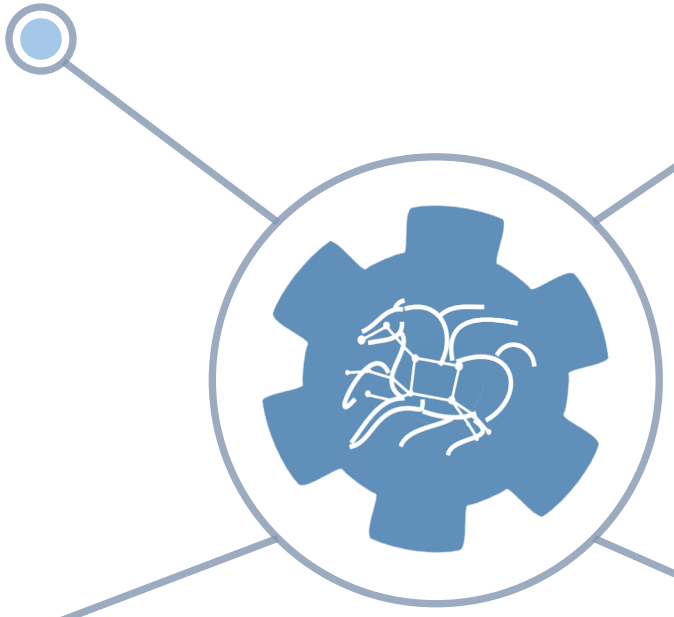


Tree

PE Instance

4 PEs & 10 processes

Pegasus workflow system



Automation

Automates pipeline executions
Parallel, distributed computations
Automatically executes data transfers
Heterogeneous resources
Task-oriented model
Application is seen as a black box

Debugging

Workflow execution and job performance metrics
Real-time monitoring, graphs, provenance

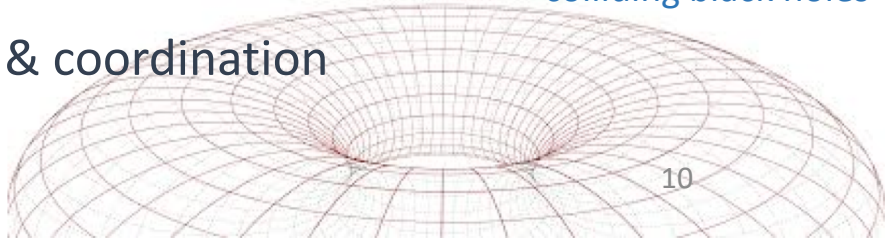
Recovery

Job failure detection
Checkpoint Files
Job Retry
Rescue DAGs

Optimisation

Job clustering
Data cleanup

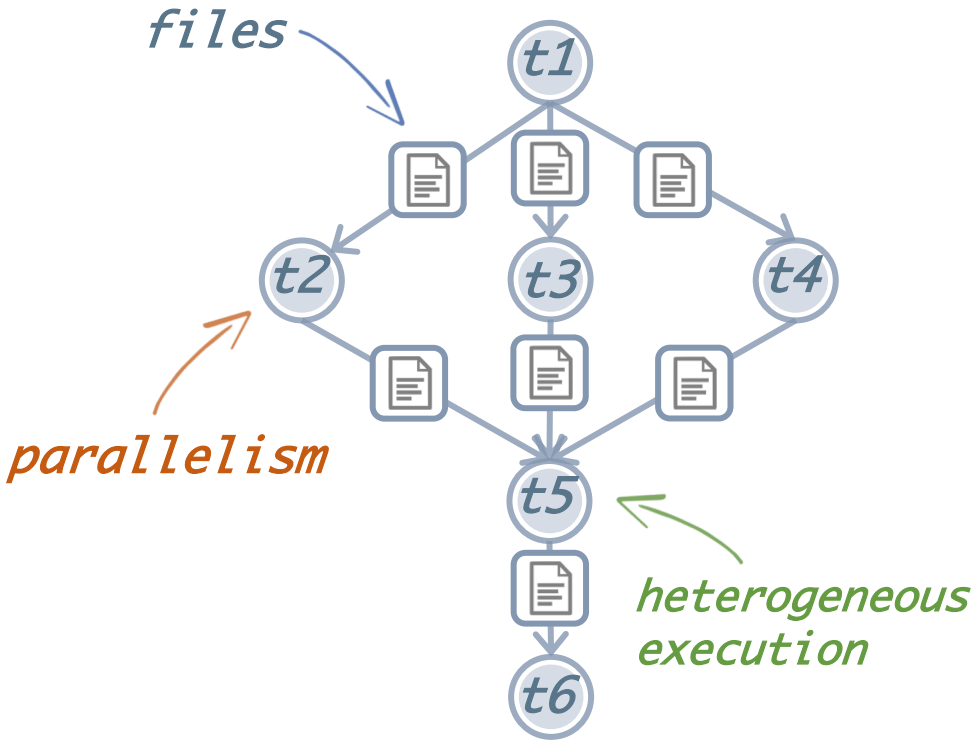
LIGO project:
First **detection of gravitational waves** from colliding black holes



Key-features: Automatic data movement, cleanup, heterogeneous & coordination

http://pegasus.isi.edu

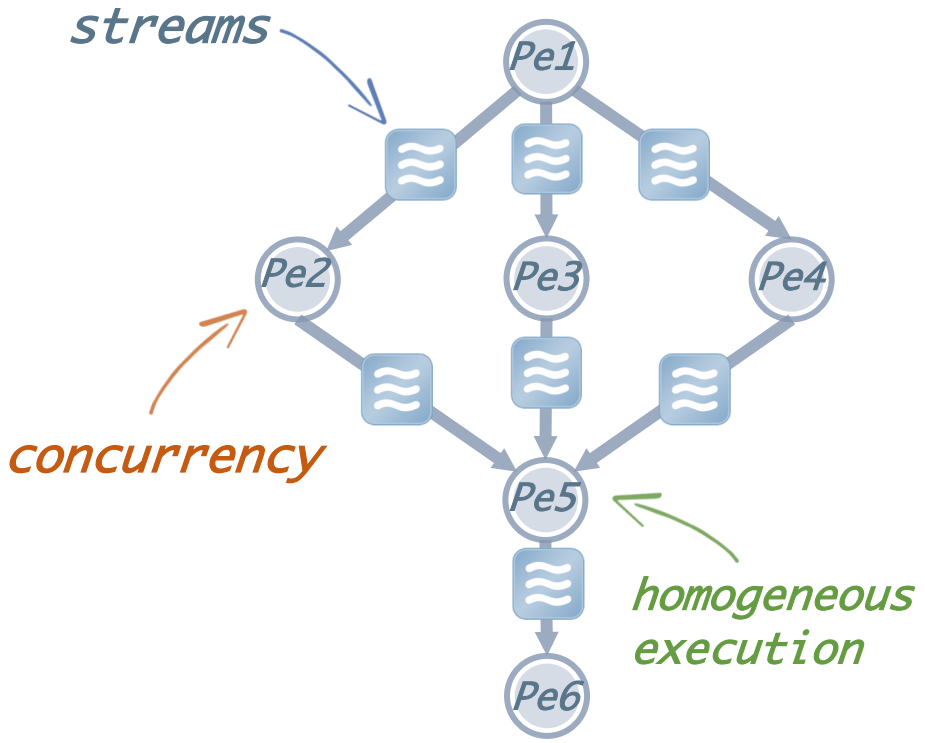
Complementary systems



Task-flow

Task: Executable (black box)

dispel4py



Data-flow

Processing Elements: python objects

epcc

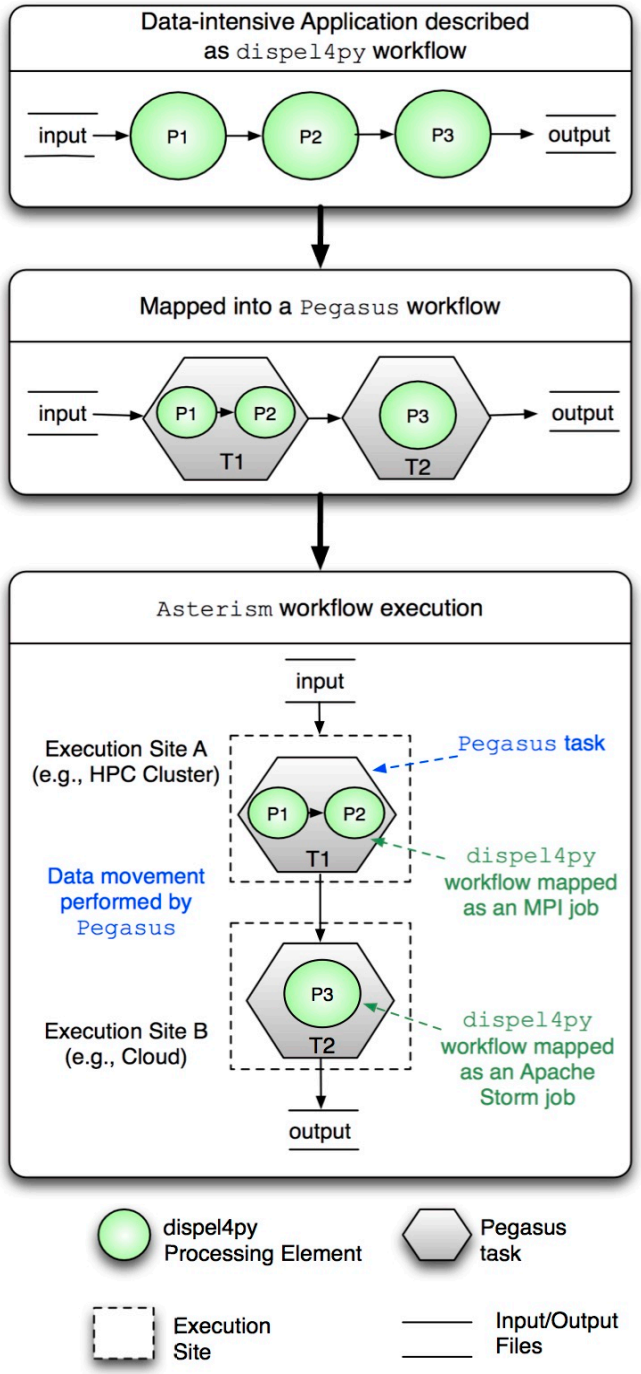
dispel4py

+

Pegasus

=

ASTERISM

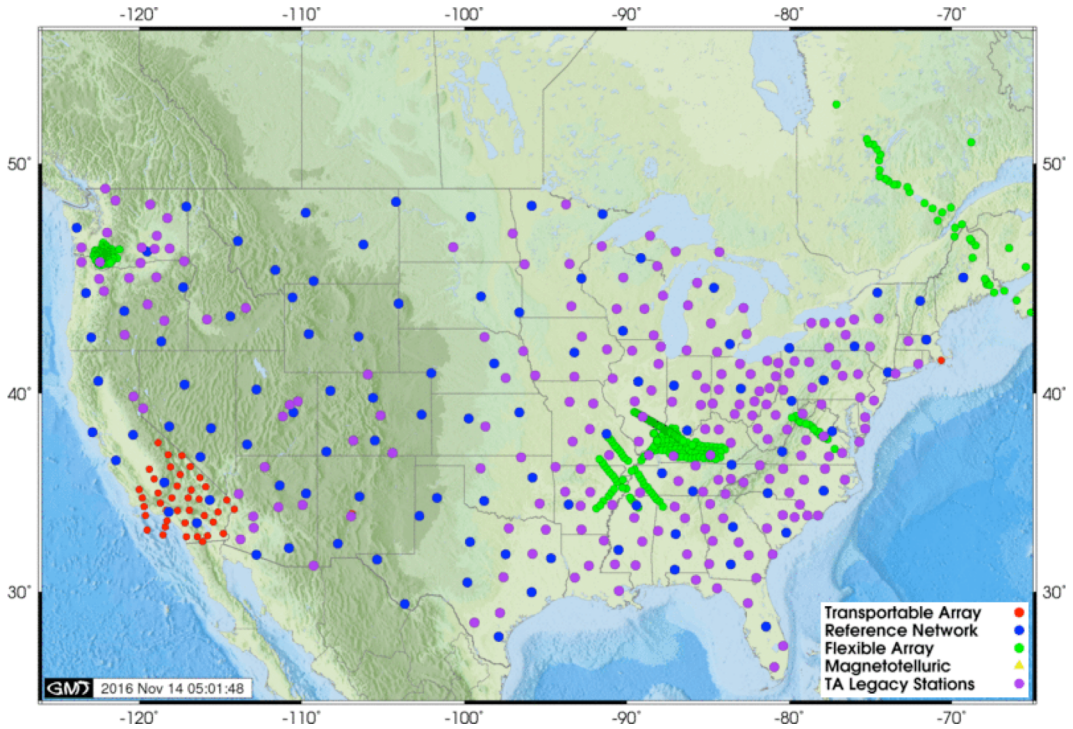


dispelpy to represent different parts of applications

Pegasus to distribute and execute each dispel4py workflow

epcc

Seismic Ambient Noise Cross-Correlation

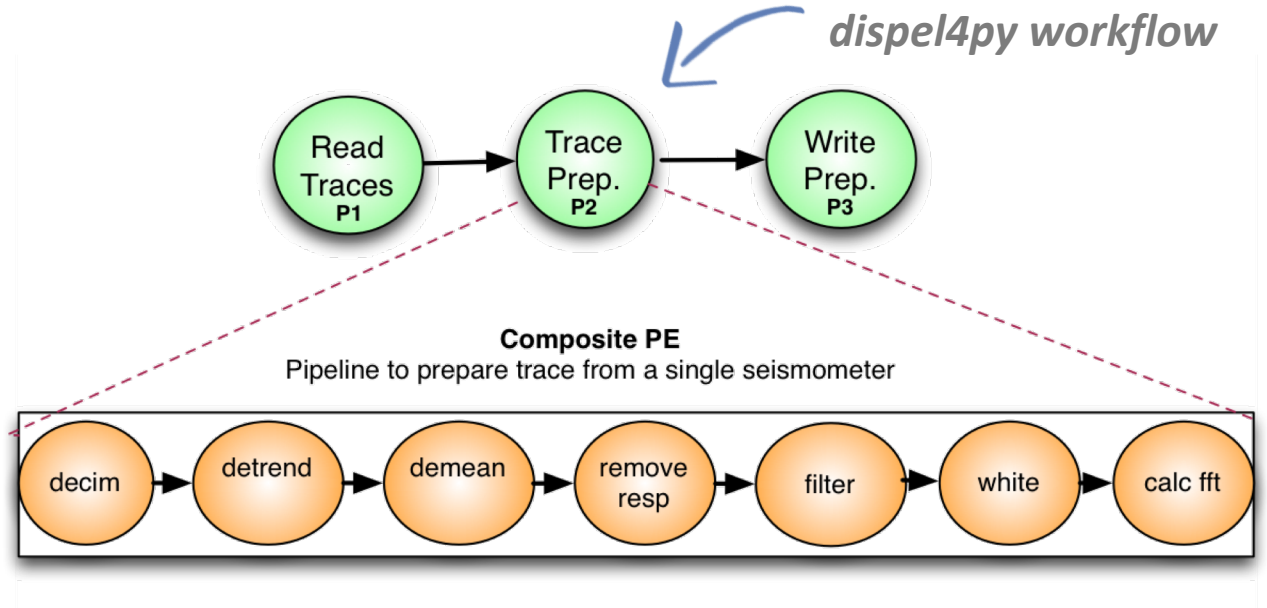


IRIS USA TA array – 1000 stations- 4999500 cross-correlations per hour

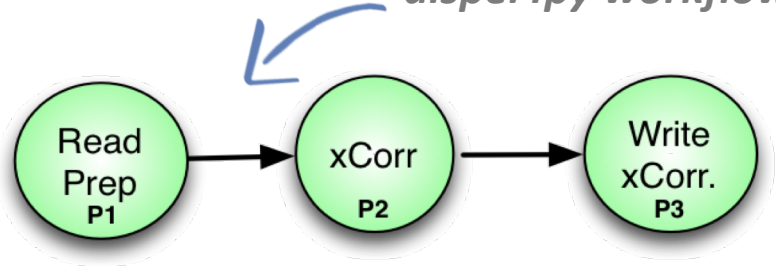
Preprocesses (Phase 1) and cross-correlates traces (Phase 2) from multiple seismic stations

VERCE project both phases on the same HPC resource

Phase 1
dispel4py workflow

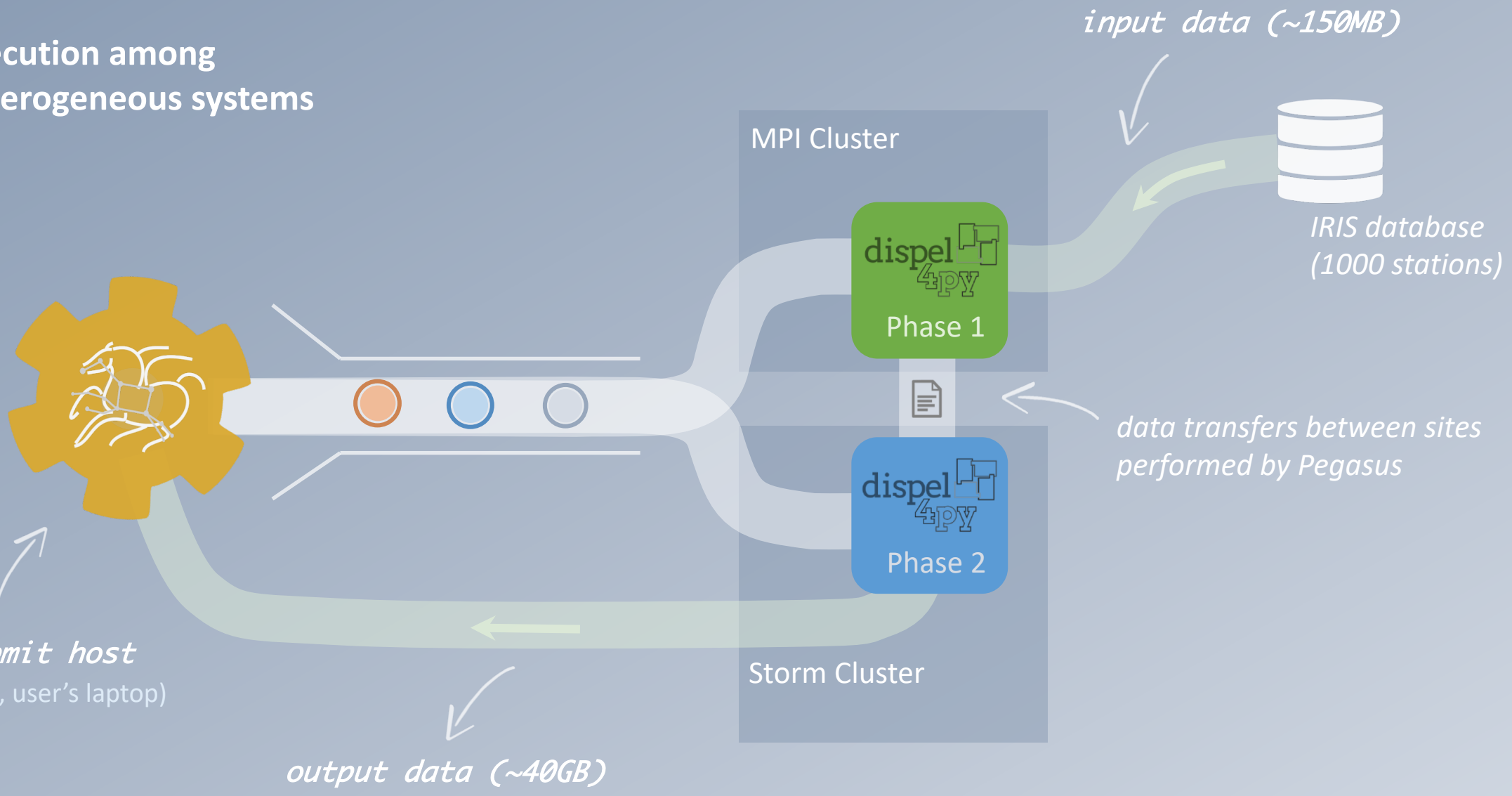


Phase 2
dispel4py workflow



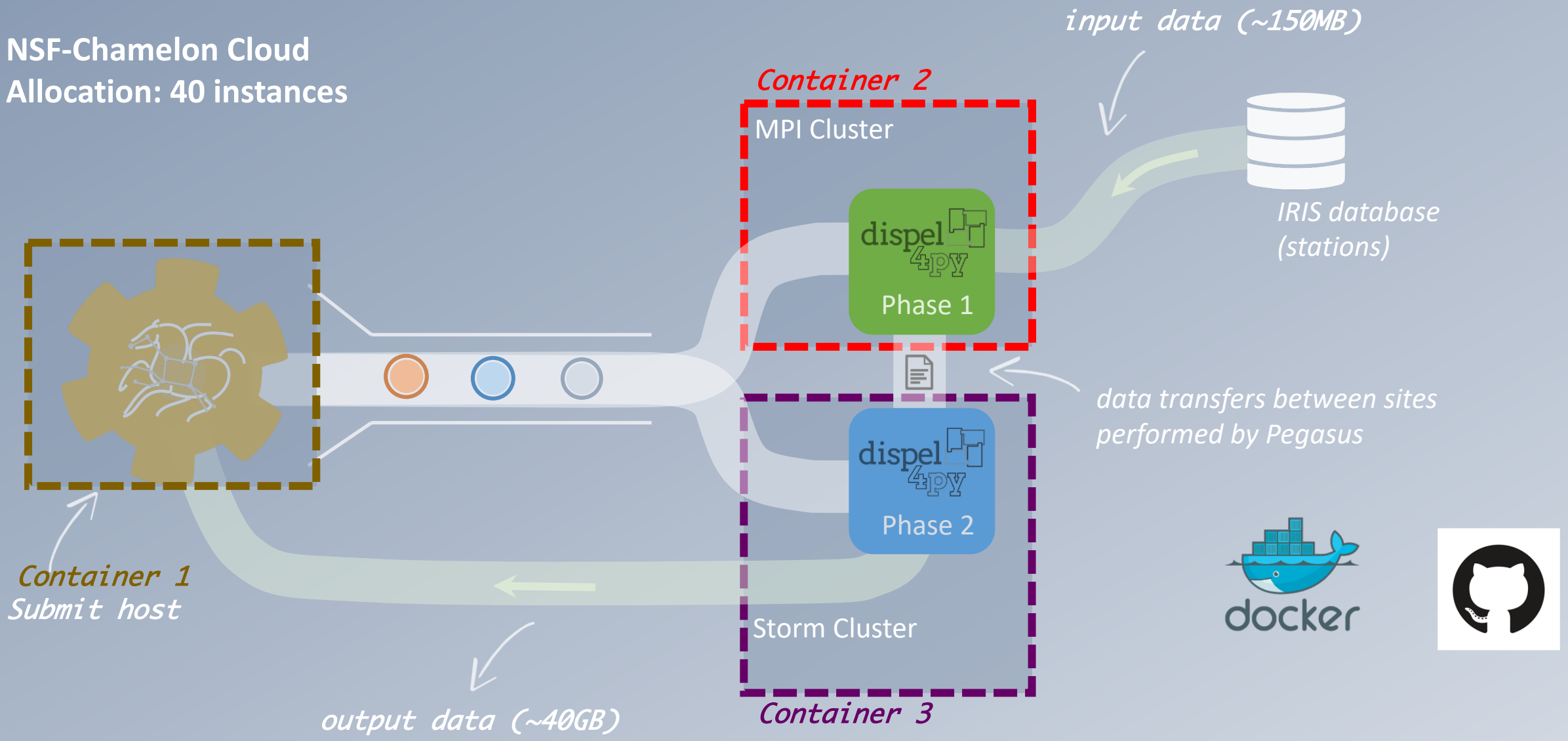
Evaluation- Seismic Ambient Noise Cross-Correlation

Execution among heterogeneous systems



Evaluation- Seismic Ambient Noise Cross-Correlation

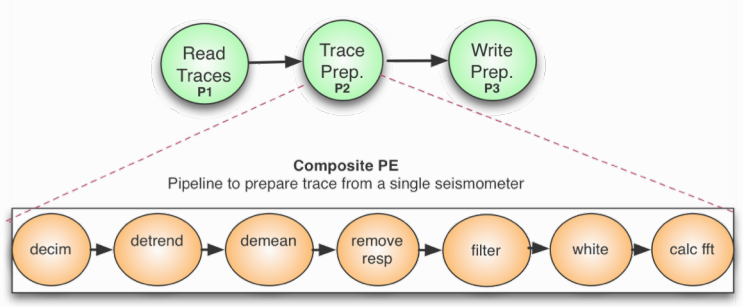
NSF-Chamelon Cloud
Allocation: 40 instances



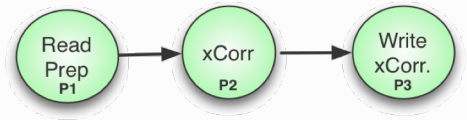
https://github.com/dispel4py/pegasus_dispel4py

Reminder

Data-Intensive Application



dispel4py preproc. (Phase 1)



dispel4py proc. (Phase 2)

Container 1

Submit Site

Container 2

MPI Cluster Phase 1

Storm Cluster Phase2

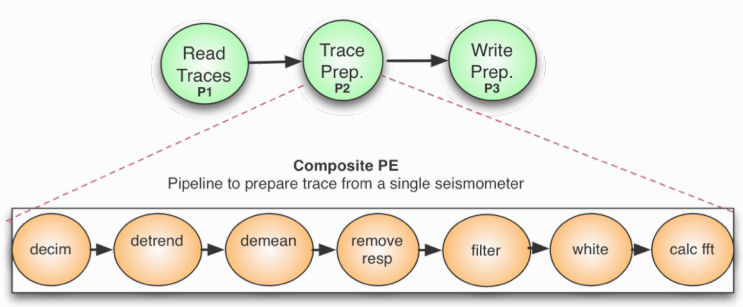
Container 3

NSF-Chameleon cloud 1 node – 40 cores

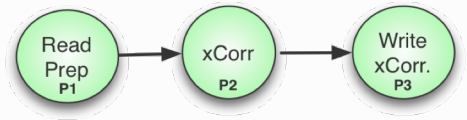
Dockerfiles to configure containers **images** → Stored in our **GitHub** → Linked to **DockerHub** → stored/share/download images

Reminder

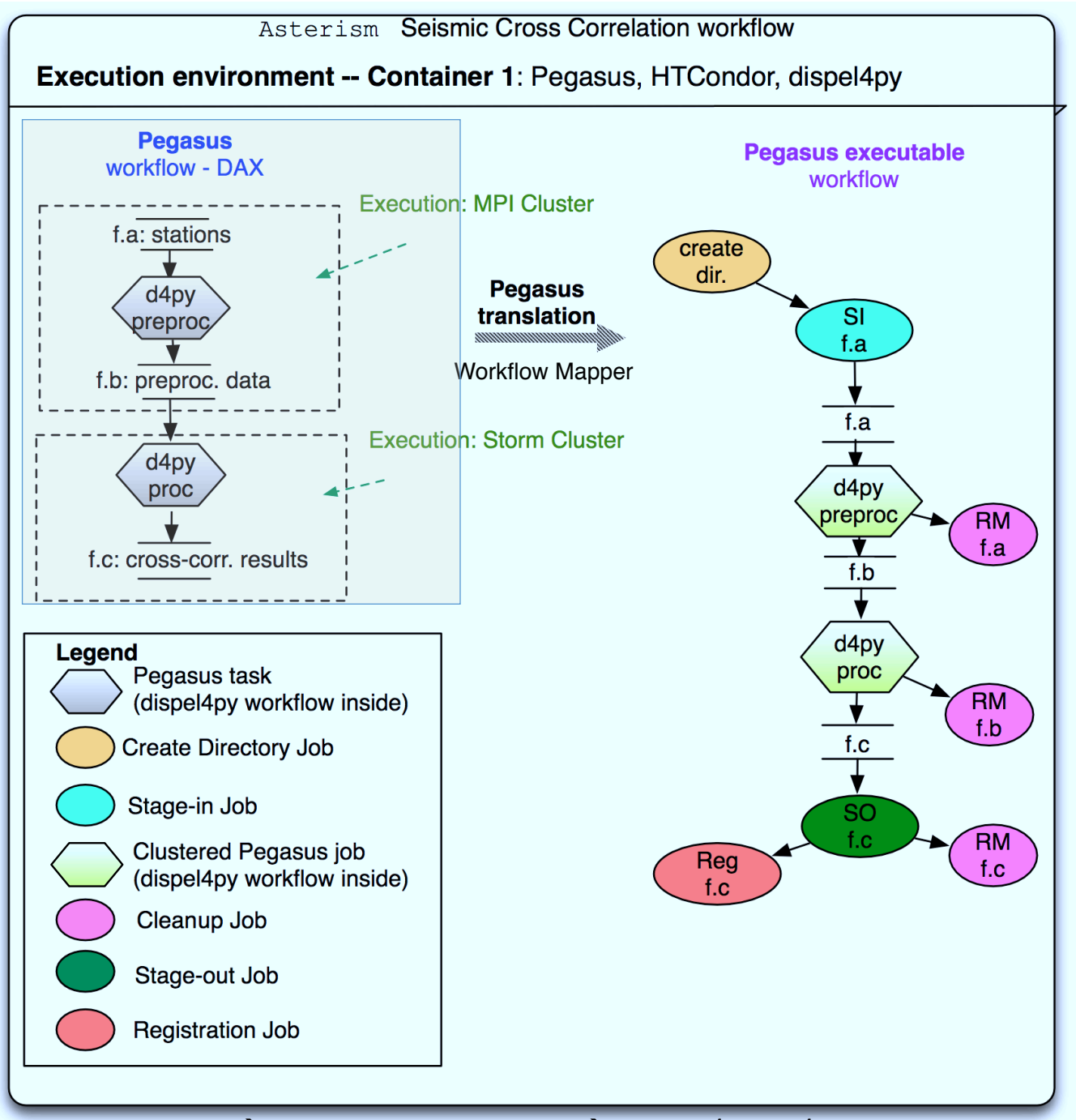
Data-Intensive Application



dispel4py preproc. (Phase 1)



dispel4py proc. (Phase 2)



1 instance as Container 1

Container 1

Submit Asterism

Container 2

MPI Cluster

Storm Cluster

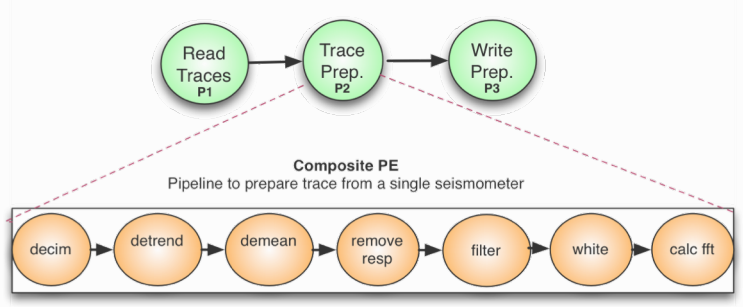
Container 3

NSF-Chameleon cloud
1 node – 40 cores

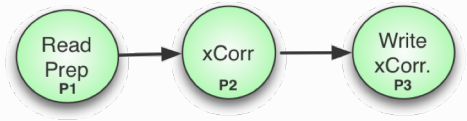
Dockerfiles to configure containers **images** → Stored in our **GitHub** → Linked to **DockerHub** → stored/share/download images

Reminder

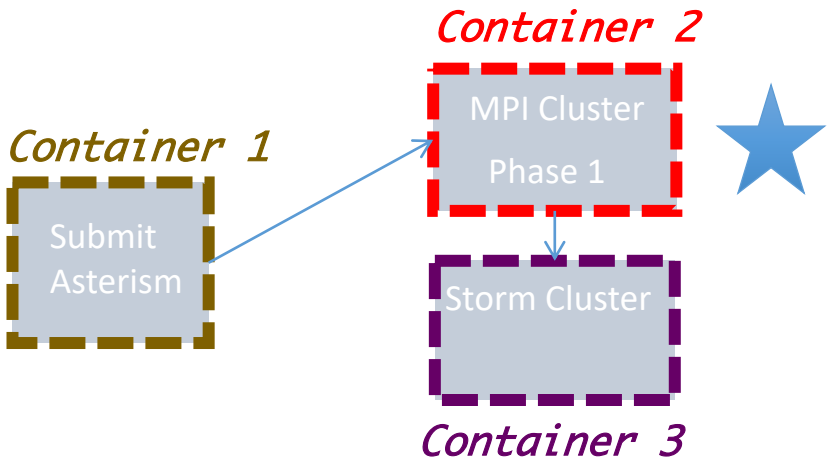
Data-Intensive Application

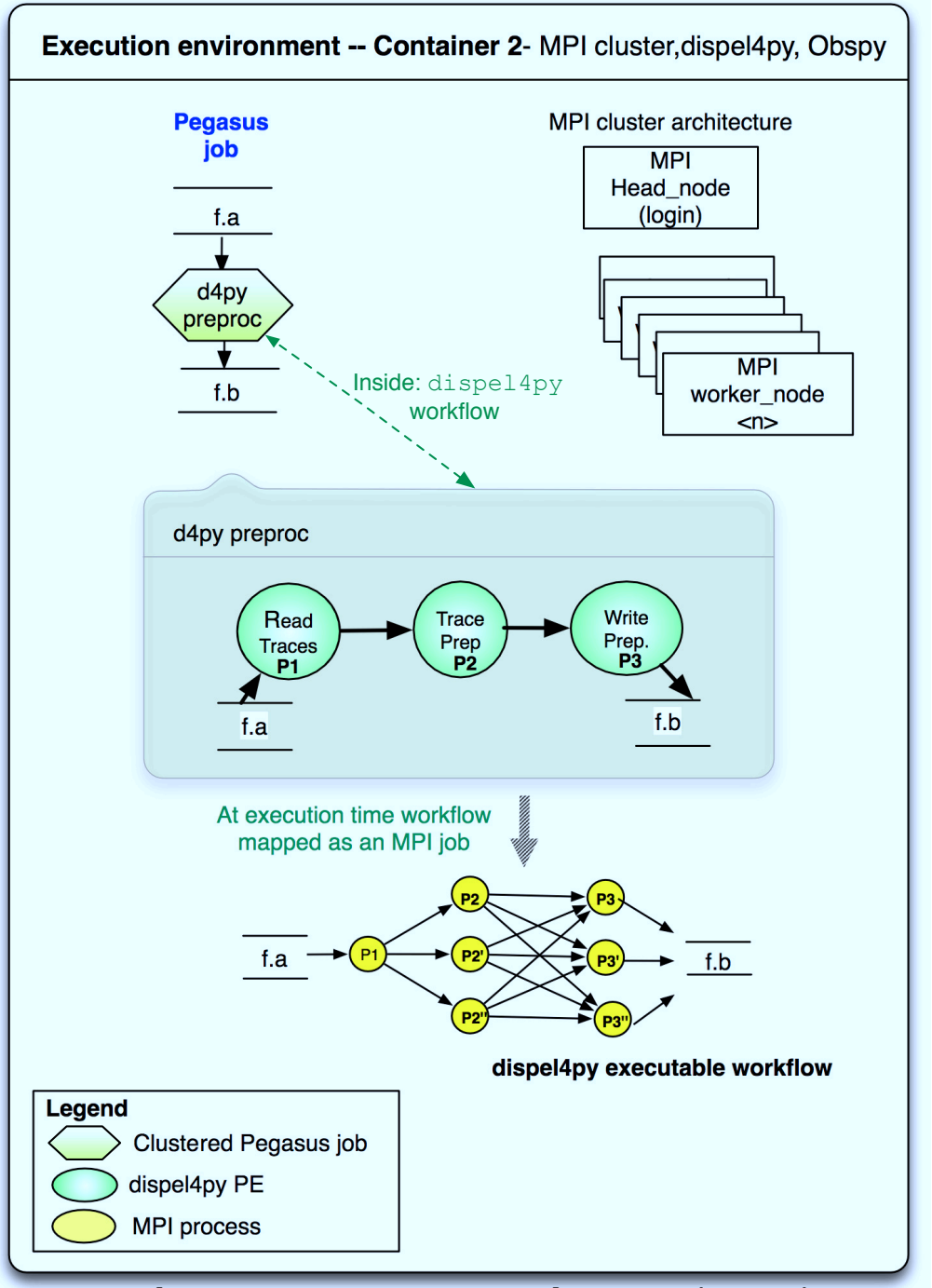


dispel4py preproc. (Phase 1)



dispel4py proc. (Phase 2)





1 instance as Container 2 (MPI head node)

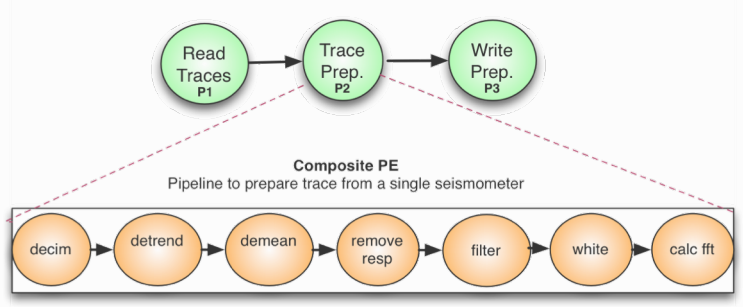
16 instances as Container 2 (MPI workers)

NSF-Chameleon cloud
1 node – 40 cores

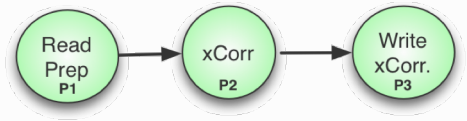
Dockerfiles to configure containers **images** → Stored in our **GitHub** → Linked to **DockerHub** → stored/share/download images

Reminder

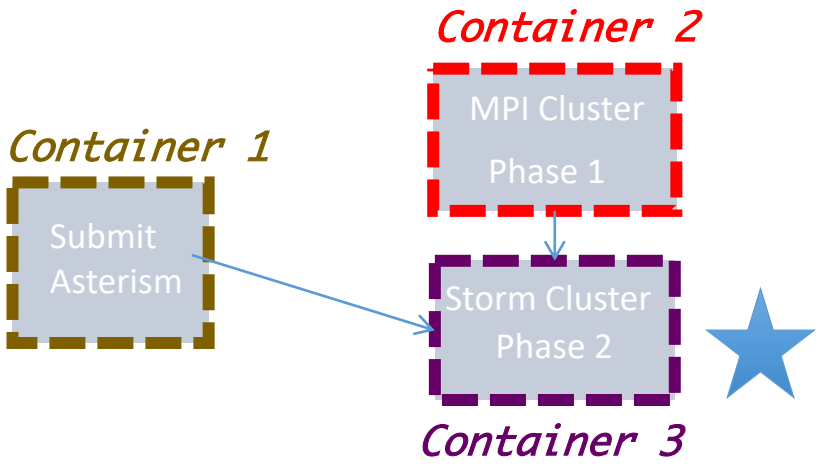
Data-Intensive Application

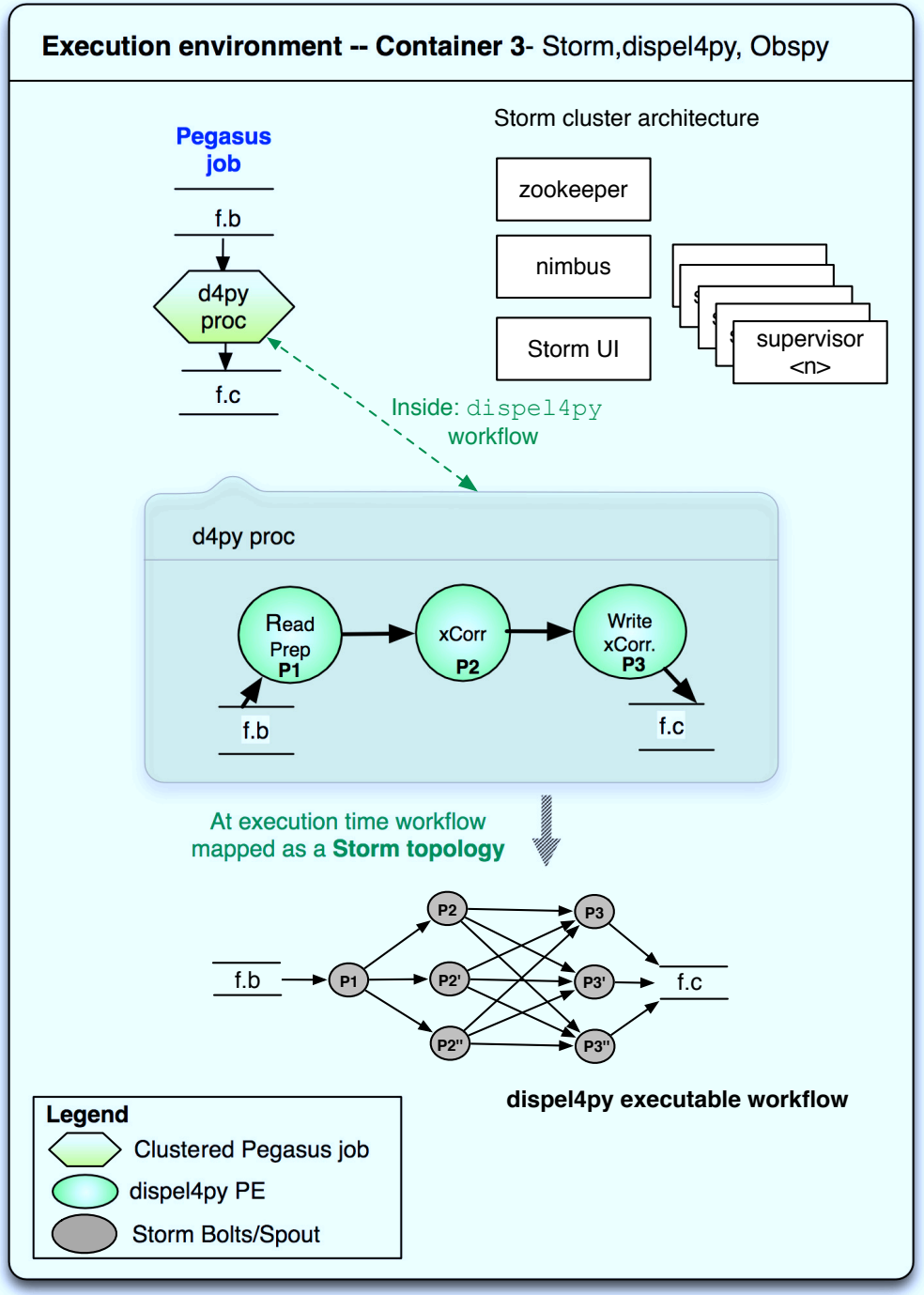


dispel4py preproc. (Phase 1)



dispel4py proc. (Phase 2)





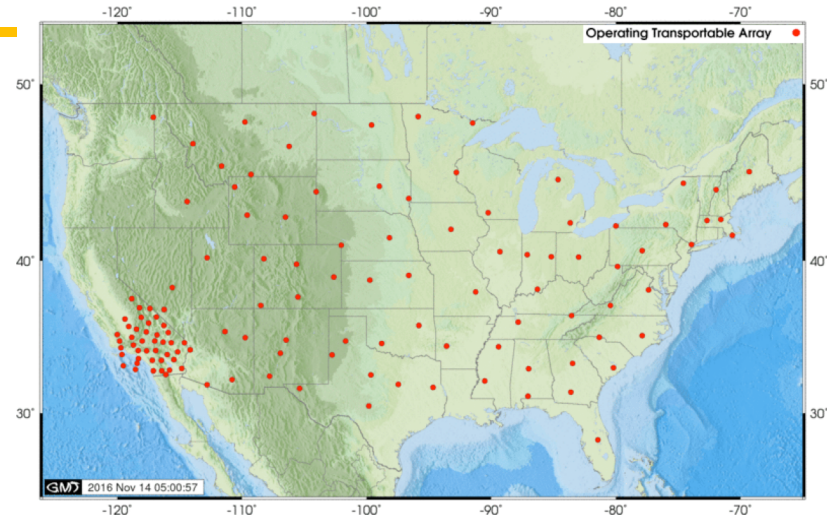
3 instances as Container 3 (zookeper, nimbus, Storm UI)

16 instances as Container 3 (Supervisors)

NSF-Chamelon cloud
1 node – 40 cores

Dockerfiles to configure containers **images** → Stored in our **GitHub** → Linked to **DockerHub** → stored/share/download images

Asterism Evaluations



Experiment 1: Data from IRIS services (394 stations)

Time

Phase 1 – 8 minutes
Phase 2 – 2 hours
Moving data < 1 minute

Data size

Input data 150MB
Output data 39GB

Experiment 2: Workflow for 3 days requesting data every 2 hours

Scope of this work

Executing & paralyzing automatically data-intensive applications

in heterogeneous systems with different enactment engines

NSF-Chamelon cloud
1 node – 40 cores

Maximizing performance
- both phases in the MPI cluster
- increasing the number of Storm Supervisors

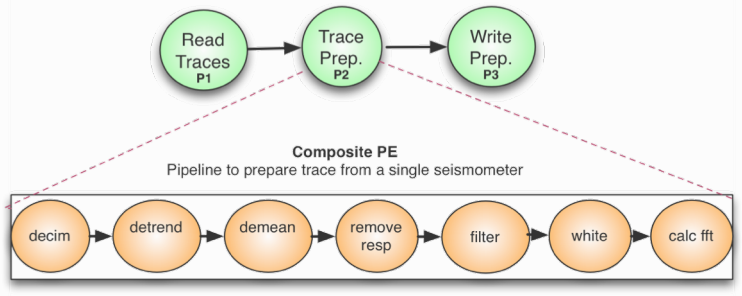
epcc

dispel4py Performance Evaluations

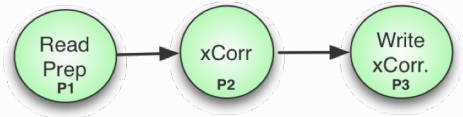
Computing Resources	Terracorrelator	SuperMuc	Amazon EC2	EDIM1
Type	Shared-memory	Cluster	Cloud	Cloud
Enactment Systems	MPI, multi	MPI, multi	MPI, Storm, multi	MPI, Storm, multi
Nodes	1	16	18	14
Cores per Node	32	16	2	4
Total Cores	32	256	36	14
Memory	2TB	32GB	4GB	3GB

dispel4py Performance Evaluations

Data-Intensive Application



dispel4py preproc. (Phase 1)



dispel4py proc. (Phase 2)

1000 stations
Input 150MB
Output 39GB

Both workflows (Phase 1 and Phase 2) executed in the same computing resource and the same mapping.

Mode	Terracorrelator (32 cores/Node)	SuperMuc (256 cores 16 cores/node)	Amazon (36 cores 2 cores/node)	EDIM1 (14 cores 4 cores/node)
MPI	1501.32 (~25minutes)	1093.16 (~**19minutes**)	16862.73 (~5hours)	38656.94 (~11 hours)
multi	1332 .20 (~23minutes)			
Storm			27898.89 (~8 hours)	120077.123 (~33 hours)

Asterism: Easy-to-use system to empower data-driven research

New framework that automatically

manage the entire workflow, monitor its execution

handle data transfers between different platforms

map to different enactment engines at runtime

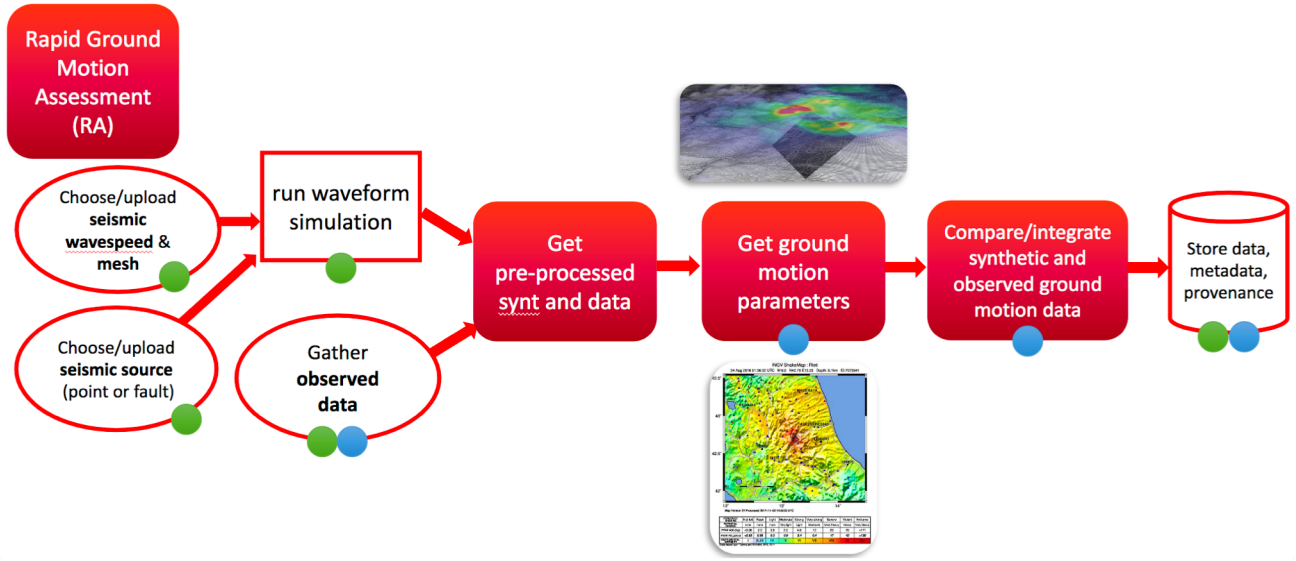
DARE (Delivering Agile Research Excellence on European e-Infrastructures)

Provide scientific communities with tools/frameworks/APIs to allow for data-driven experiments, and rapid prototyping:

Address the requirements of European RIs, initially of EPOS, on Earth science, and IS/ENES2, on climate.

epcc

Rapid Ground Motion Assessment (RA)



Aims:

Model the strong ground motion after large earthquakes

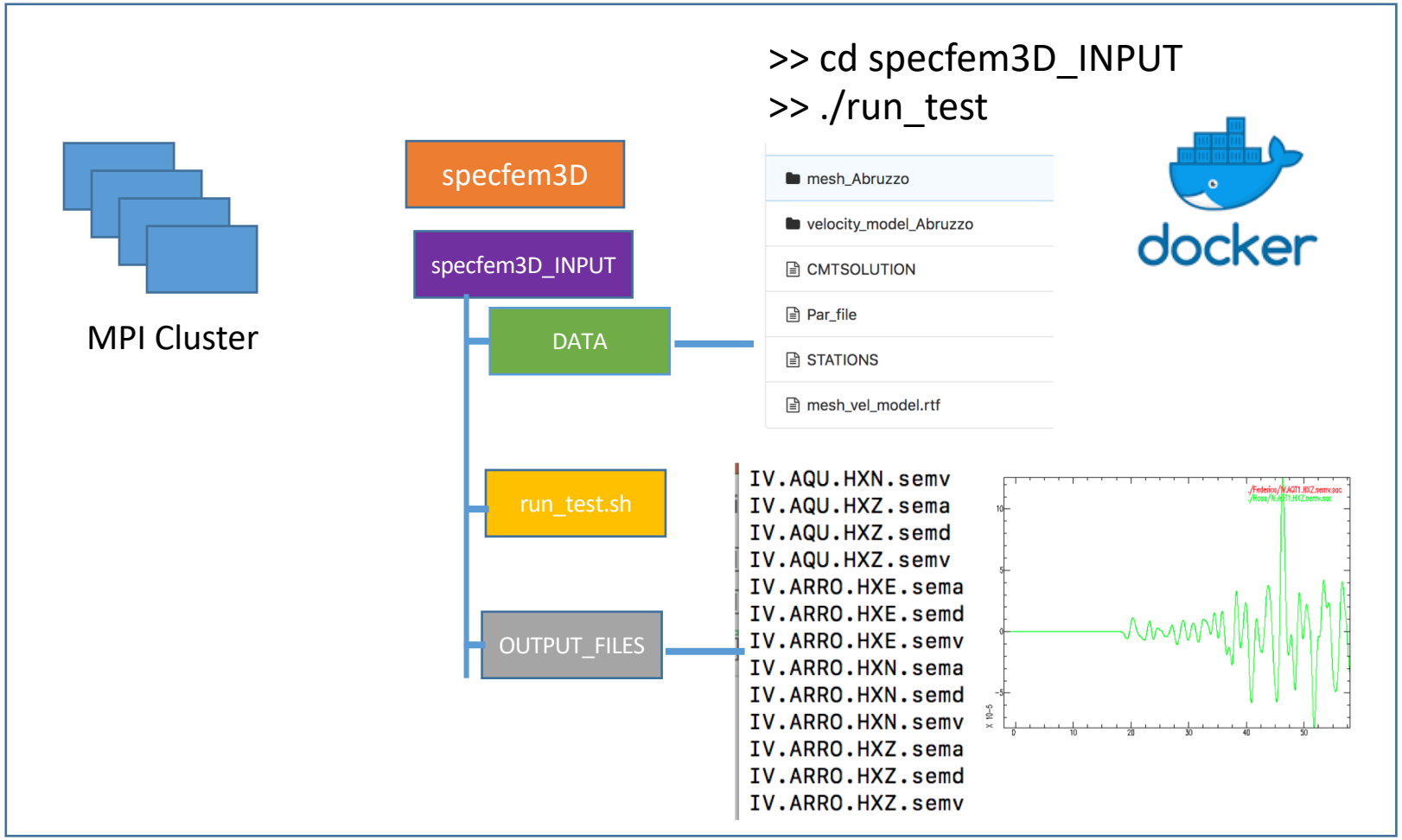
Rapid assessment of earthquakes' impact, and emergency response

Steps:

Build dispel4py workflows to test them locally – using small dataset.

Scale them up:
-Run the workflows using HPC/Cloud
  ** Using dispel4py parallel mappings

Waveform simulation: Specfem3D + MPI cluster



Test Case: RA

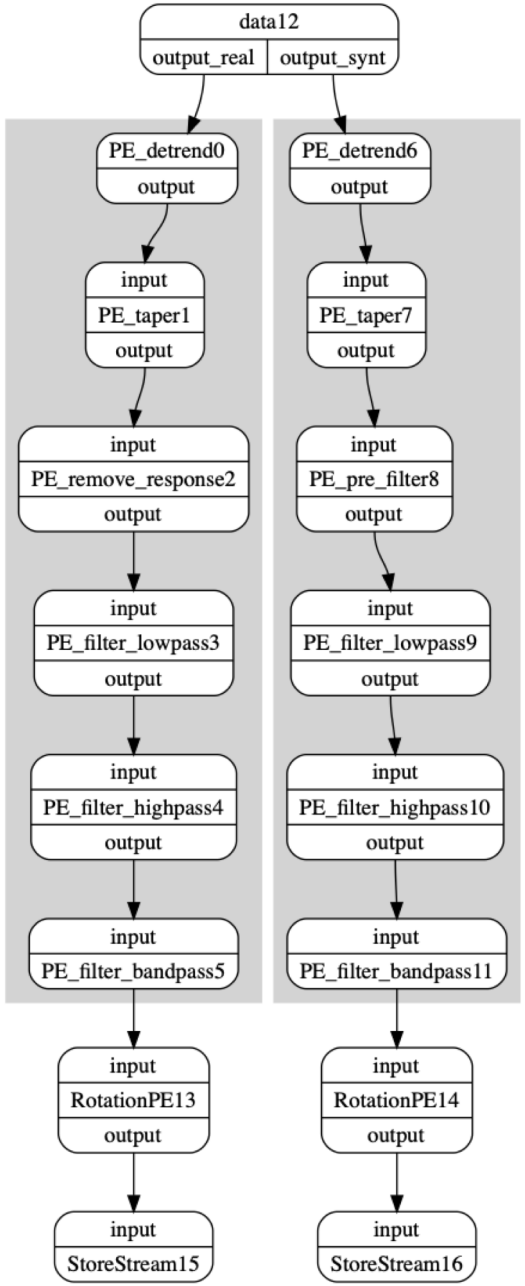
run waveform simulation

- Virtual Machine
  - (Bare-metal Instance)
  - 24 Cores
- Config script to install docker, pip & python.

- Clone the WP6_EPOS gitlab repo
- Docker info: Alpine 3.8, OpenMPI, Specfem3D
- Build the image
- Copy the Specfem3D_INPUT in the container
- Run the docker container

epcc

Get Pre-Preprocessed Synthetic and Data



Test Case: RA

Get pre-processed synt and data

Get Pre-Preprocessed Synthetic and Data

run_preprocess_misfit.sh 175 Bytes

```
#!/bin/bash

export PYTHONPATH=$PYTHONPATH
export MISFIT_PREP_CONFIG="pr
echo $MISFIT_PREP_CONFIG
dispel4py simple create_misfi

```

misfit_input.jsn 848 Bytes — Edit | Web IDE

```
{
    "data": [
        {
            "input": {
                "data_dir": "/Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/misfit_data/data",
                "synt_dir": "/Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/misfit_data/synth",
                "events": "/Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/misfit_data/events_simulation_CI_CI_test_0_1507128030823",
                "event_id": "smi:webservices.ingv.it/fdsnws/event/1/query?eventId=1744261",
                "stations_dir": "/Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/misfit_data/stations",
                "output_dir" : "/Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/misfit_data/output",
                "network": [
                    "IV"
                ],
                "station": [
                    "ARRO"
                ]
            }
        }
    ]
}
```

data

- IV.ARRO..EHE.mseed
- IV.ARRO..EHN.mseed
- IV.ARRO..EHZ.mseed

synth

- IV.ARRO.HXE.sema
- IV.ARRO.HXE.semd
- IV.ARRO.HXE.semv
- IV.ARRO.HXN.sema
- IV.ARRO.HXN.semd
- IV.ARRO.HXN.semv
- IV.ARRO.HXZ.sema
- IV.ARRO.HXZ.semd
- IV.ARRO.HXZ.semv

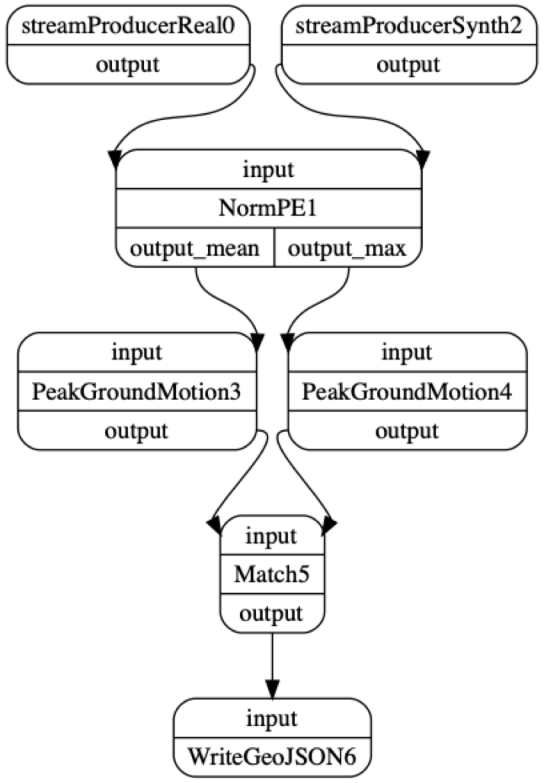
Note: Those are the synth seismograms generated in the previous step (slide)

output

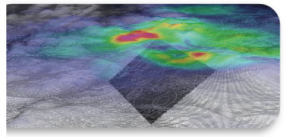
- IV.ARRO.HXZ.synth
- IV.ARRO.HXR.synth
- IV.ARRO.HXT.synth
- IV.ARRO.EHZ.data
- IV.ARRO.EHR.data
- IV.ARRO.EHT.data

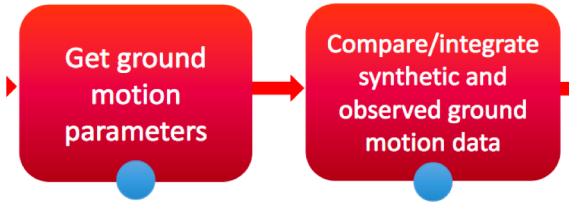
Pre-preprocessed synthetic and observed data
(Underline files are used in the next step (slide))

Get and Compare Ground Motion Parameters



Test Case: RA





Get and Compare Ground Motion Parameters

run_RA.sh 210 Bytes

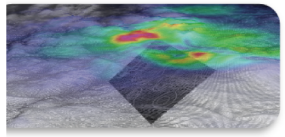
Lock | Edit | Web IDE | Replace | Delete

```
1 dispel4py simple dispel4py_RA.pgm_story.py -d '{"streamProducerReal": [ {"input": "./misfit_data/output/IV.ARRO.EHR.data"} ], "streamProducerSynth":
```

output

```
ARRO_max.json    ARRO_mean.json
```

Test Case: RA



Get ground motion parameters → Compare/integrate synthetic and observed ground motion data

Get and Compare Ground Motion Parameters

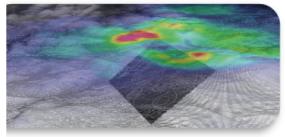
output


```
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:                0.00003889272805005096
    PGV:                0.00011736045694475592
    PGA:                0.0003549366539822615 5
    p_norm:             "max"
    PSA_0.3Hz:          0.0003942182089108563
    PSA_1.0Hz:          0.0007176179285863899
    PSA_3.0Hz:          0.0003707452407479844
  difference:
    PGD:                -0.00000830957268584994 6
    PGV:                0.00003651316895170355
    PGA:                0.0004486364987864541
    PSA_0.3Hz:          -0.0002223374318992273
    PSA_1.0Hz:          0.0012964651798472158
    PSA_3.0Hz:          0.000610498457992085 9
  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:                0.00003889272805005096
    PGV:                0.00011736045694475592
    PGA:                0.0003549366539822615 5
    p_norm:             "mean"
    PSA_0.3Hz:          0.0003942182089108563
    PSA_1.0Hz:          0.0007176179285863899
    PSA_3.0Hz:          0.0003707452407479844
  difference:
    PGD:                -0.00000830957268584994 6
    PGV:                0.00003651316895170355
    PGA:                0.0004486364987864541
    PSA_0.3Hz:          -0.0002223374318992273
    PSA_1.0Hz:          0.0012964651798472158
    PSA_3.0Hz:          0.000610498457992085 9
  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:        []
```

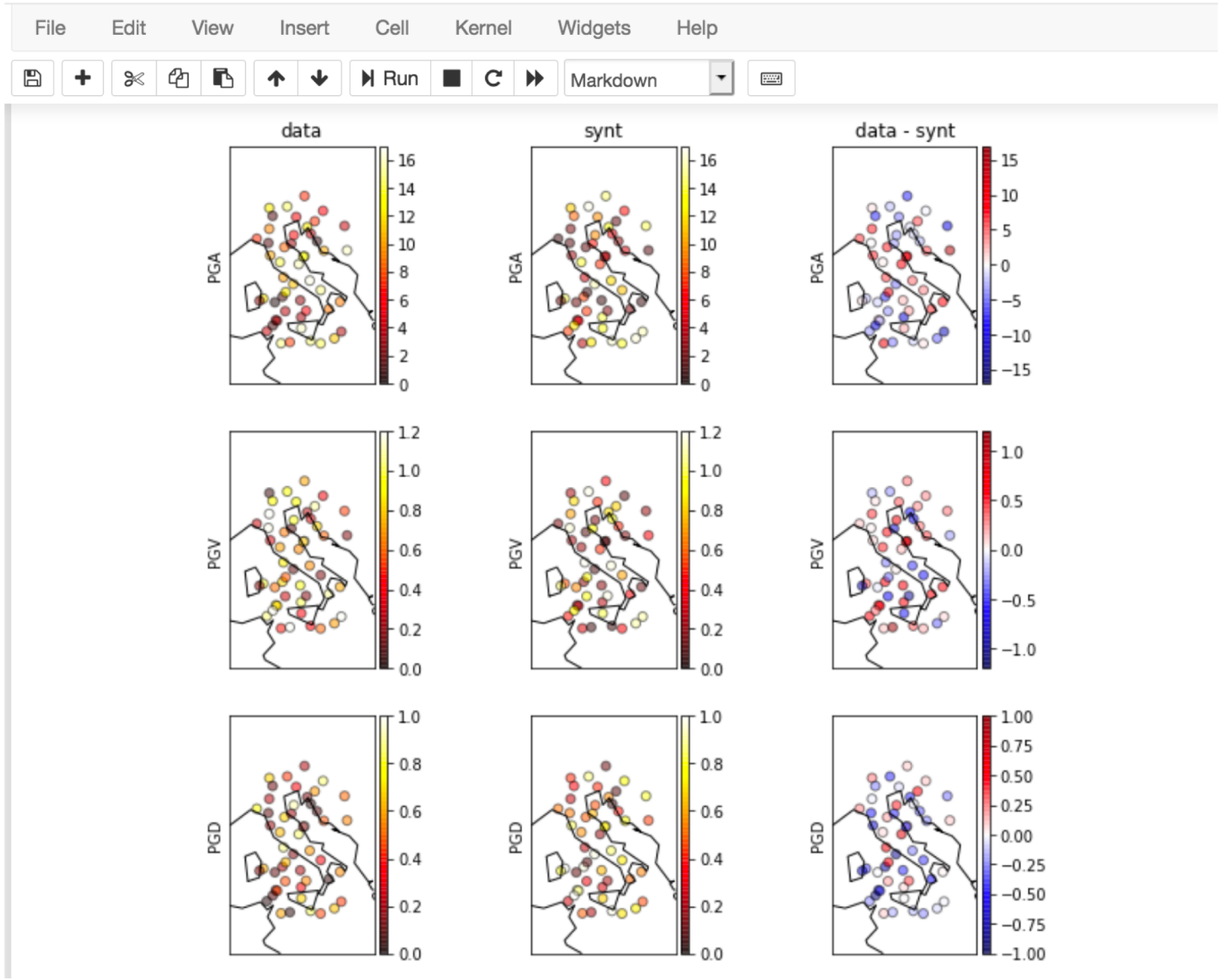

Test Case: RA



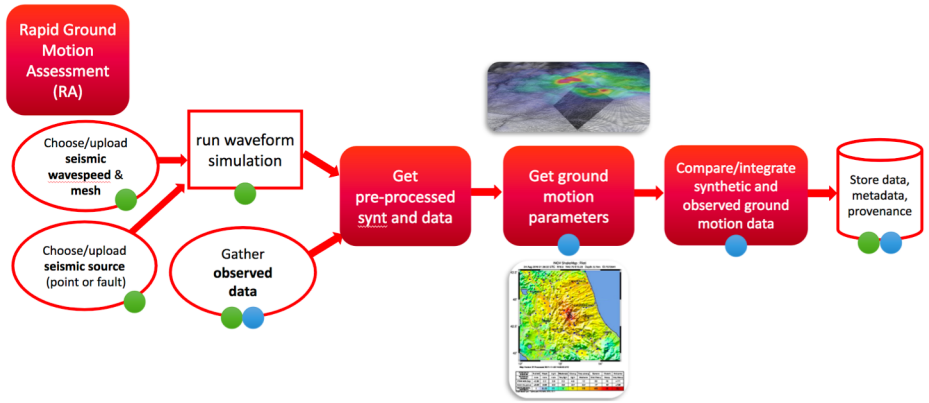
Get ground motion parameters

Compare/integrate synthetic and observed ground motion data

RA Maps


File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Run
Markdown
data
synt
data - synt
PGA
PGV
PGD

Rapid Ground Motion Assessment (RA)

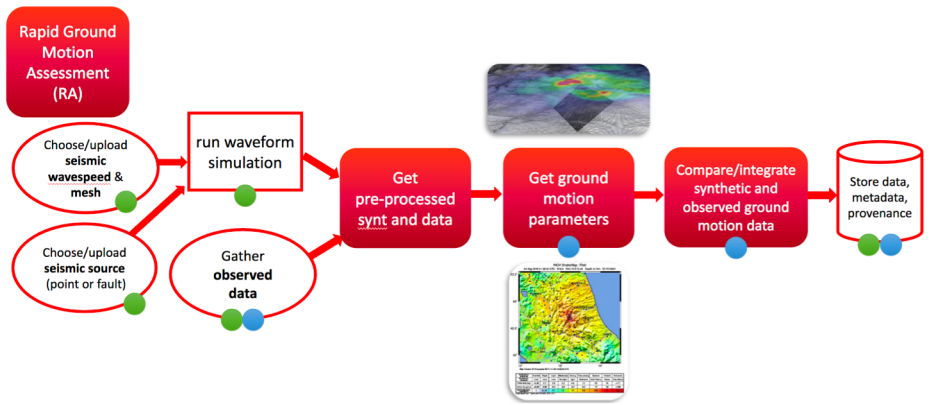


dispel4py + COMMON WORKFLOW LANGUAGE → semantics and description

CWL is a specification for describing the
data and execution model of workflows/command tools

Provides a consistent way to connect programs

Rapid Ground Motion Assessment (RA)



dispel4py + COMMON WORKFLOW LANGUAGE → semantics and description

CWL is a specification for describing the
data and execution model of workflows/command tools

Provides a consistent way to connect programs

dispel4py-RA-pgm_story-job.yml 372 Bytes

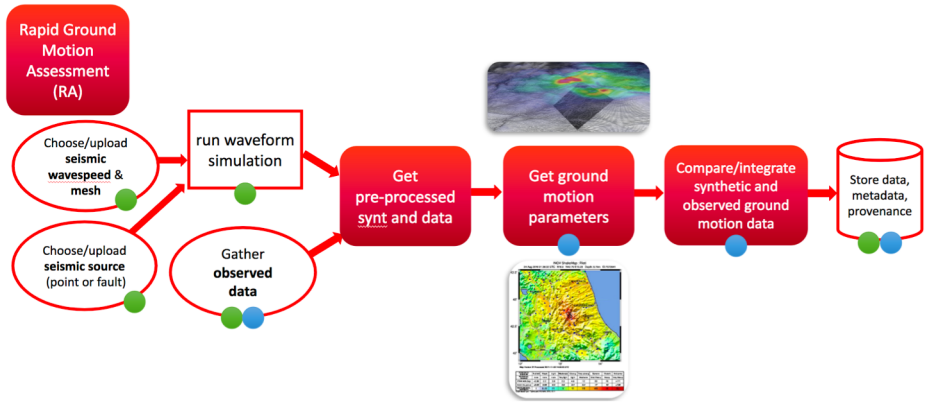
```yaml
script:
  class: File
  path: /Users/rosafilgueira/EPCC/DARE/WP6/test/MISFIT_RA/dispel4py_RA.pgm_story.py


input: '{"streamProducerReal": [ {"input": "/Users/rosafilgueira/EPCC/DARE/WP6/test/MI
```

dispel4py-RA-pgm_story.cwl 437 Bytes

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

cwlVersion: v1.0
class: CommandLineTool
baseCommand: [dispel4py, simple]
requirements:
  EnvVarRequirement:
    envDef:
      PYTHONPATH: $(inputs.script.dirname)

inputs:
- id: script
  type: File
  inputBinding:
    position: 1
- id: input
  type: string
  inputBinding:
    prefix: -d
    position: 2

outputs:
  output:
    type:
      type: array
      items: File
    outputBinding:
      glob: "*.json"
```

```
cwl-runner dispel4py-RA-pgm_story.cwl dispel4py-RA-pgm_story-job.yml
```

Rapid Ground Motion Assessment (RA)



Future development:

Optimization of workflows → dynamic deployment
→ mapping selection

Once tested all the workflows locally (seq. map),
They can be scaled up automatically → Next step.

Provenance data is also collected in runtime (optional)

Metadata, Input and Output files --> registry/catalog

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

Dr. Rosa Filgueira, University of Edinburgh, EPCC

Extra Slides

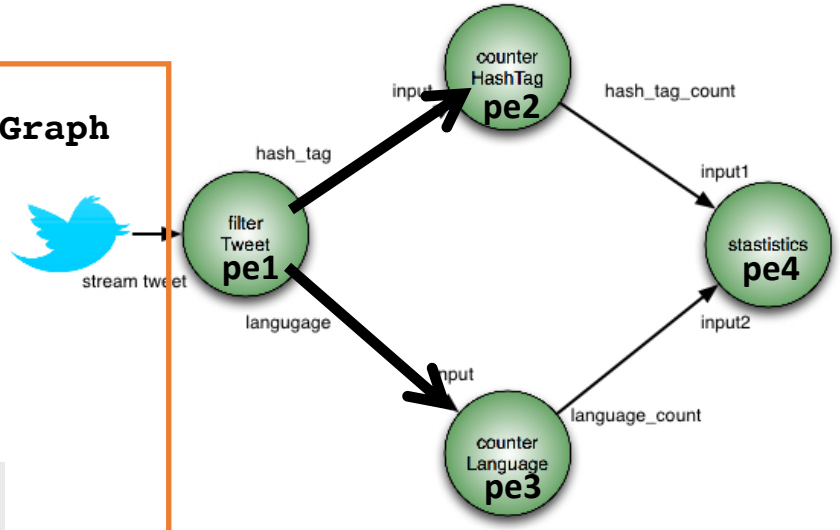
dispel4py parallel stream-based dataflow system

```
from dispel4py.workflow_graph import WorkflowGraph


pe1 = filterTweet ()
pe2 = counterHashTag ()
pe3 = counterLanguage ()
pe4 = statistics ()

graph = WorkflowGraph ( )

graph.connect(pe1,'hash_tag',pe2,'input')
graph.connect(pe1,'language',pe3,'input')
graph.connect(pe2,'hash_tag_count',pe4,'input1')
graph.connect(pe3,'language_count',pe4,'input2')
```

PEs objects

Graph

Connections



Users only have to implement:

- PEs
- Connections

https://github.com/dispel4py/dispel4py

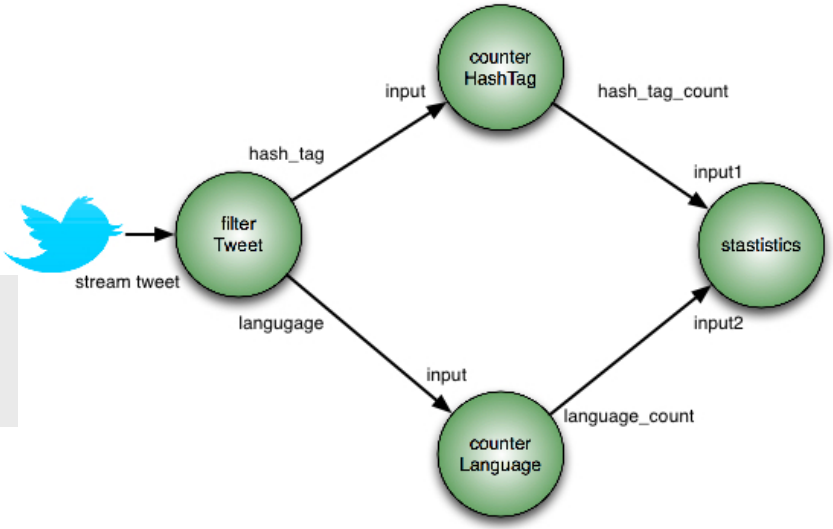
dispelp4y basic concepts– Example of a PE

```
Class filterTweet(GenericPE):
def __init__( self ):
    GenericPE.init (self)
    self.add_output('hash_tags ')
    self.add_output('language')

def process ( self , inputs ):
        twitterDataFile= inputs['input ']
        tweet file = open(twitterDataFile)
        for line in tweet file :
        tweet = json.loads( line )
                language = ' '
                hashtags =[]
                language = tweet[u'lang '].encode('utf -8')
                text = tweet[u'text '].encode('utf-8')
            hashtags=re.findall(r"#(\w+)", text)

                self.write('hash tag', hashtags)
                self.write('language', language)
```

Inputs & outputs

Logic of PE

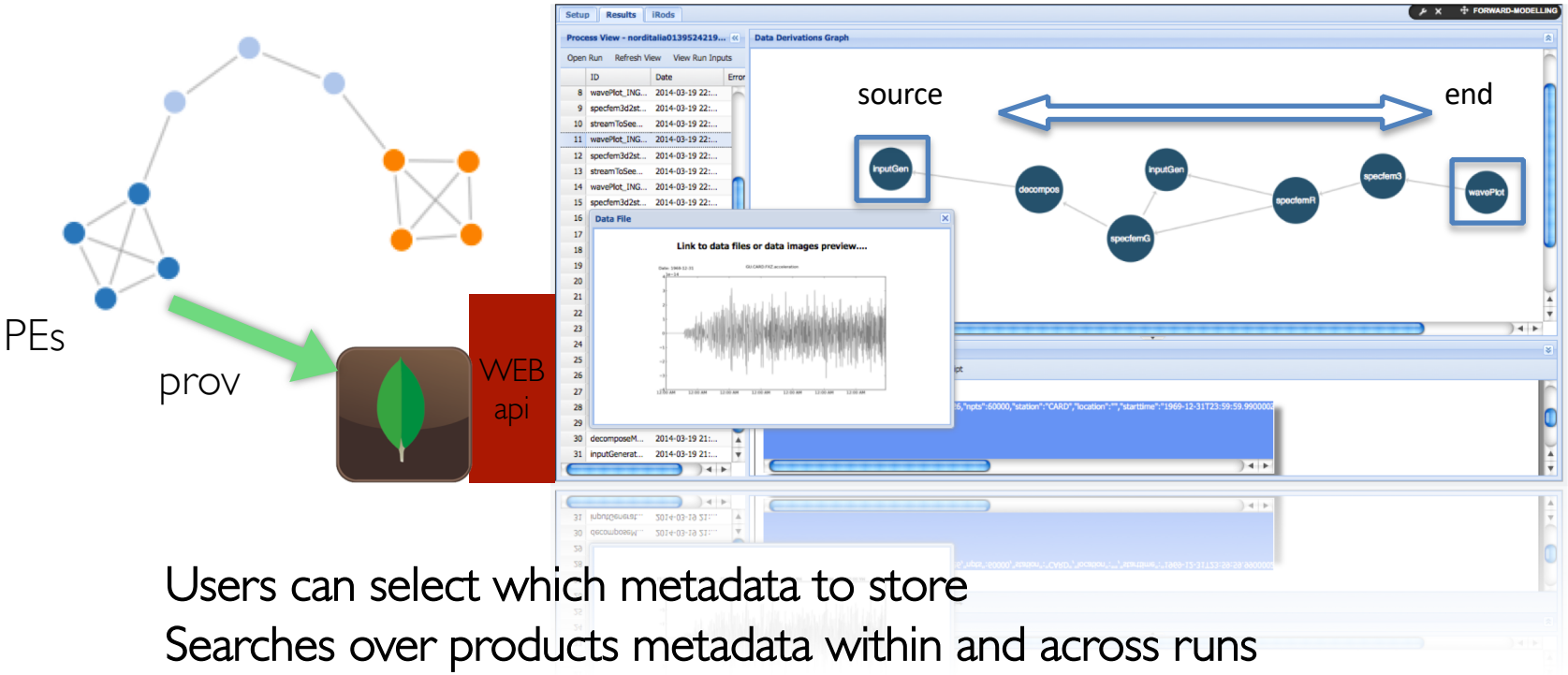
Stream out data



Users only have to implement:

- PEs
- Connections

dispel4py advance concepts – Provenance



Users can select which metadata to store
Searches over products metadata within and across runs
Data download and preview
Capturing of Errors for Diagnostic purposes
Data Fabric: Multi directional navigations across data dependencies
W3C PROV-DM as reference model.