Developing a convincing story for DARE future

DARE: sustained power from abstraction and mapping

at
Creating platform-driven eInfrastructure innovation on EOSC

NCSR Demokritos campus

Malcolm Atkinson, University of Edinburgh

10 July 2019

Outline

- Vision and Goals
- Key insights
- Architecture
- Achievements and Work in Progress

Vision

Vision

- Growth unlimited and sustained
  - Data
  - Computation
  - Complexity

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  - Computation
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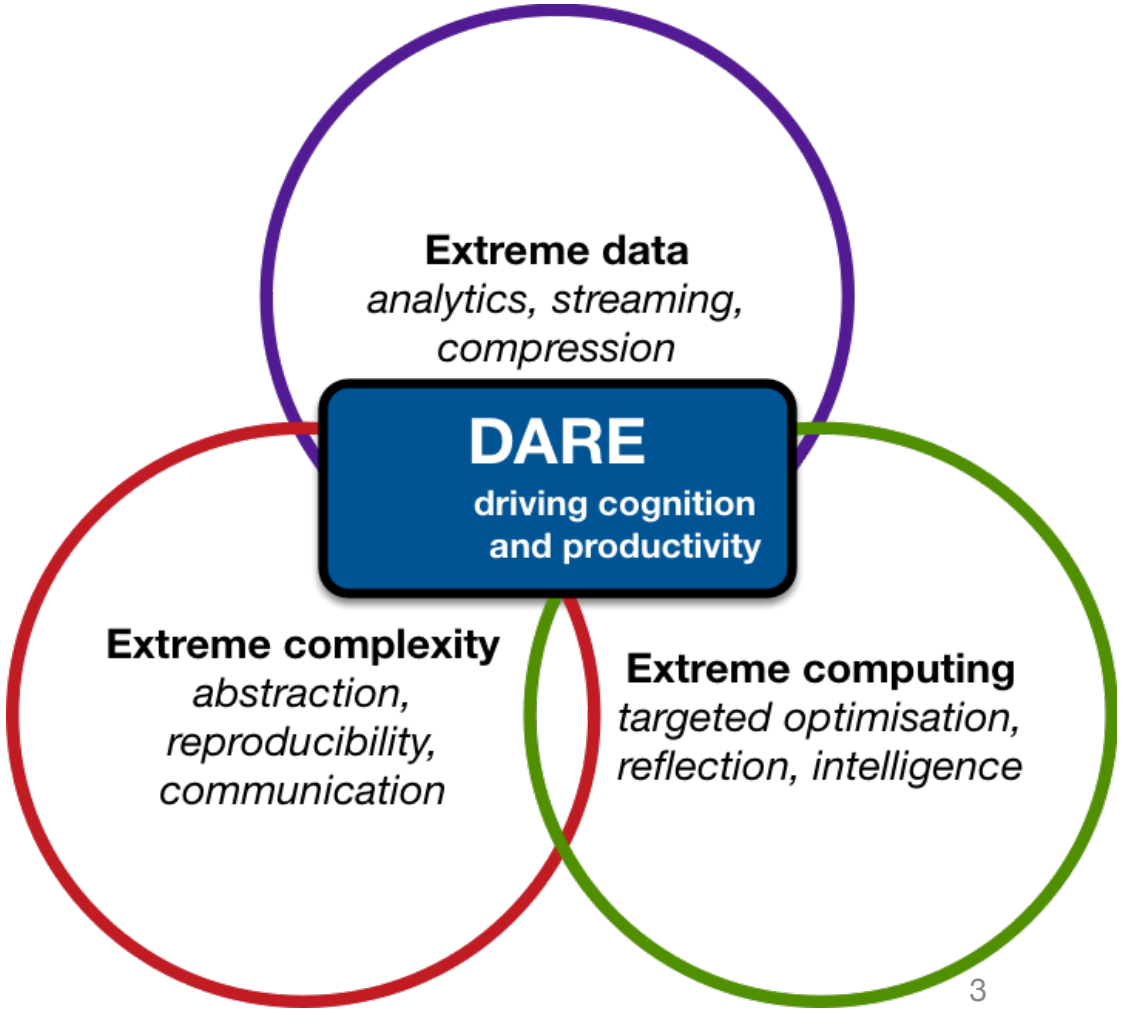
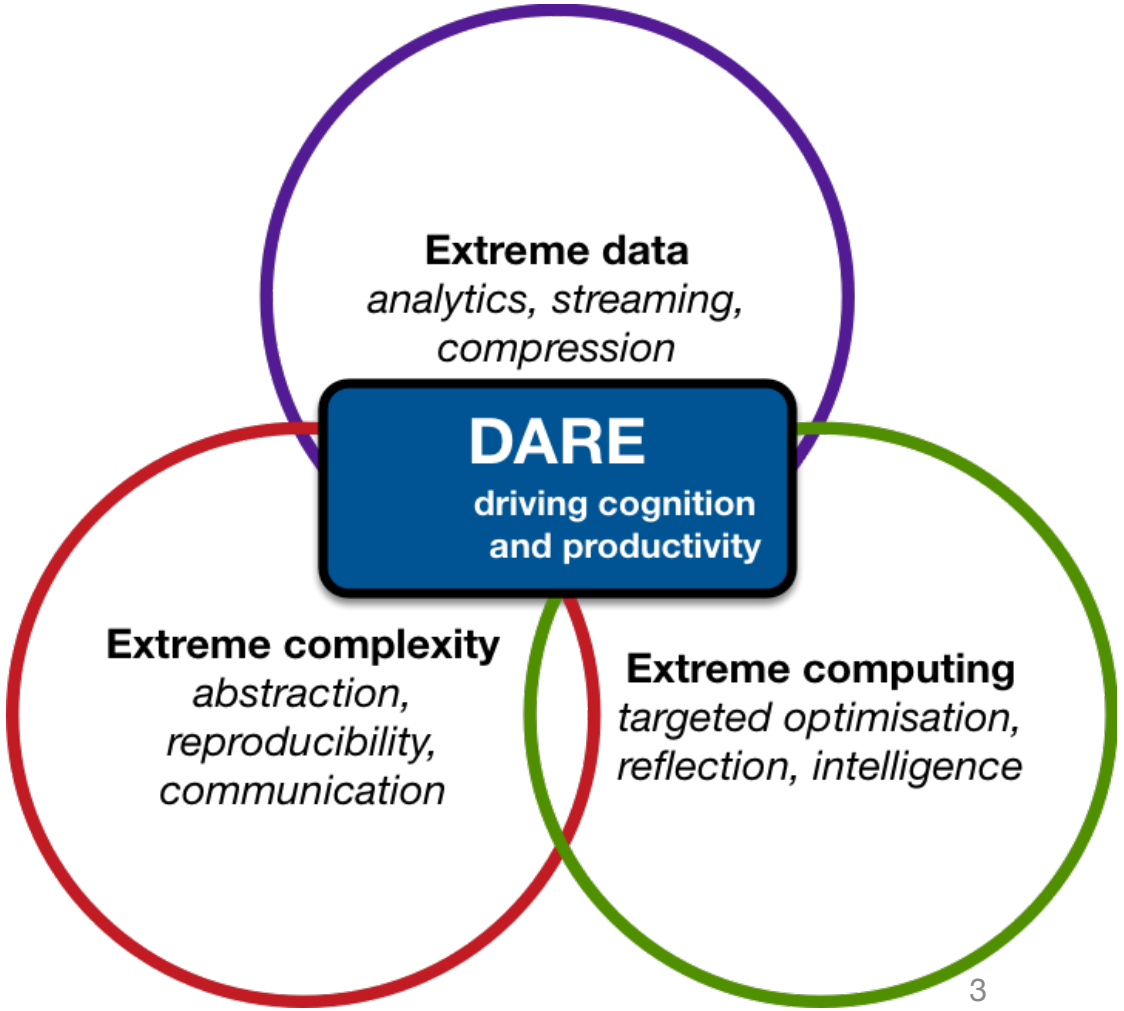
- Challenges demanding and urgent



Vision

- Growth unlimited and sustained
  - Data
  - Computation
  - Complexity
- Challenges demanding and urgent
- Conserving scarce resources
  - Human intellectual effort
  - Willingness to collaborate
  - Energy / GHG emissions



Science and collaborations

"Black Hole Image Makes History; NASA Telescopes Coordinated Observations"

A black hole and its shadow have been captured in an image for the first time, a historic feat by an international network of radio telescopes called the Event Horizon Telescope.

"Collaboration is the key to cancer research"

To fight the disease effectively, researchers from across the scientific spectrum and beyond must join forces.

nature International journal of science 2018, Neal Savage

"Science is powerful"

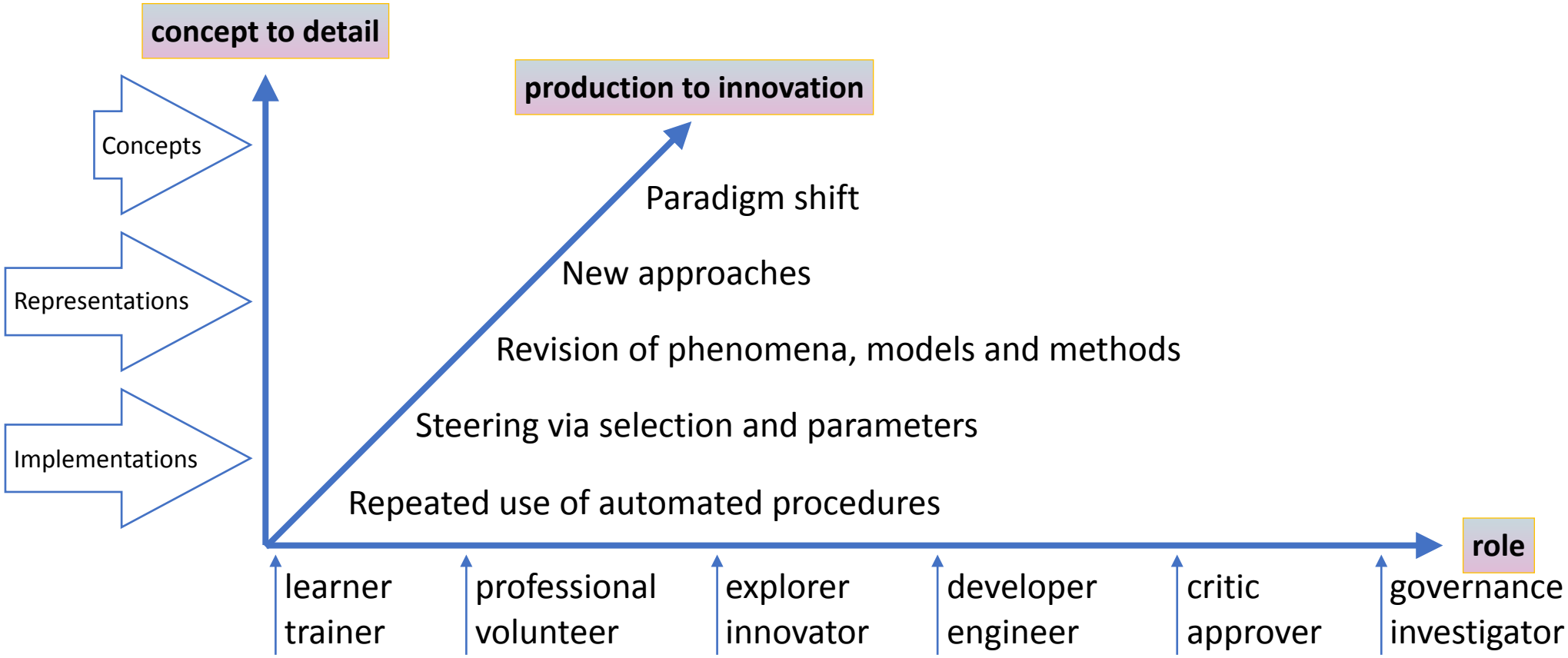
TOGETHER SCIENCE CAN

Science can solve some of the world's most complex problems, but only when the best ideas are brought together.

#TogetherScienceCan

Acknowledge Luca Trani, KNMI & EPOS

Respond to community complexity



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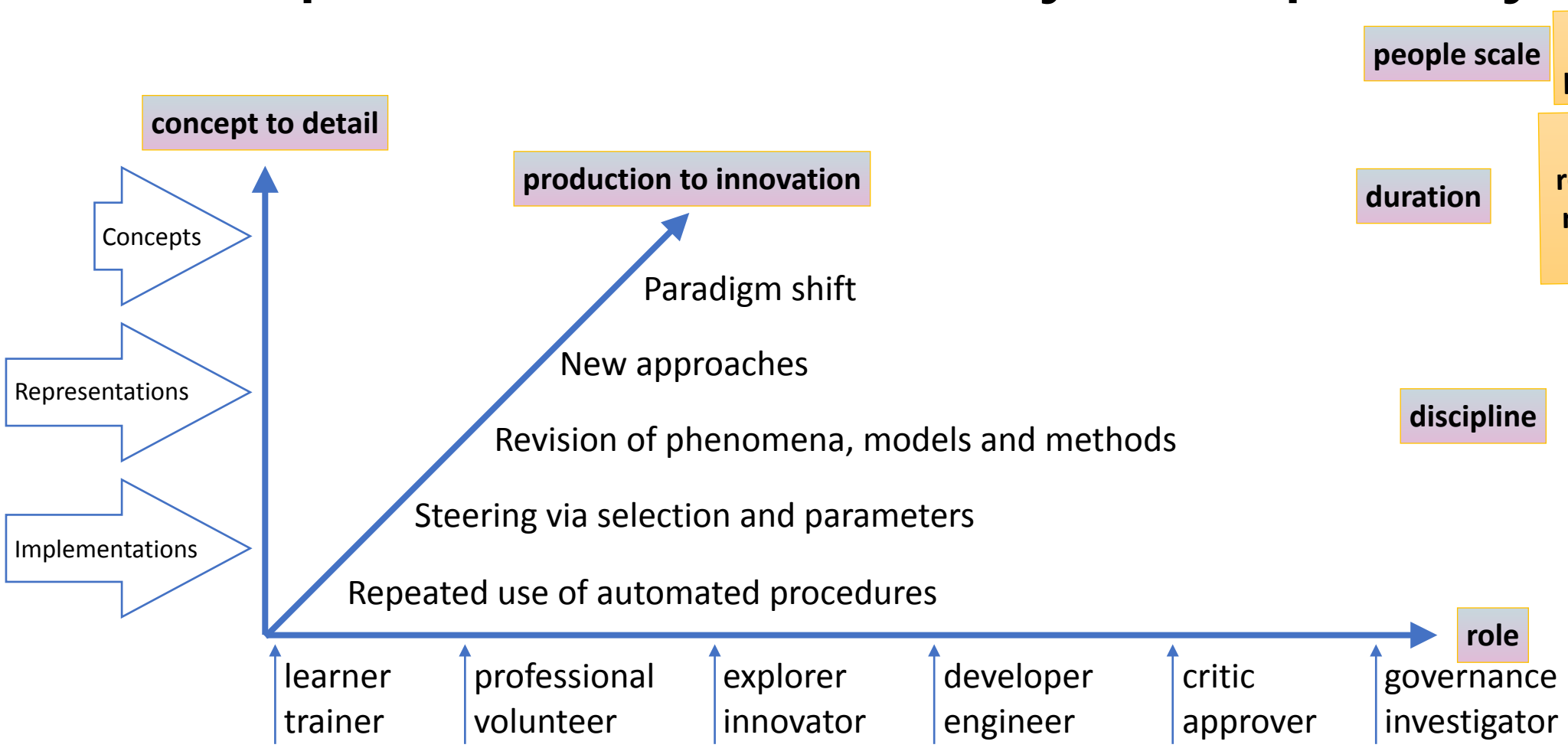


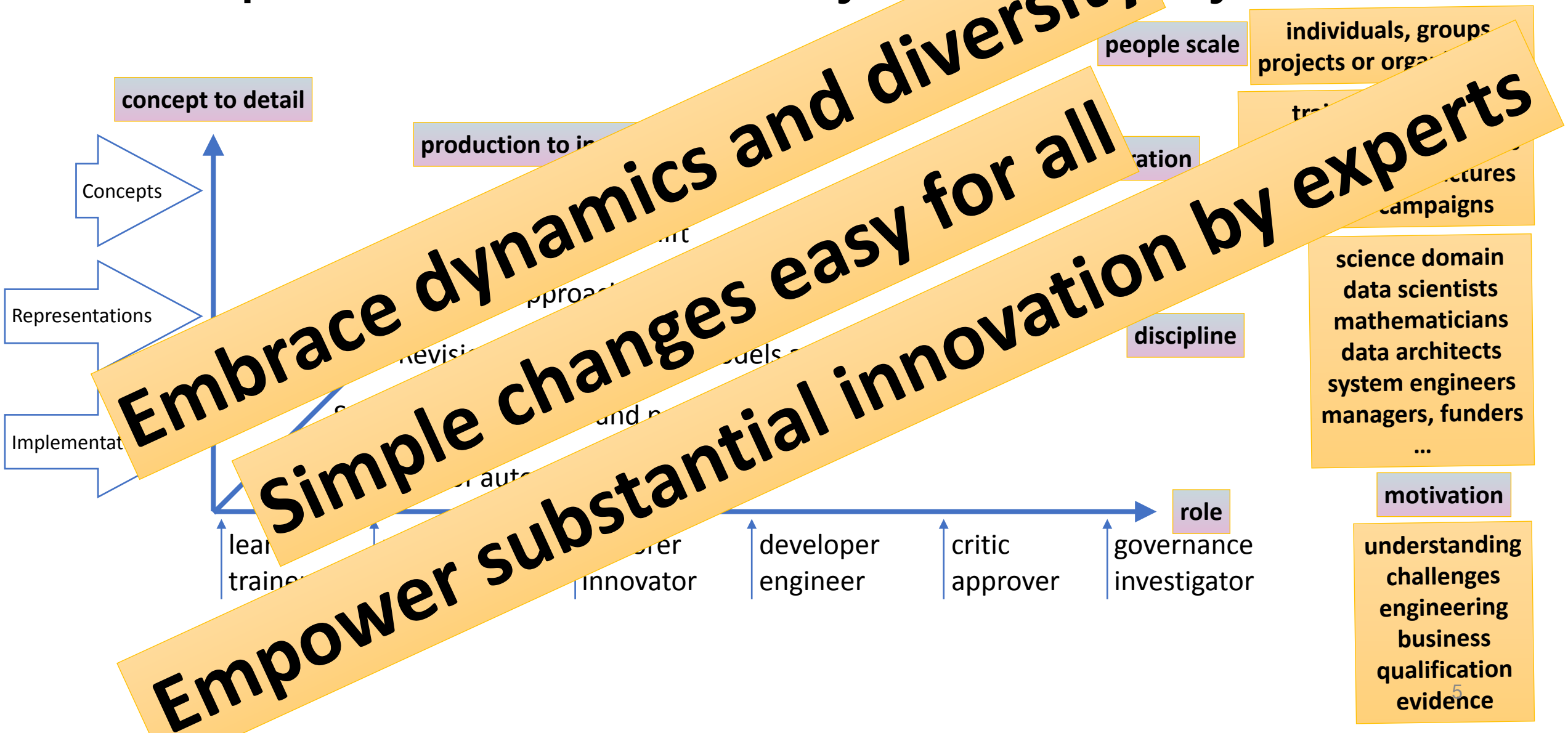
people scale — **individuals, groups, projects or organisations**

duration — **training sessions, real-time, PhDs, projects research infrastructures research campaigns**

discipline — **science domain data scientists mathematicians data architects system engineers managers, funders …**

motivation — **understanding challenges engineering business qualification evidence**

Respond to community co kity

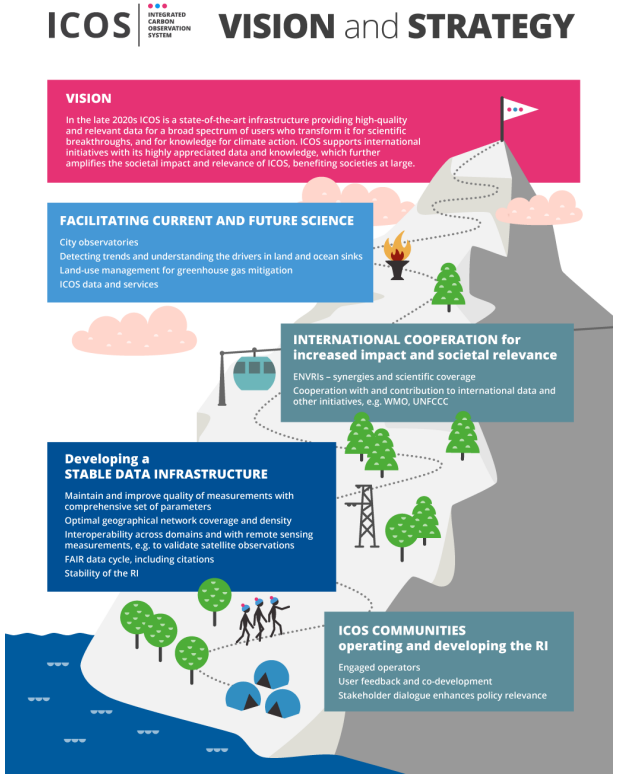


Embrace dynamics and diversity

Simple changes easy for all

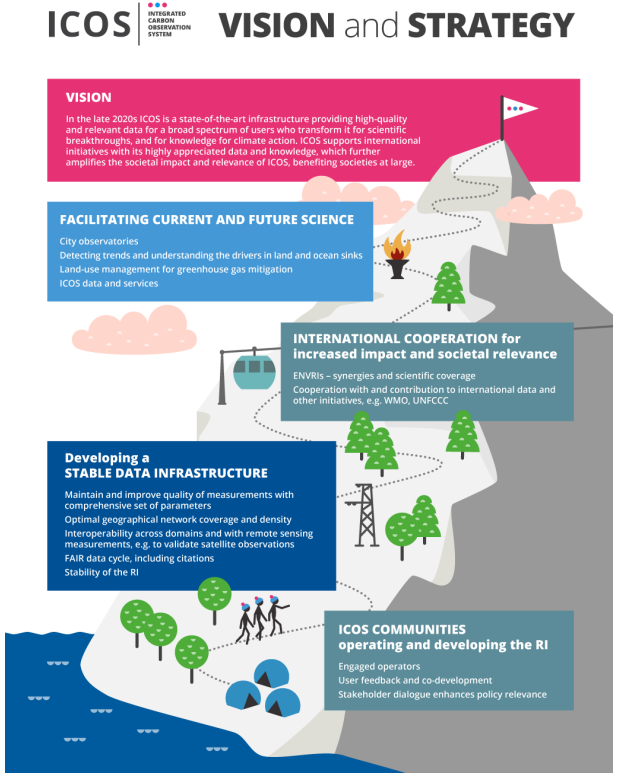
Empower substantial innovation by experts

Deliver benefits Avoid disruption Be adopted



Deliver benefits Avoid disruption Be adopted

- Deliver stability
  - established practices unchanged
  - refined methods unchanged
  - negotiated agreements unchanged



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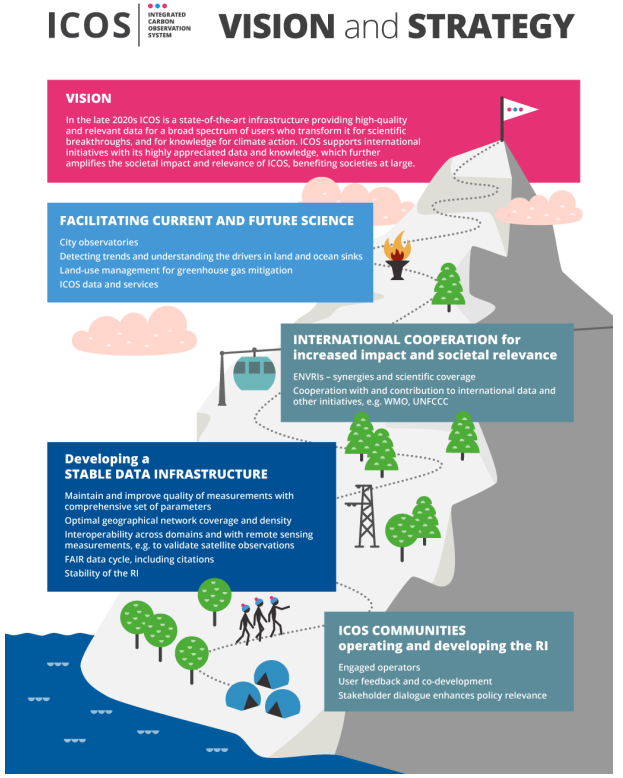

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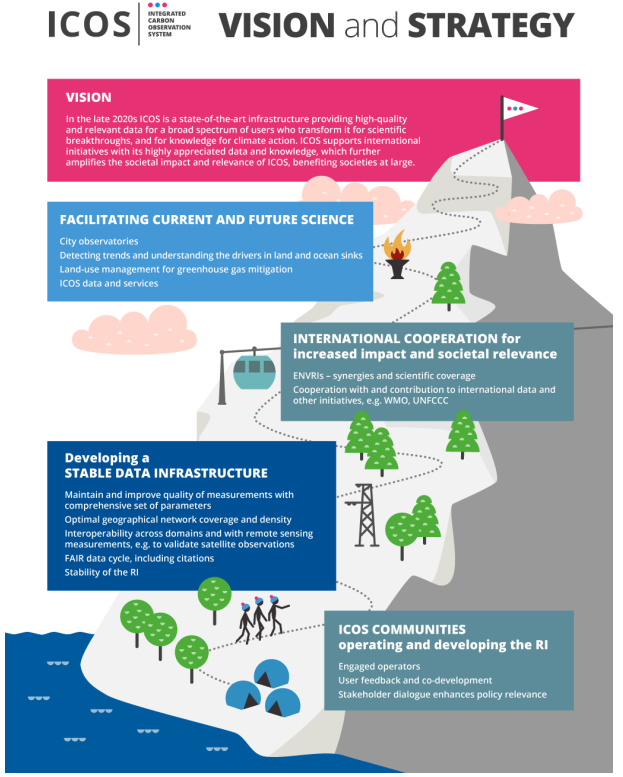
- Improved productivity



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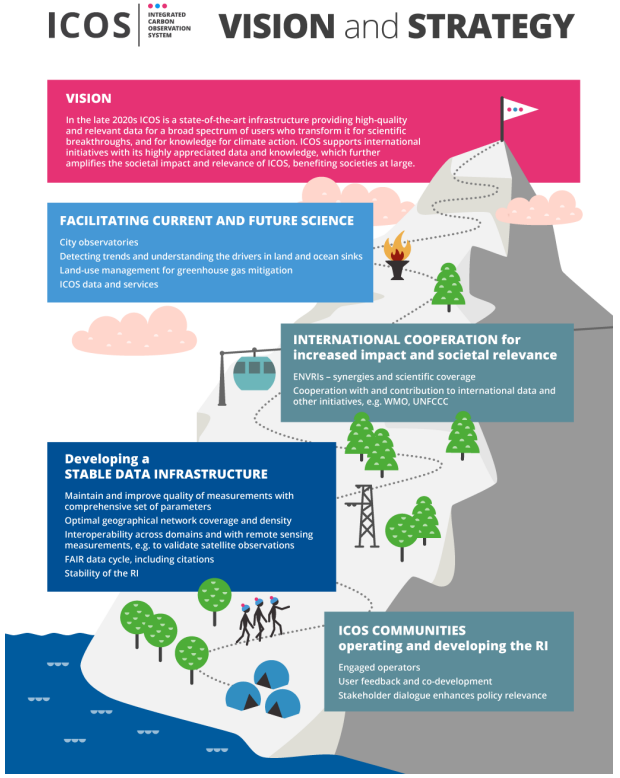
- New capabilities
- Improved productivity
- Agile response to new challenges and opportunities



Deliver benefits Avoid disruption Be adopted

- Deliver stability
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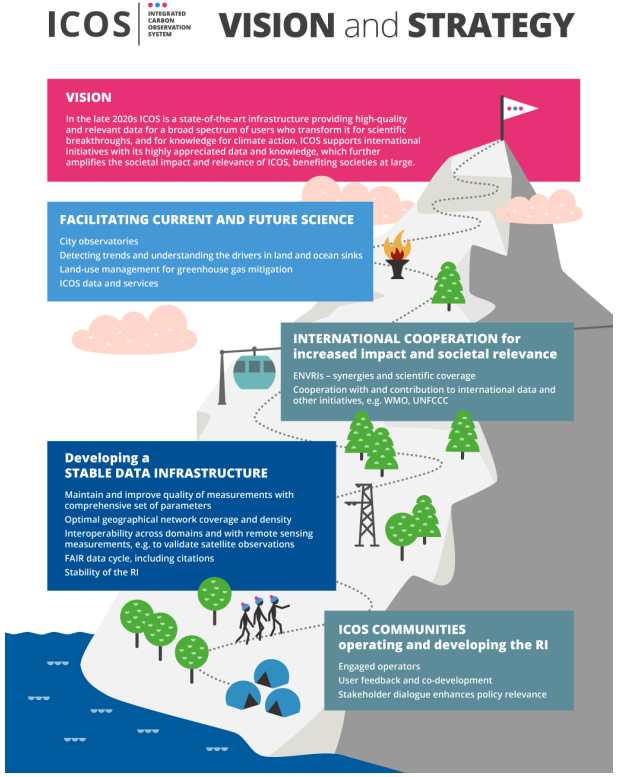
- New capabilities
- Improved productivity
- Agile response to new challenges and opportunities
- Riding the technology wave



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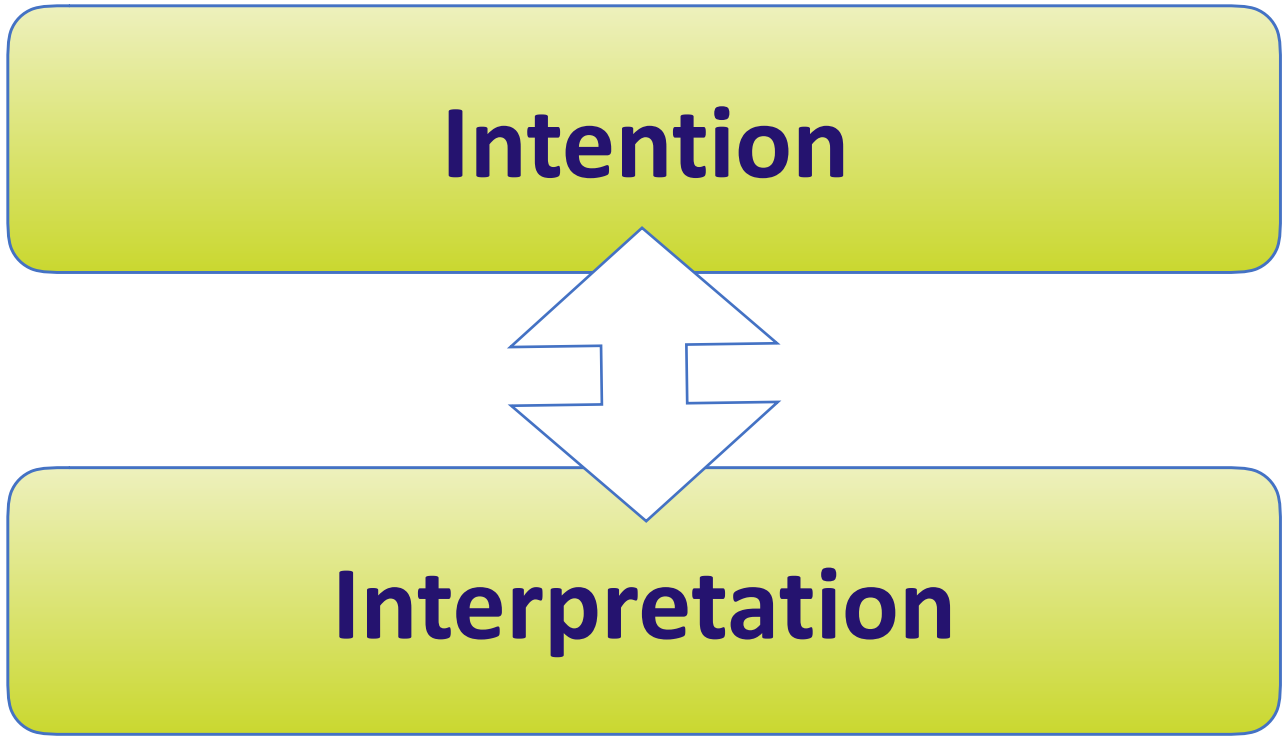
Intention

Intention

refined precise
honoured persistently
domain focused
shaped by campaigns



refined precise
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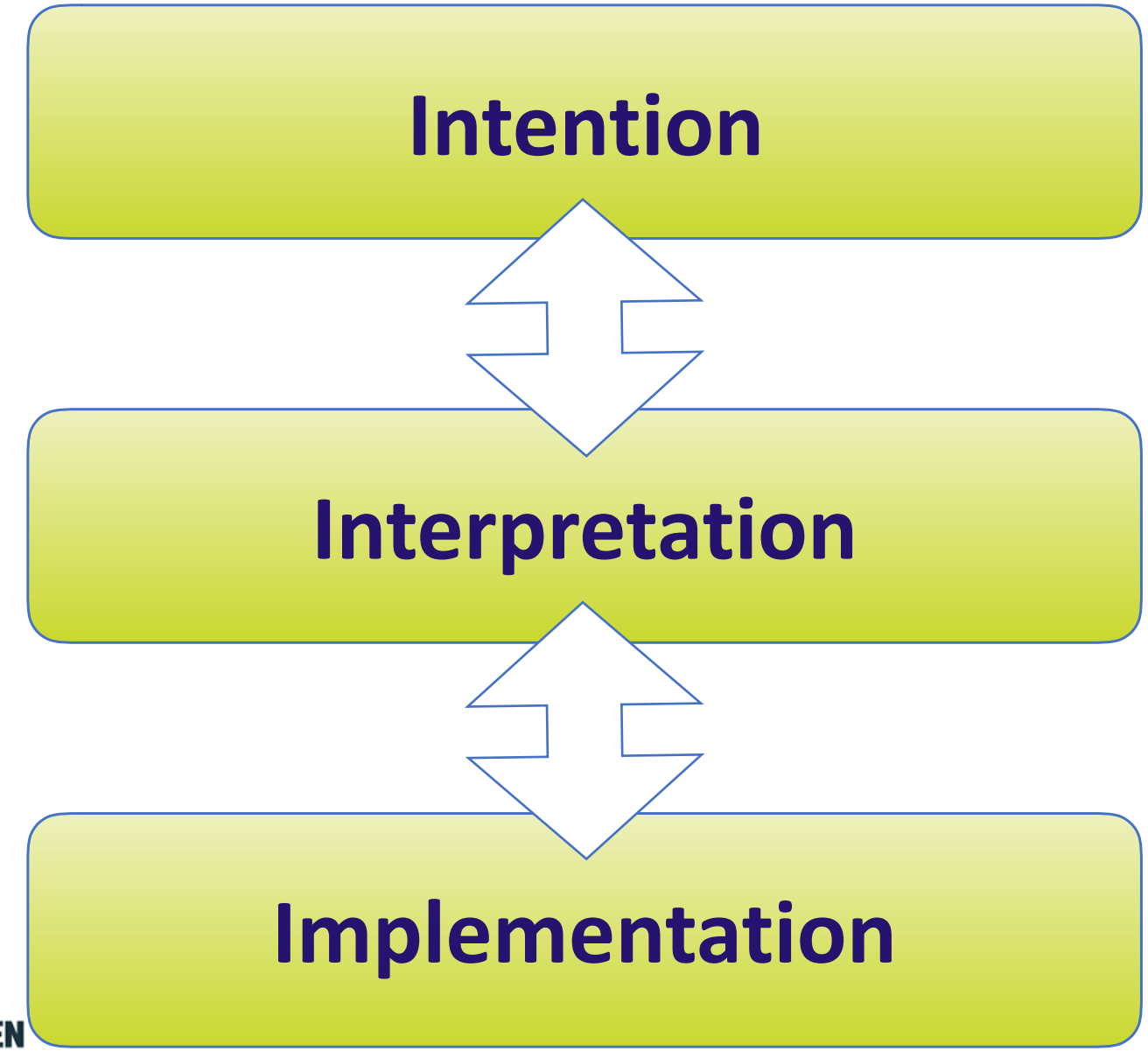
maintain intention
need scope to
optimally exploit
evolving technology

I³

DARE

Incentive



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data architecture
workflow optimisation
systems engineering
resource management
technology innovation

EUROPEAN OPEN SCIENCE CLOUD

L. Schubert and K. G. Jeffery, *New Software Engineering requirements in Clouds and large-scale systems*, IEEE Cloud Computing 2 (1) 48–58, 2015.

Outline

- ~~Vision and Goals~~
- Key insights
- Architecture
- Achievements and Work in Progress

CMDC quartet plays well

- **Concepts**
  - what a communication is about
  - precise terminology
  - precise properties
  - precise relationships
- Representations
  - how they are communicated
- Populations
  - the instances in play

Concept

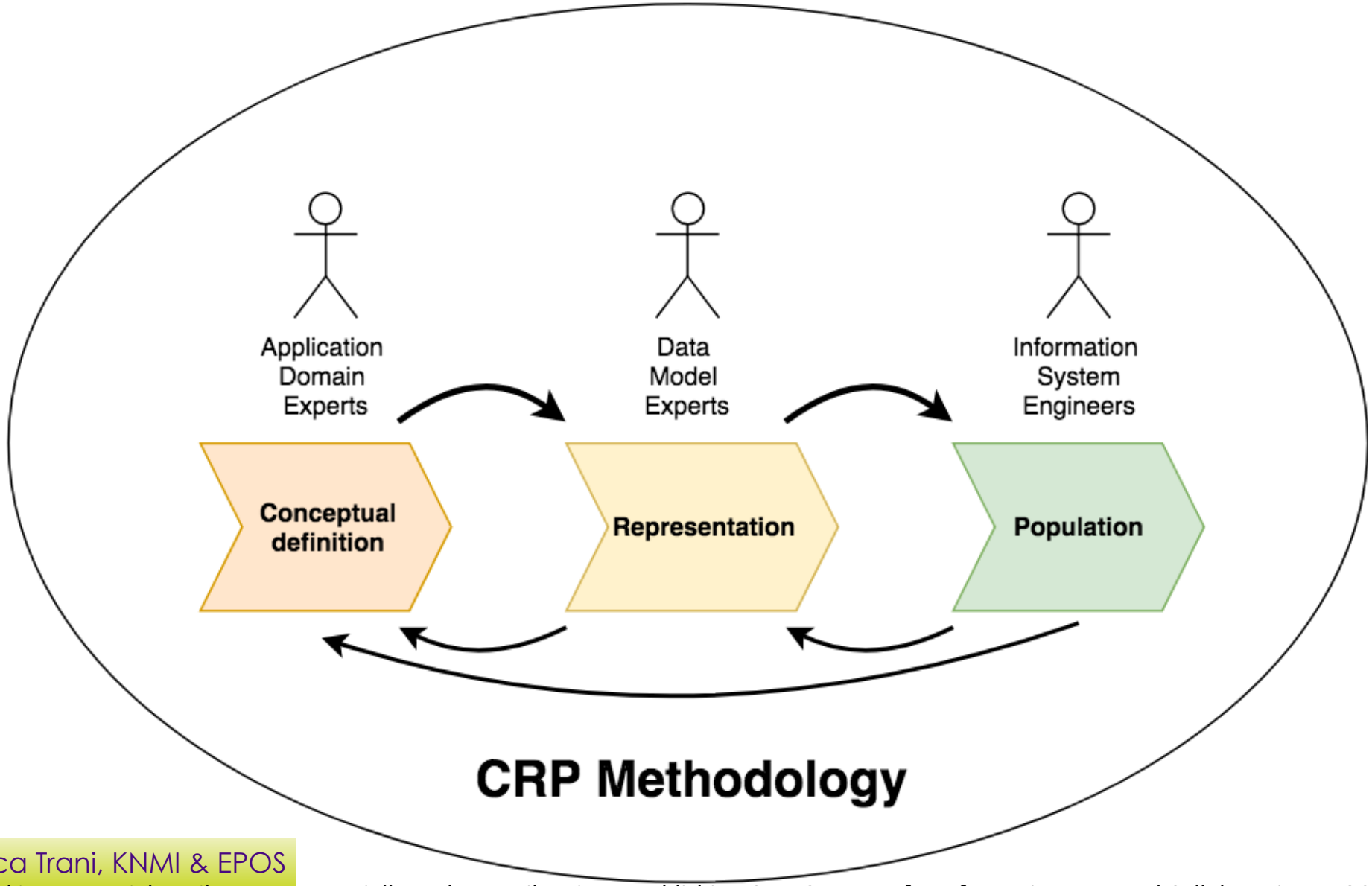
Person

Location

Depth

EQEvent

Clarifying the concepts in use



Acknowledge Luca Trani, KNMI & EPOS

Luca Trani, Malcolm Atkinson, Daniele Bailo, Rossana Paciello and Rosa Filgueira, *Establishing Core Concepts for Information-Powered Collaborations*, FGCS vol. 89, 421-437, 2018.

CMDC quartet plays well

- **Methods**
  - purpose and processes
  - conceptual inputs
  - controls, parameters and active provenance
  - conceptual results delivered
- Notations
  - creation and refinement
  - avoid distracting detail and lock-ins
  - workflows as requests for action
- Workloads
  - testing & validation
  - steered production
  - automated routine

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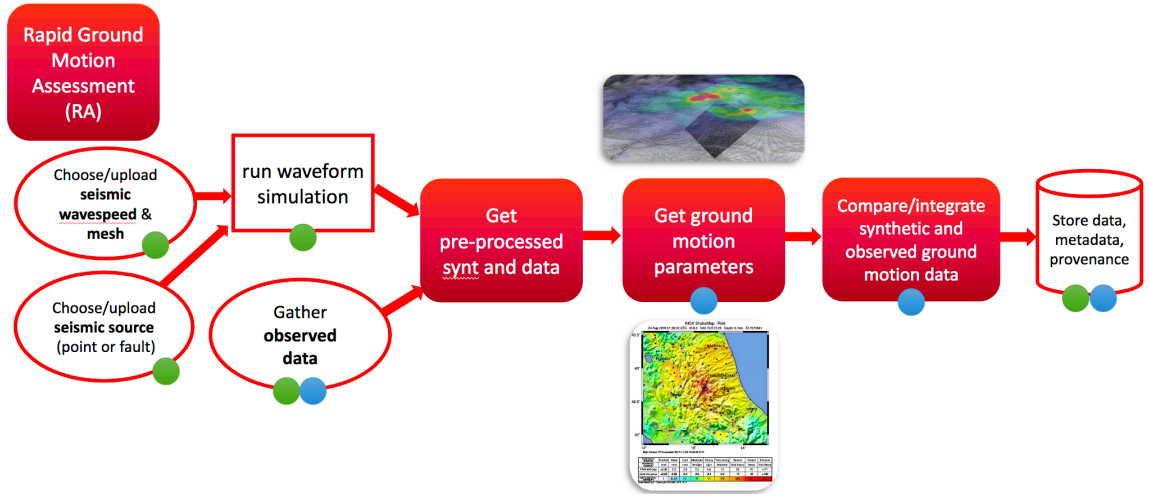

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Virtualisation for capabilities and cost saving

Immediate local action for testing

CMDC quartet plays well

- **Data**
  - primary, intermediate, evidential
  - from human input, instruments, observations, simulations and analyses
  - often standardised imperfectly
  - every possible diversity
- Organisation and structure
  - data models, metadata, storage systems, databases, document, latent
  - optimised encodings
- Populations
  - many, many instances growing in diversity, number and size

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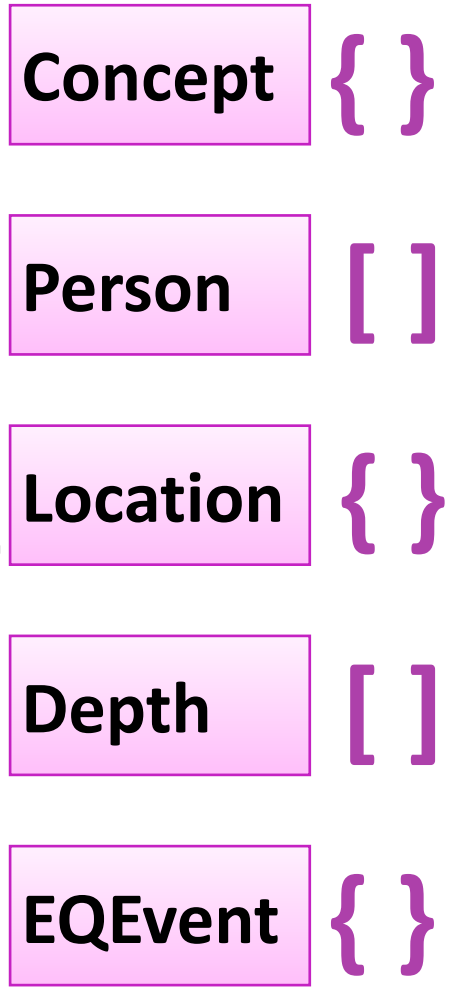
  - many, man rsity, number and size

Virtualisation for feasibility and cost saving

Local control for user judgement

CMDC quartet plays well

- **Collections**
  - users create, build, manage and use them
  - software works with them
- Representation
  - sets, bags, tuples, trees, sequences, time series, …
  - optimised encodings, scientific databases
- Populations
  - many instances growing in diversity, number & size



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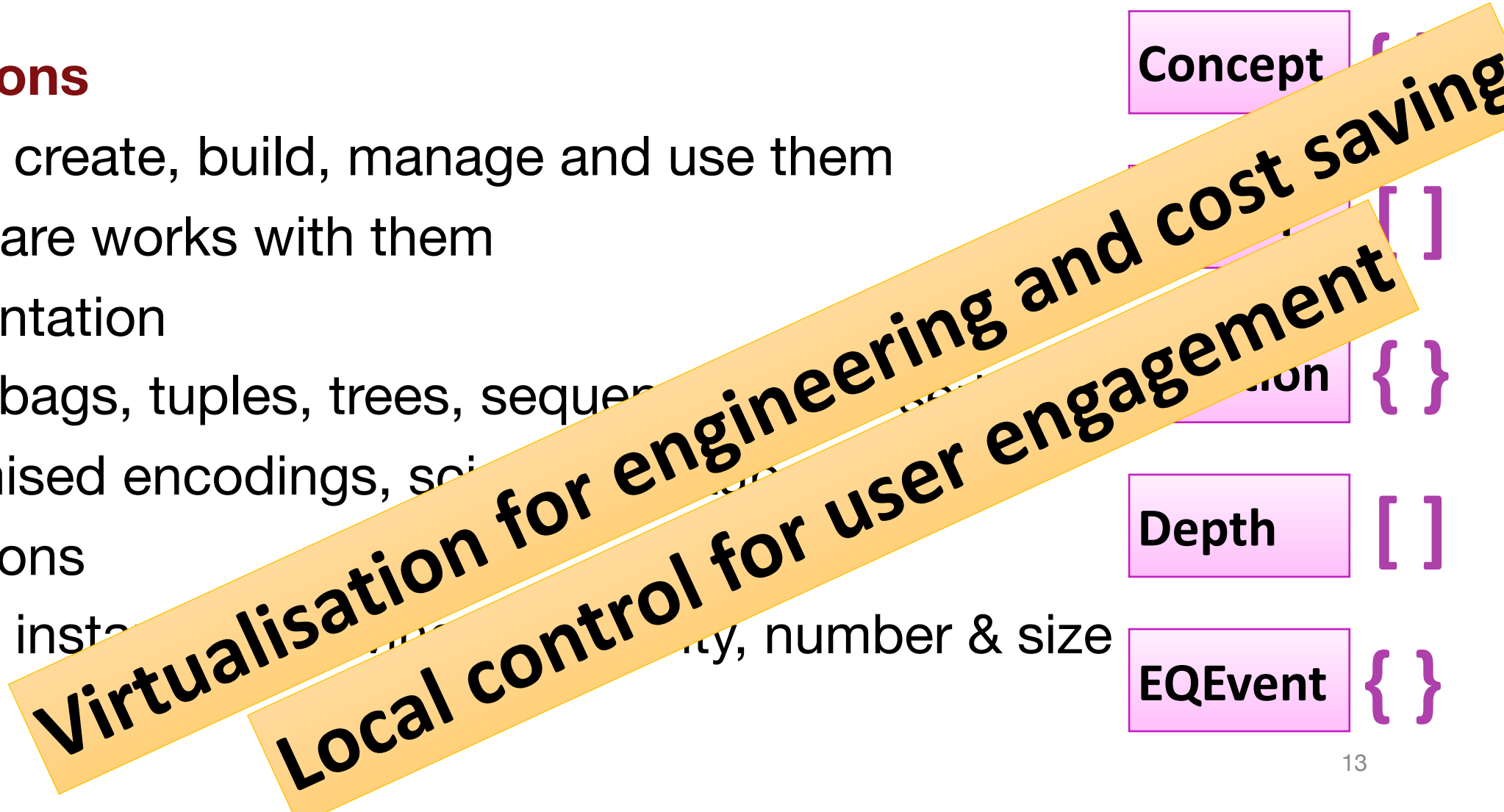


DARE

Keep CMDC in harmony

Keep CMDC in harmony for *all* in a community

Specialised *but related* work contexts

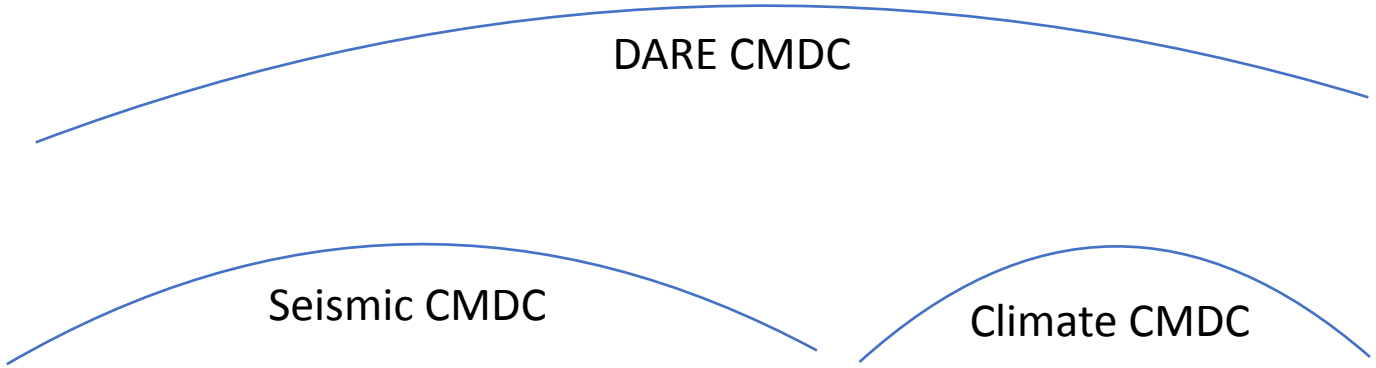
Specialised *but related* work contexts

- Delivering CMDC

CMDC **C**oncepts, **M**ethods, **D**ata and **C**ollections

Specialised *but related* work contexts

- Delivering CMDC
- Focused and tuned
  - for each community



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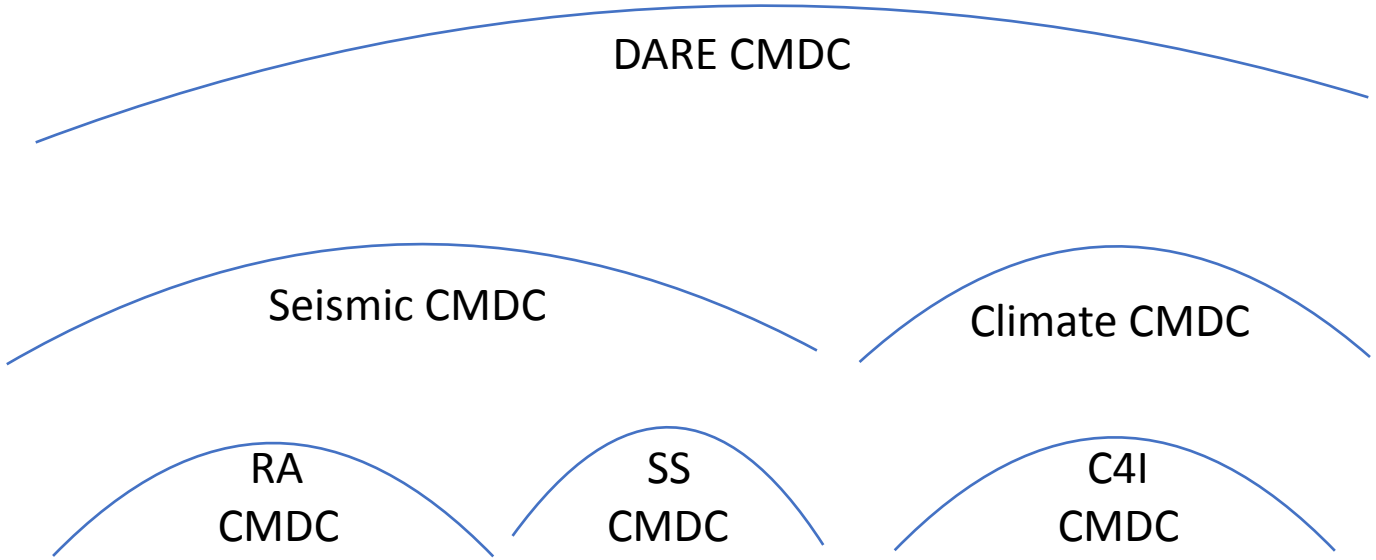

RA **R**apid **A**ssessment **SS** **S**eismic **S**ource
C4I **C**limate for **I**mpact

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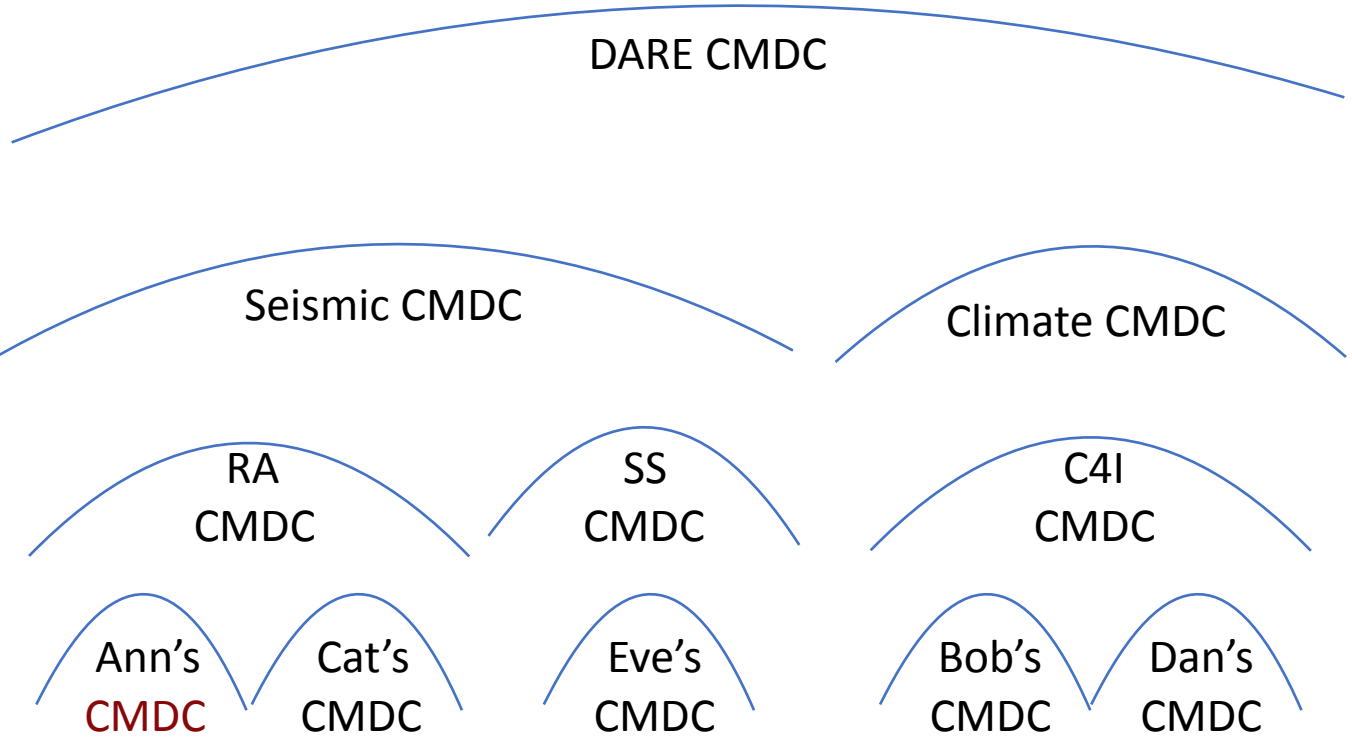
  - for each discipline / role
  - for groups and individuals



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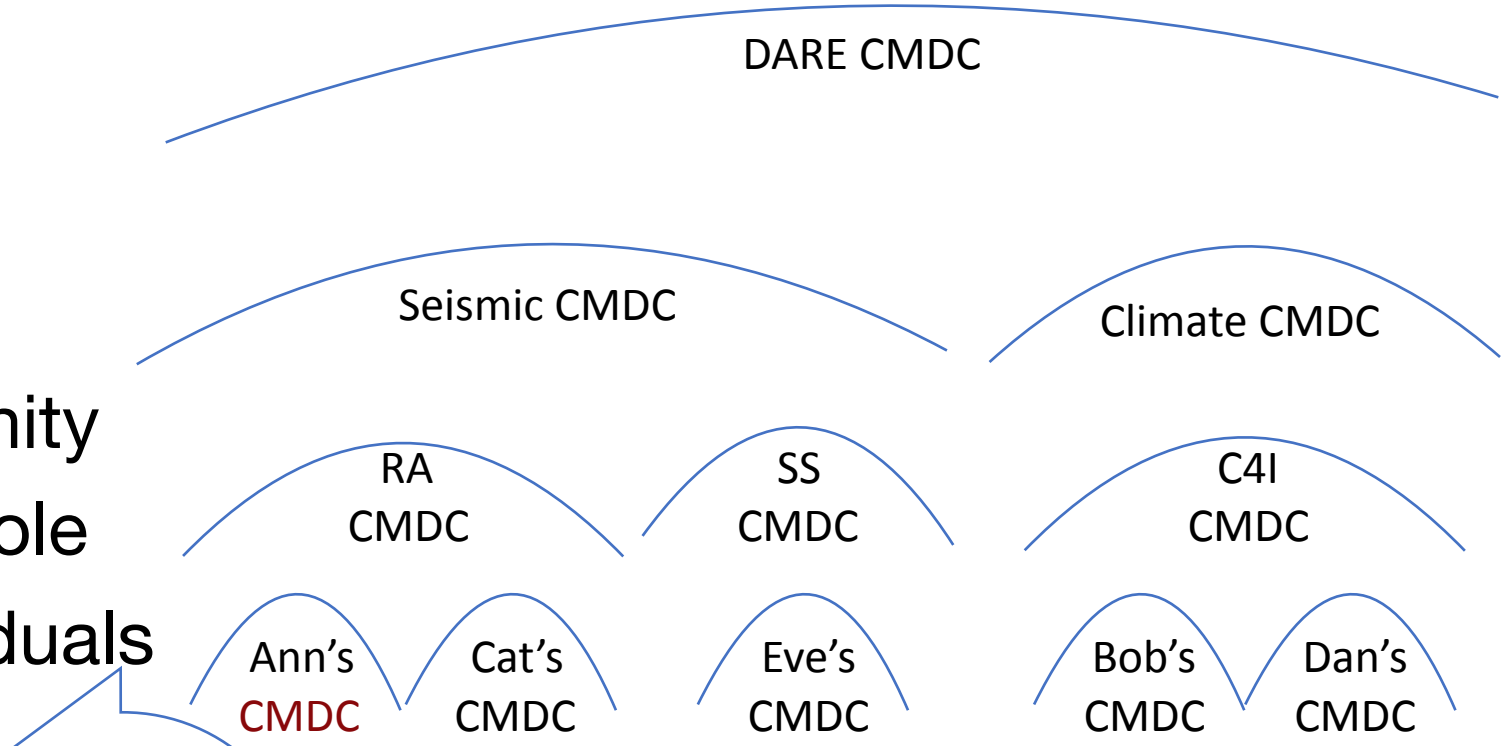
- Context-sensitive API
  - for VREs, tools & GUIs



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Outline

- ~~Vision and Goals~~
- ~~Key insights~~
- Architecture
- Achievements and Work in Progress

DARE users create, use, refine and discard

Others + DARE future: Tools & User interfaces

DARE API & Development kit

DARE Platform

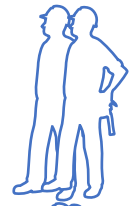
DARE Data-Intensive Technology

Virtualisation, Deployment, Orchestration & Monitoring

Domain experts
shape *their* context

Research
Developers
shape contexts

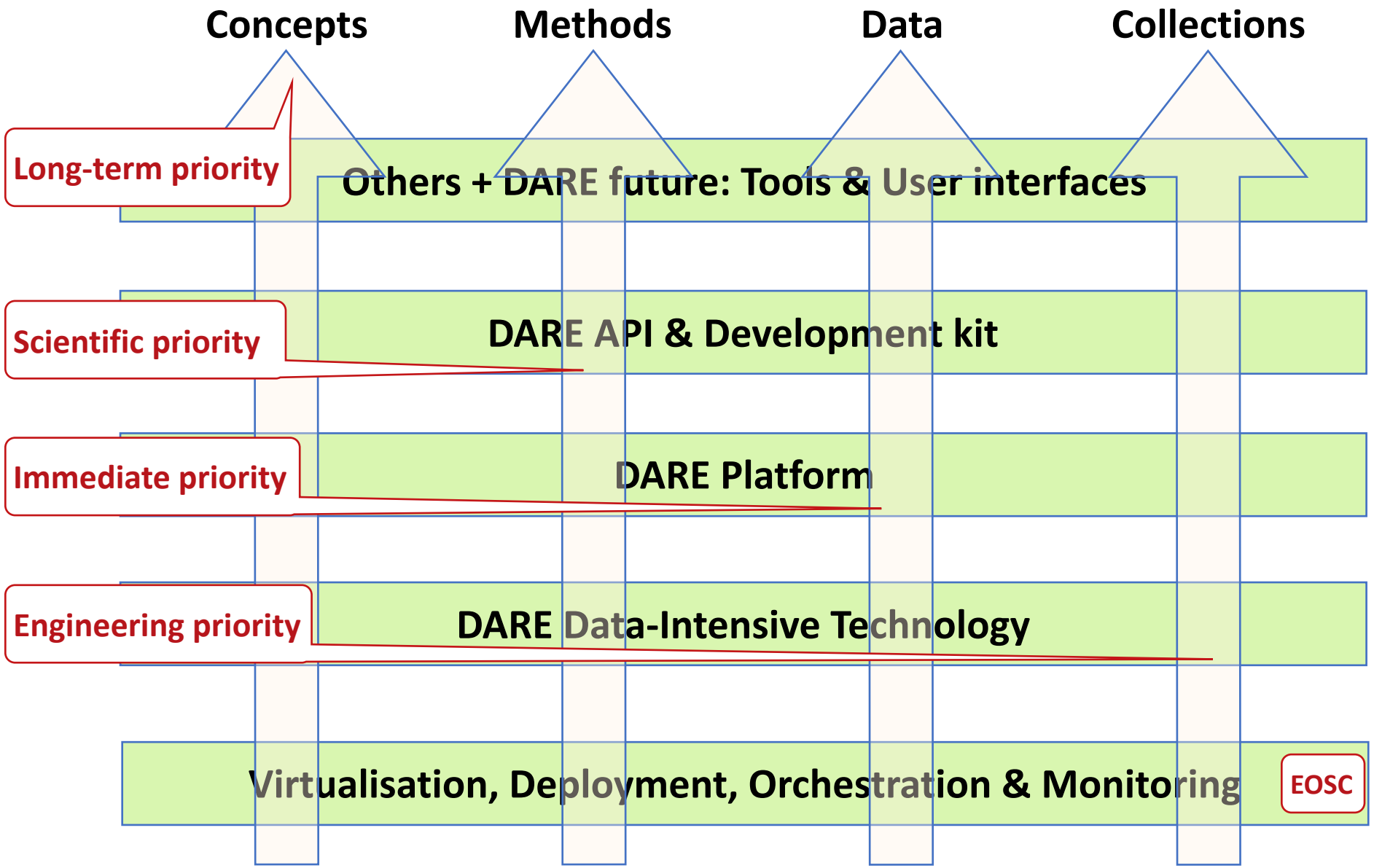
Platform
Developers
enable common
contexts



Data architects
& workflow gurus

Information system
engineers &
Resource managers

DARE users create, use, refine and discard



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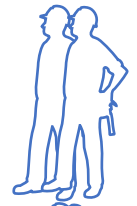

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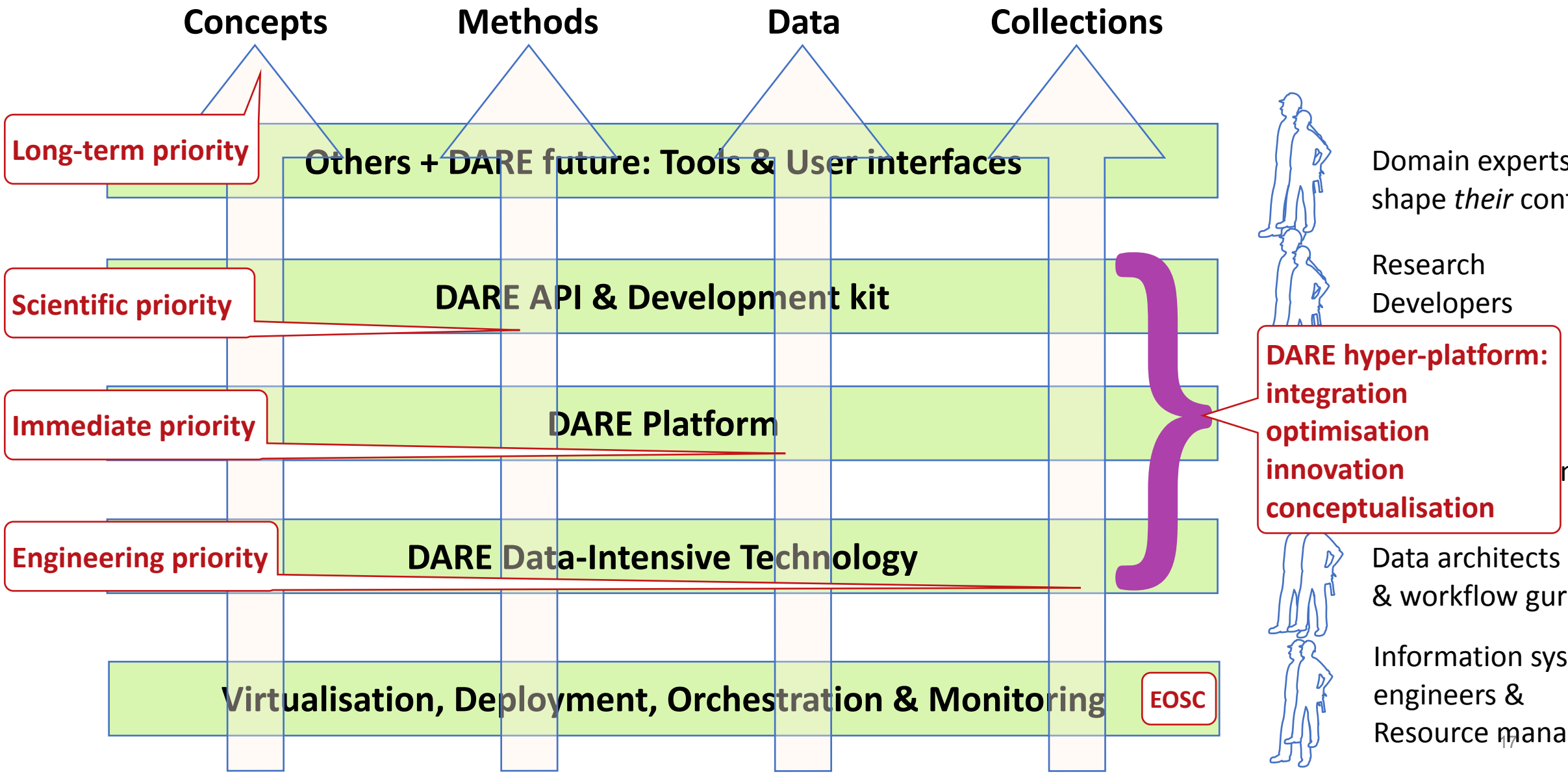
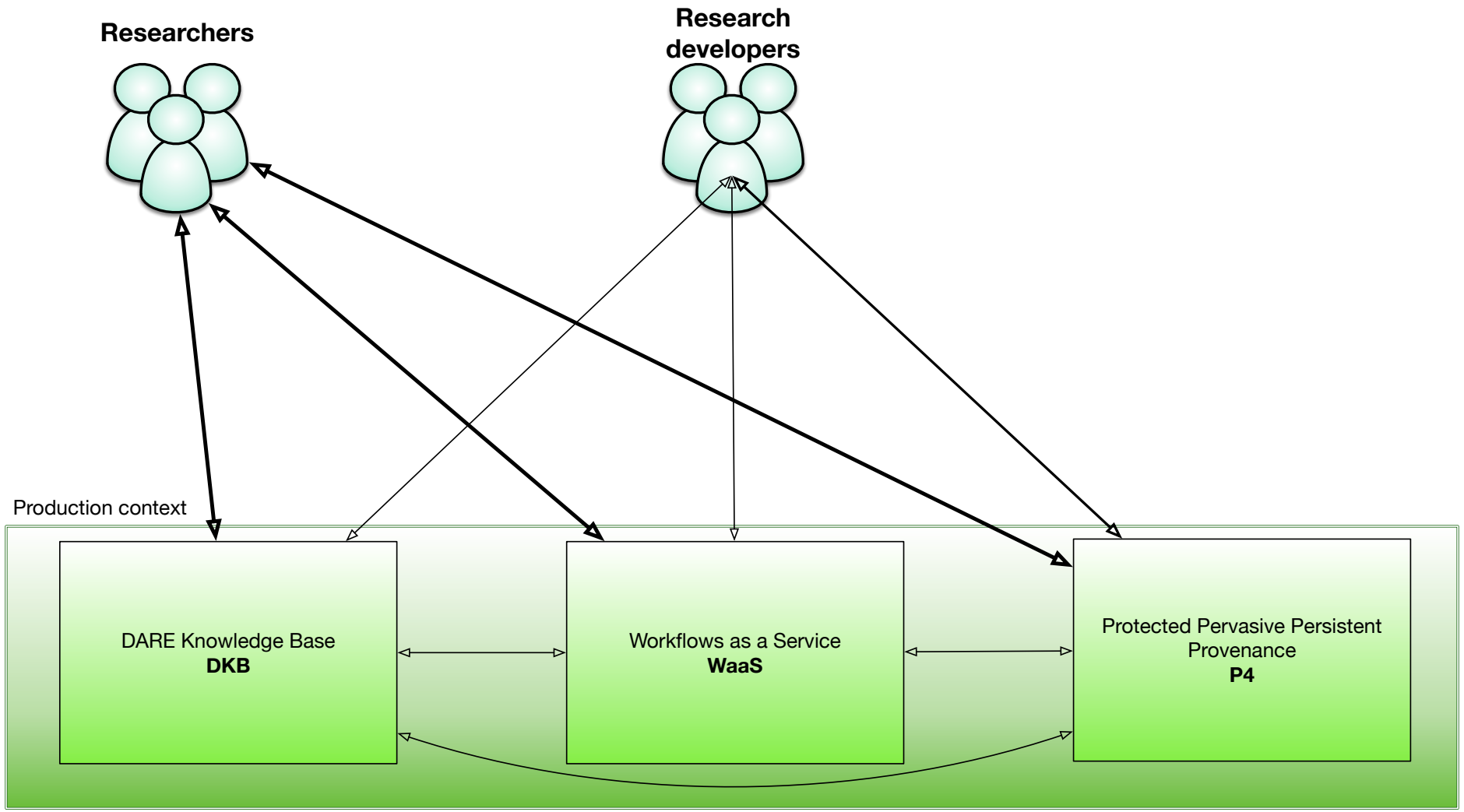
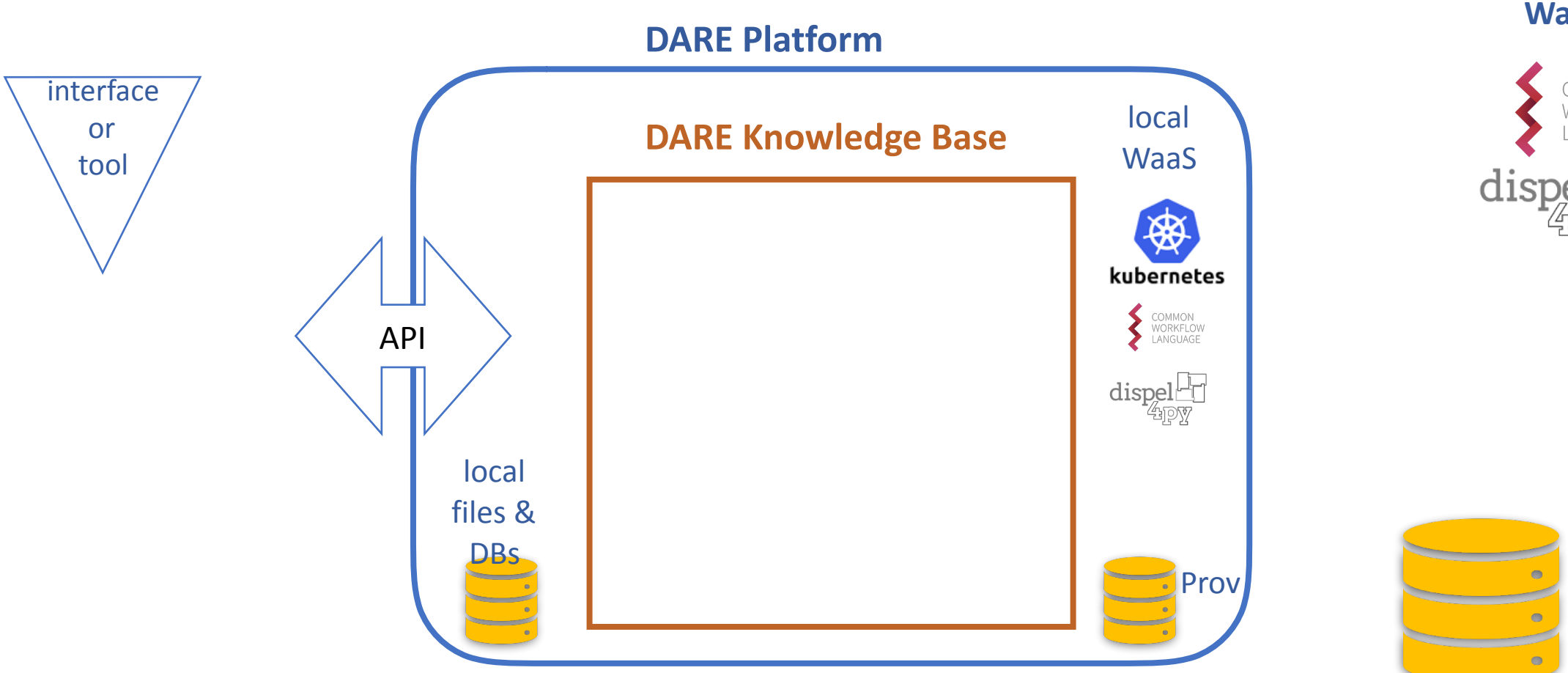


The three DARE technology pillars



DKB-mediation



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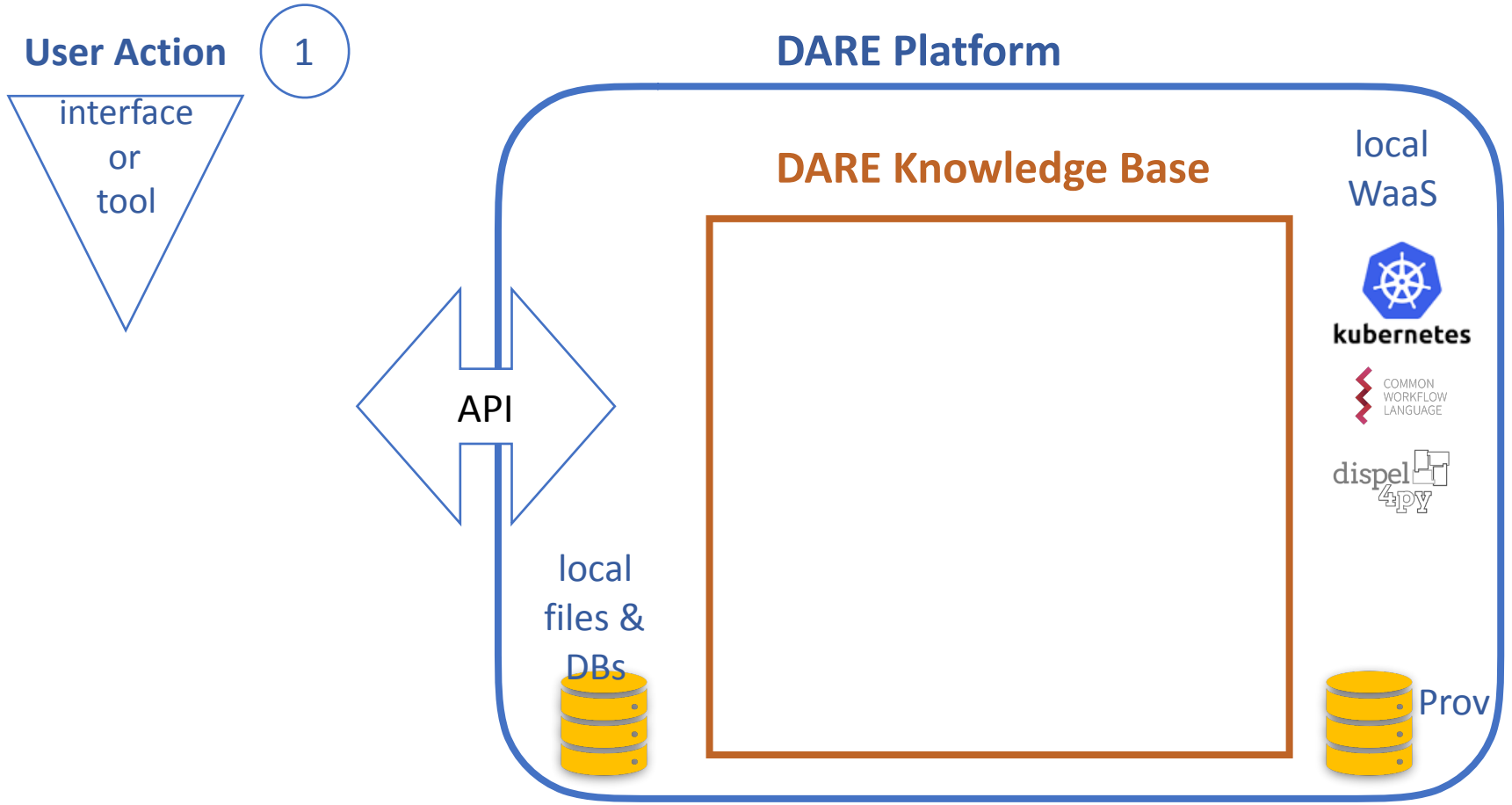

External services

Deployed
WaaS

COMMON
WORKFLOW
LANGUAGE
dispel
4py

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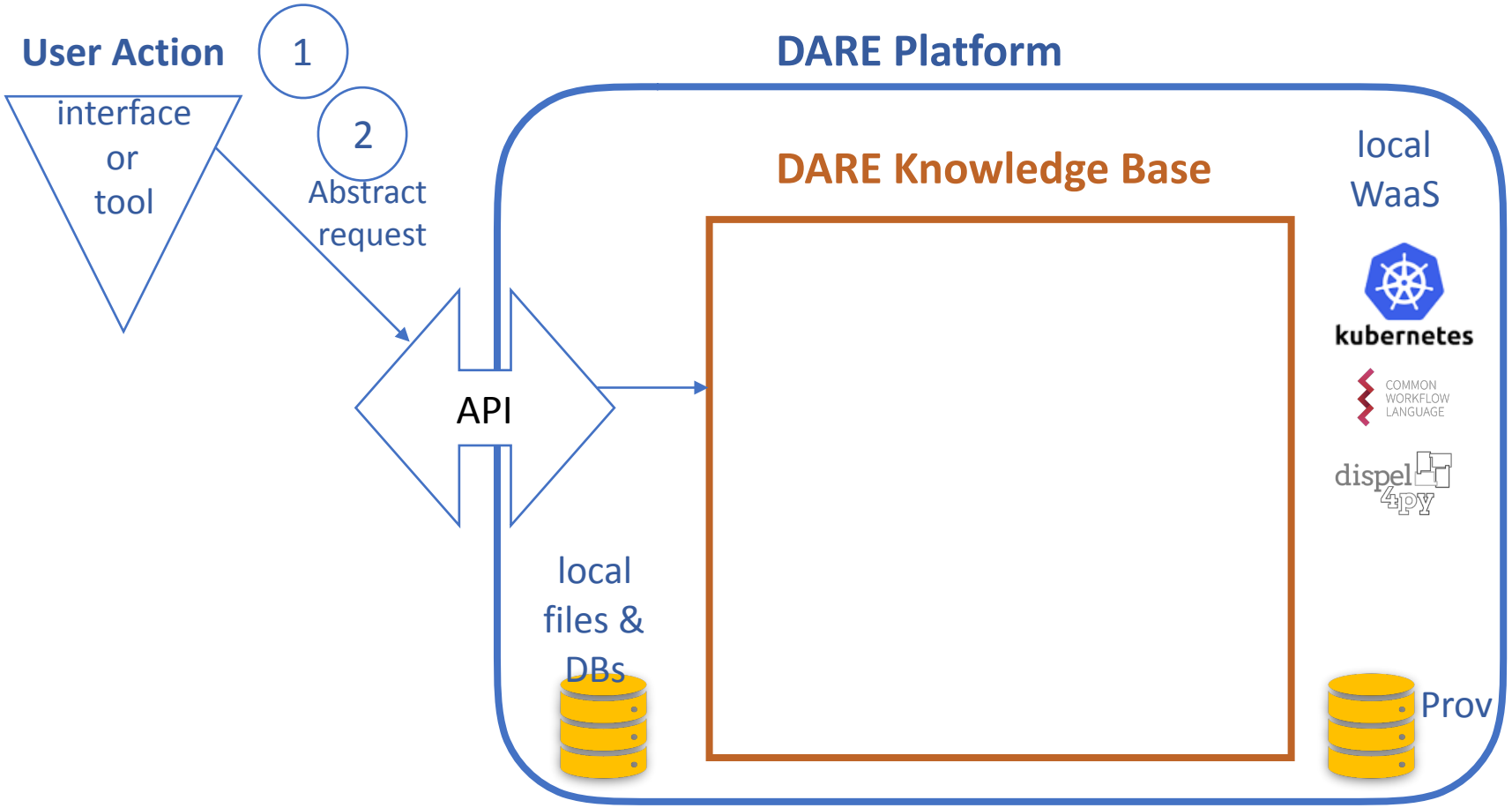
Archival
services

DKB-mediation



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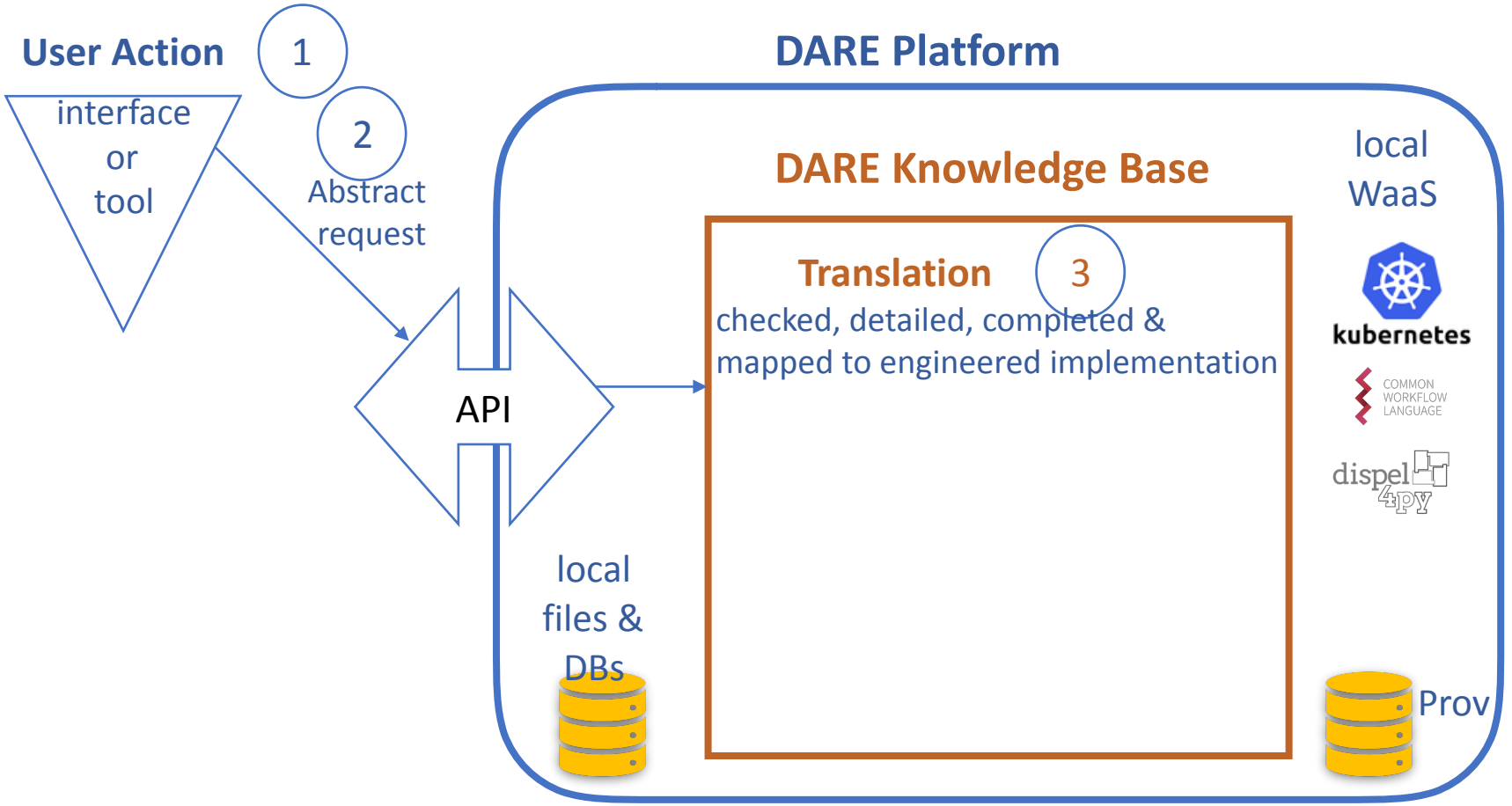

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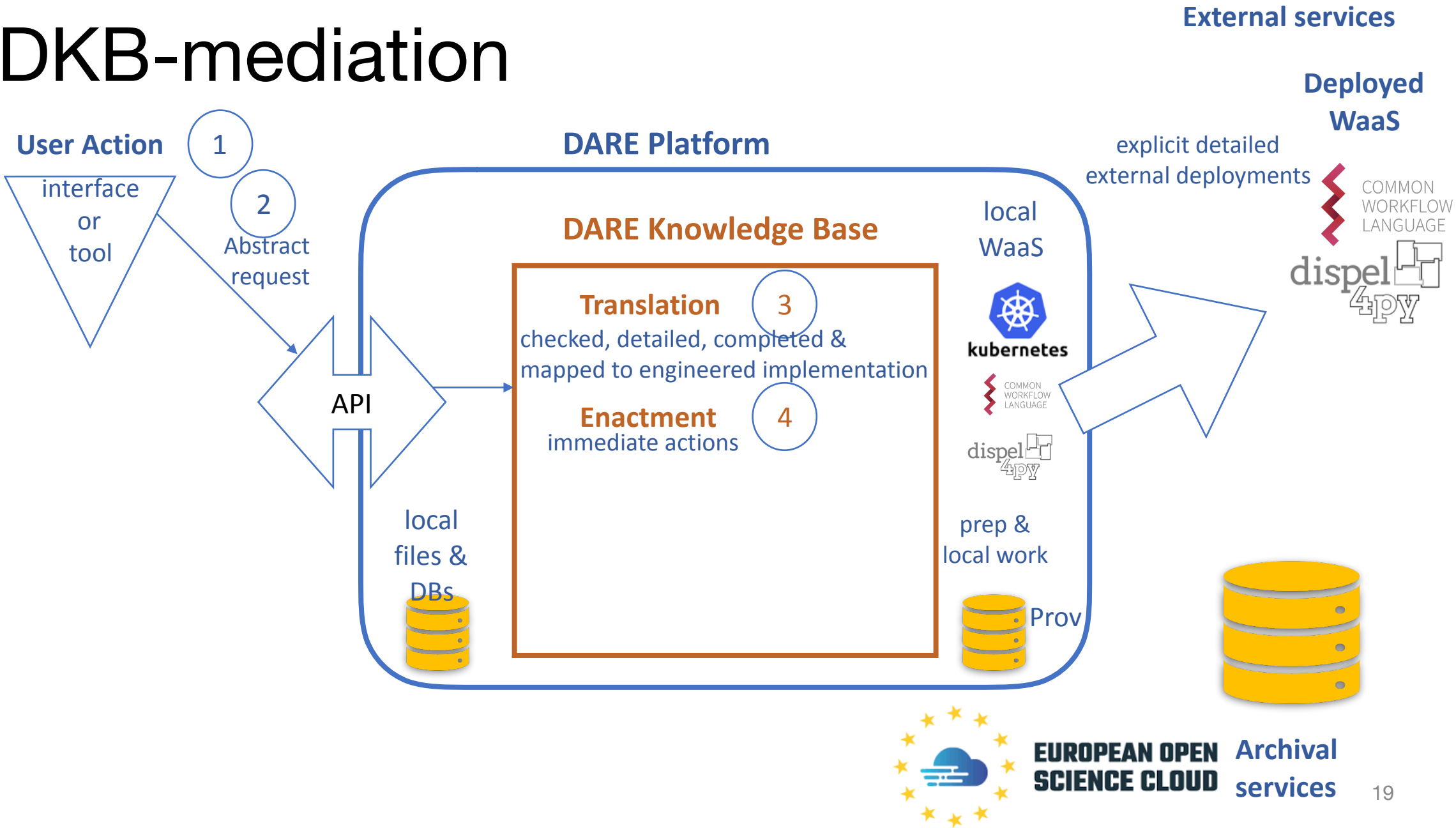

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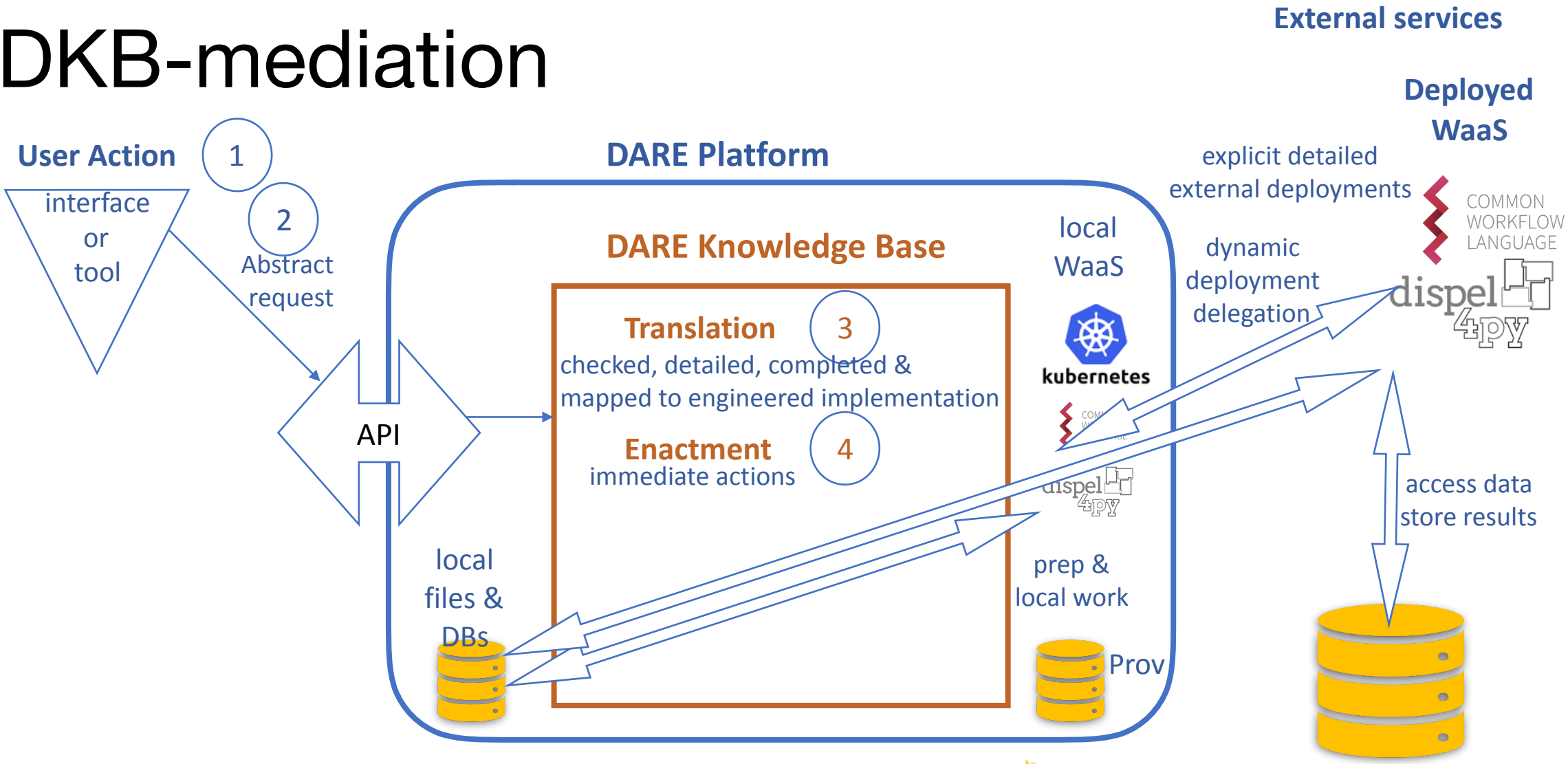

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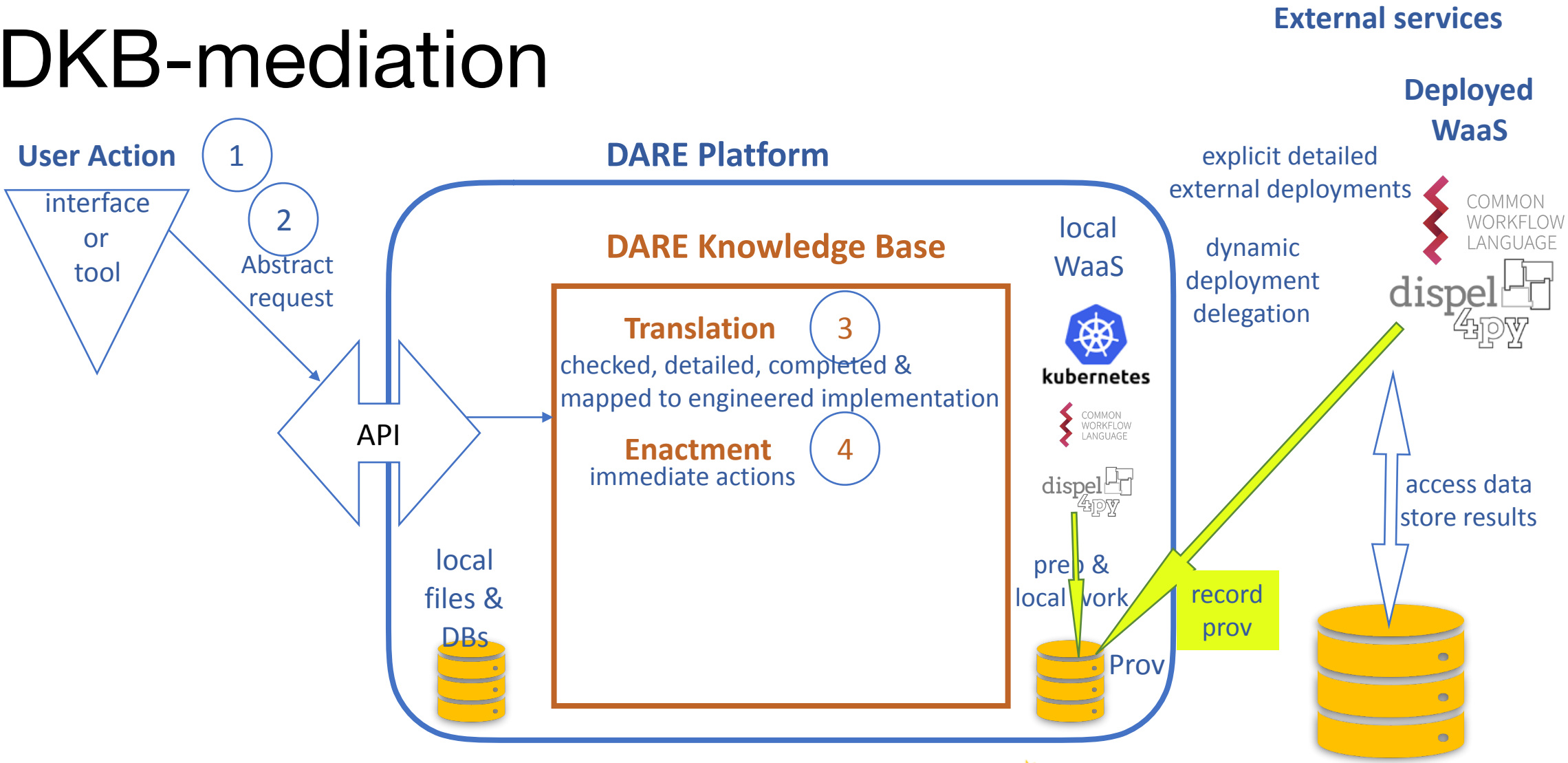

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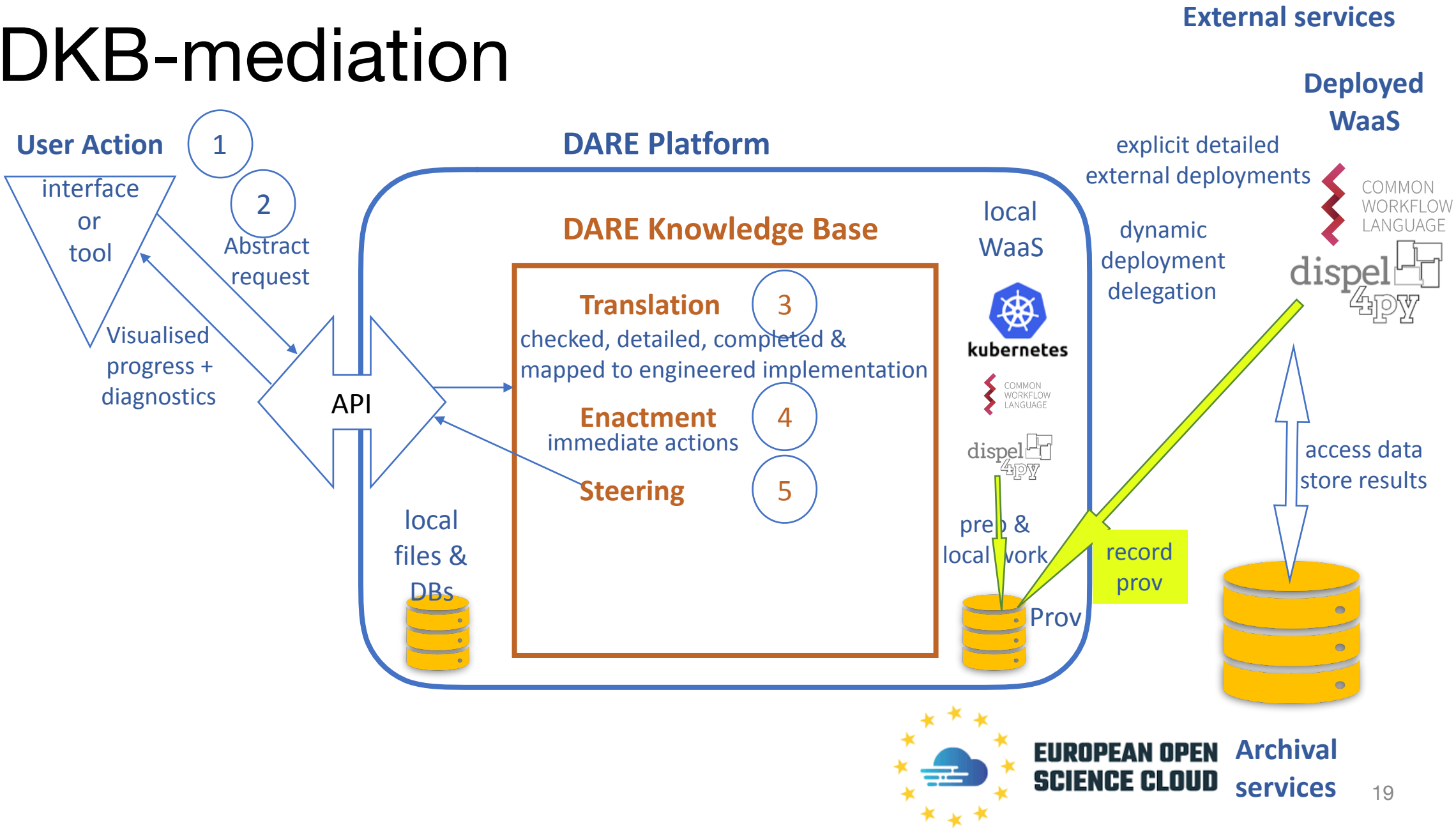

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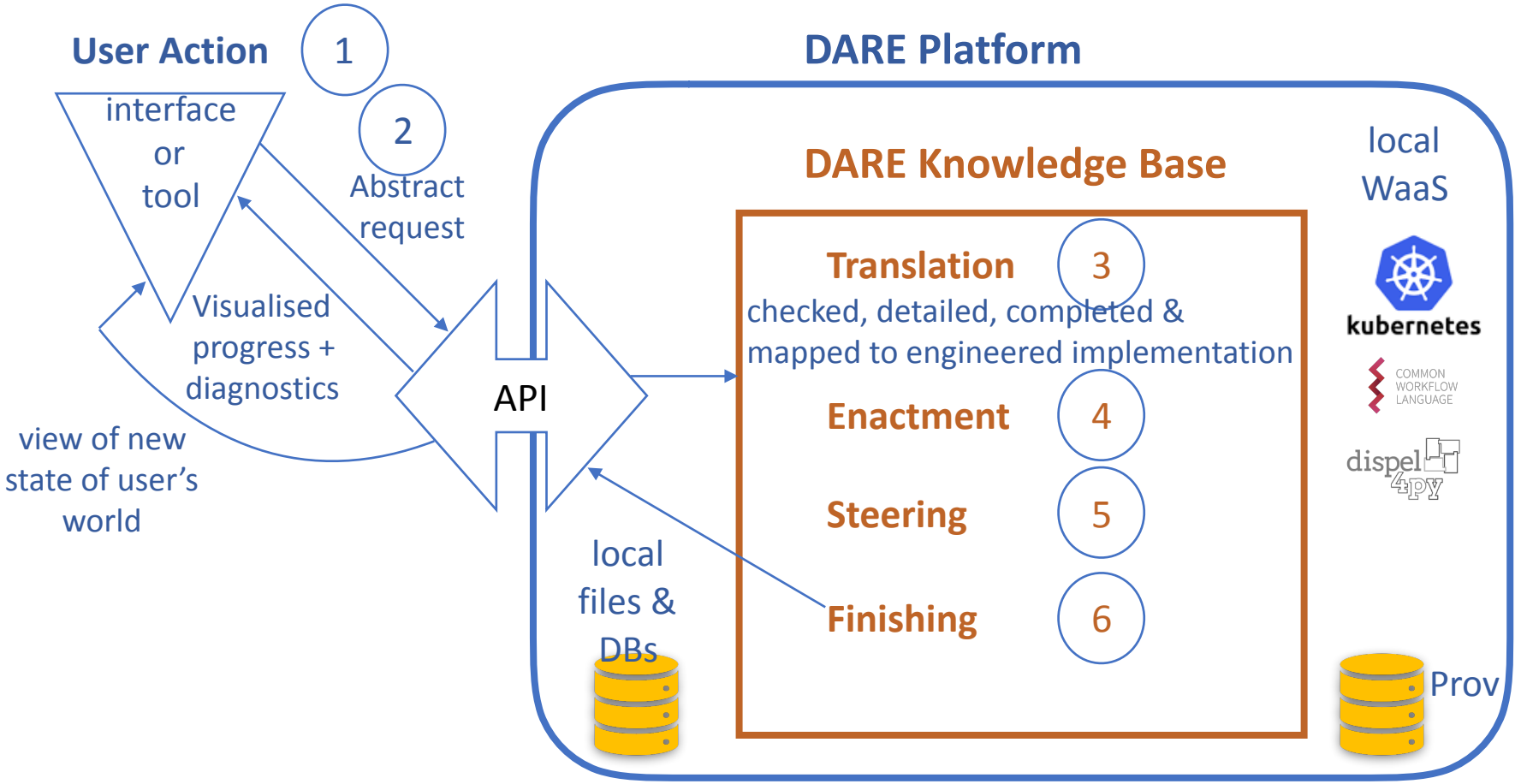

External services

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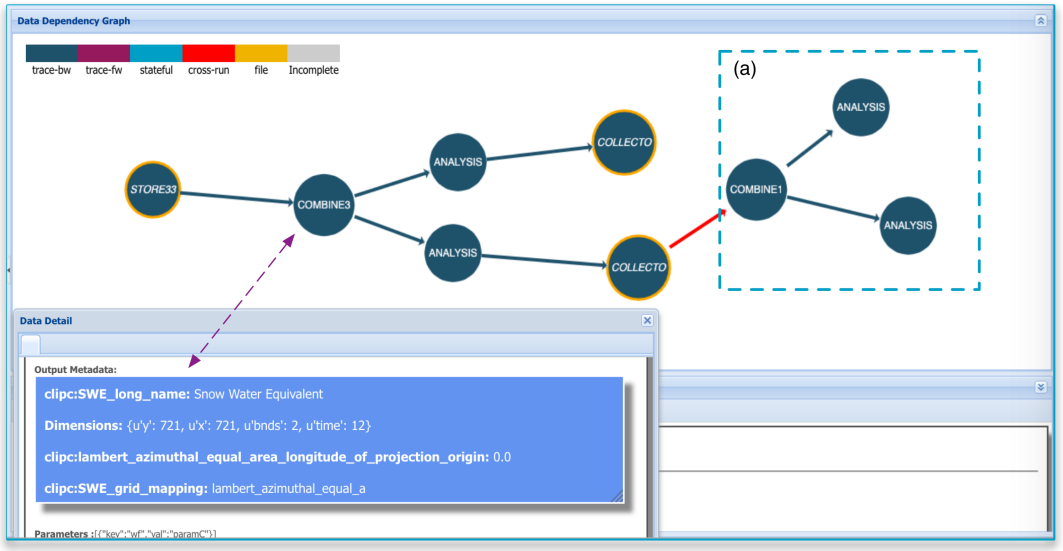
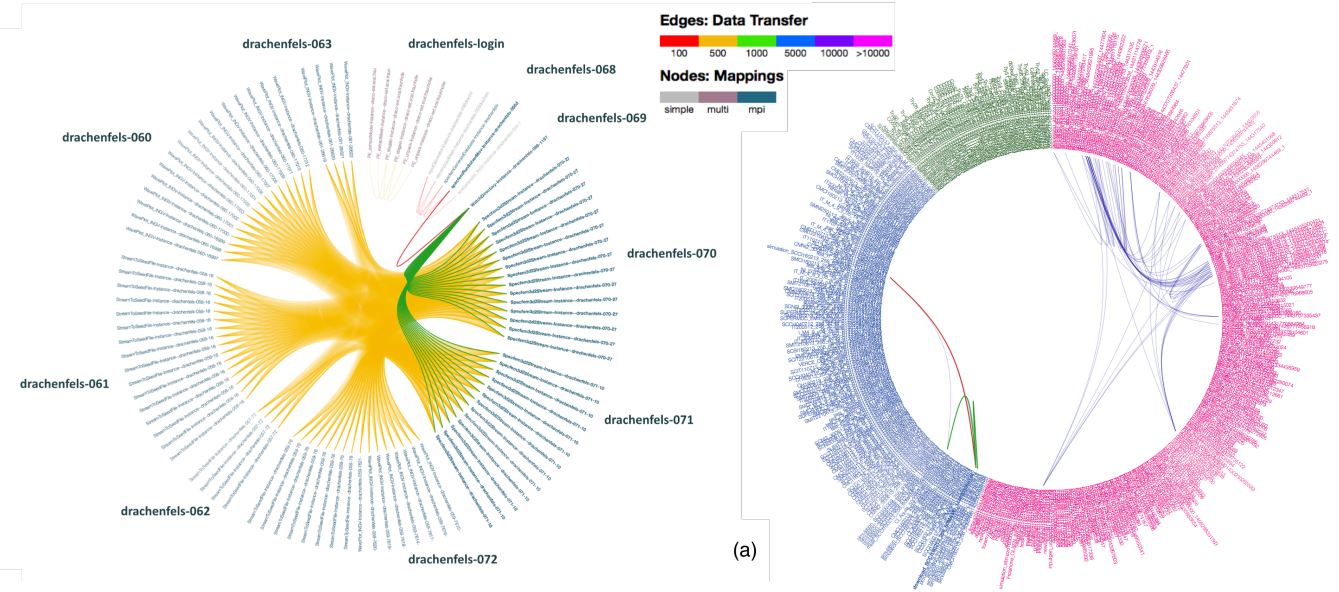
Provenance Tools





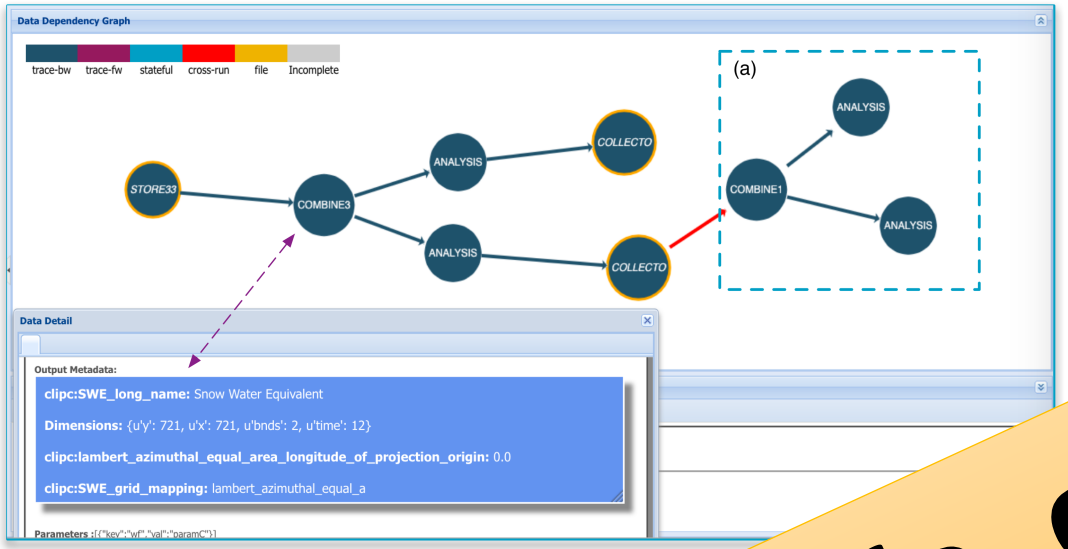
MVV - Monitoring and Validation

Focussed analysis: contextual monitoring, diagnostics and validation.
Provides metadata and indication on the production of materialised data, dependency navigation, results management and discovery

BDV — Bulk Dependencies Visualiser

Comprehensive analysis: user driven perspectives on single executions of scientific computations or involving many runs and users.
It highlights resources and data exploitation patterns

Provenance Tools



MVV - Monitoring

Focus ...textual monito...
di... ...idation.
... ...data and indicatio...
... ...ion of materialised data, d... ...ency
navigation, results management and discovery

BD... ...idencies Visualiser

...prehensive analysis: user driven perspectives on single executions of scientific computations or involving many runs and users. It highlights resources and data exploitation patterns

coping with scale, complexity and duration

delivering repeatability

Outline

- ~~Vision and Goals~~
- ~~Key insights~~
- ~~Architecture~~
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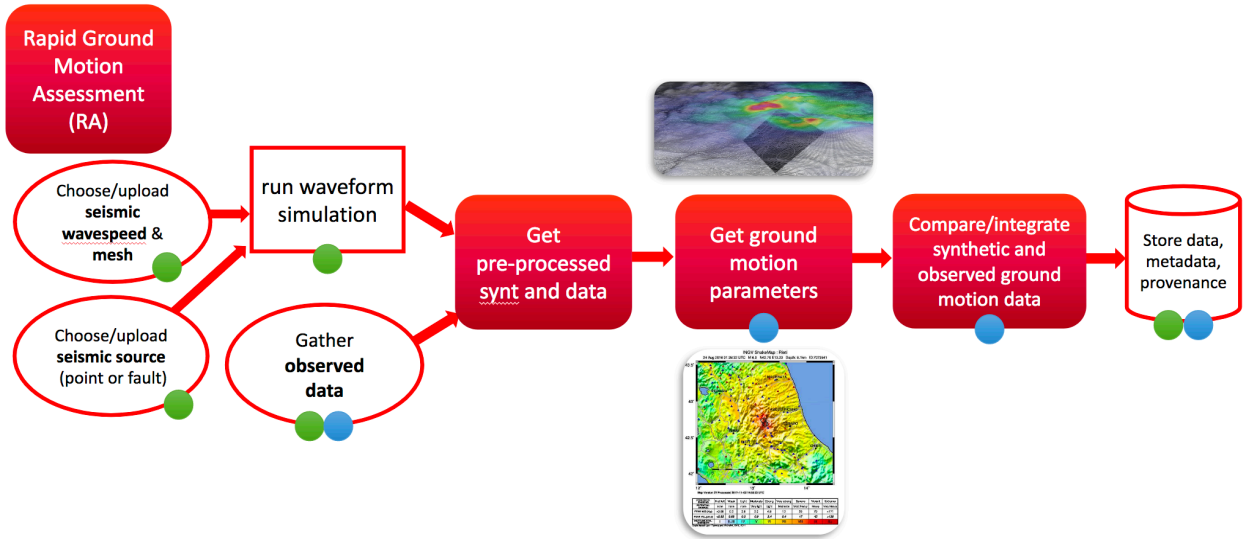
Whole seismic example

Today



Whole seismic example

Today

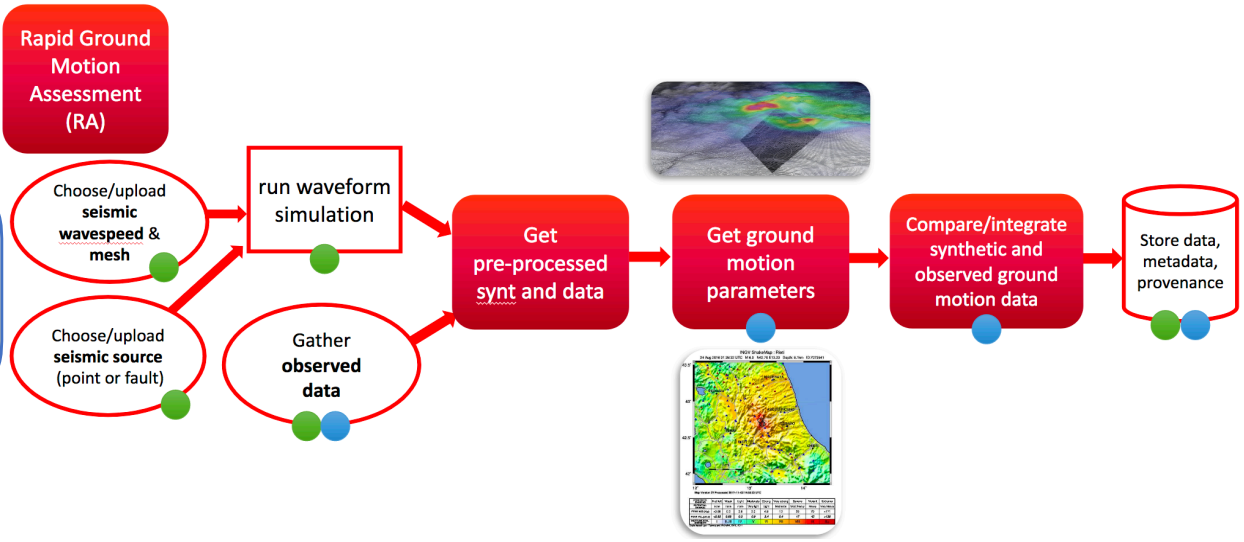
each step dispel4py linked using CWL

seismologists interact via Jupyter notebooks

targets chosen and encoded by IT experts

optimisation & mapping *fixed* by IT experts

co-developed by seismologist, developers & IT experts



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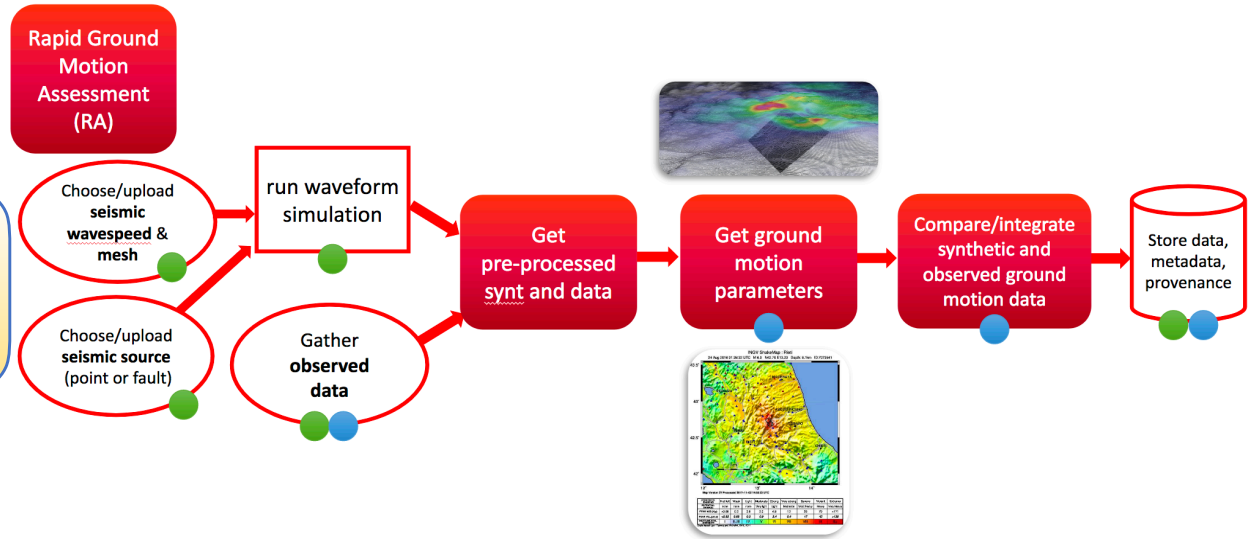
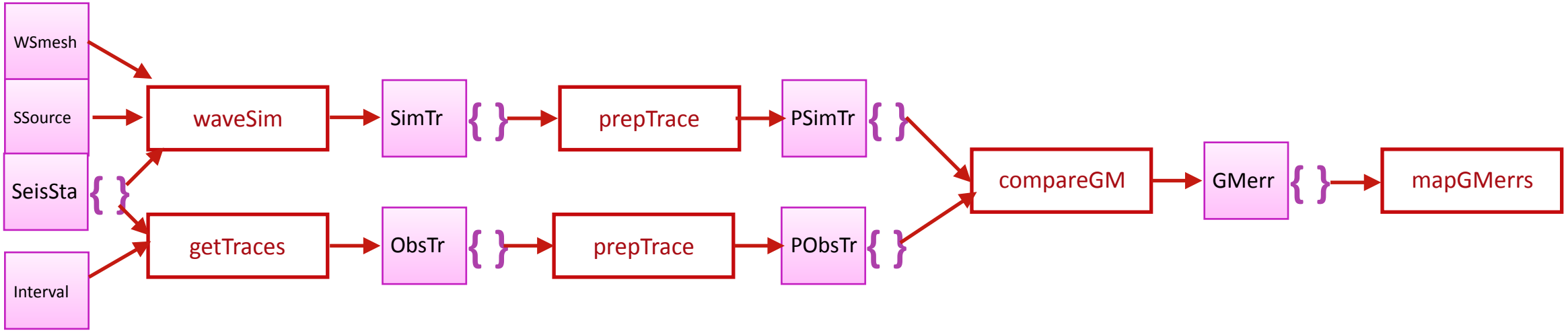


'Tomorrow'



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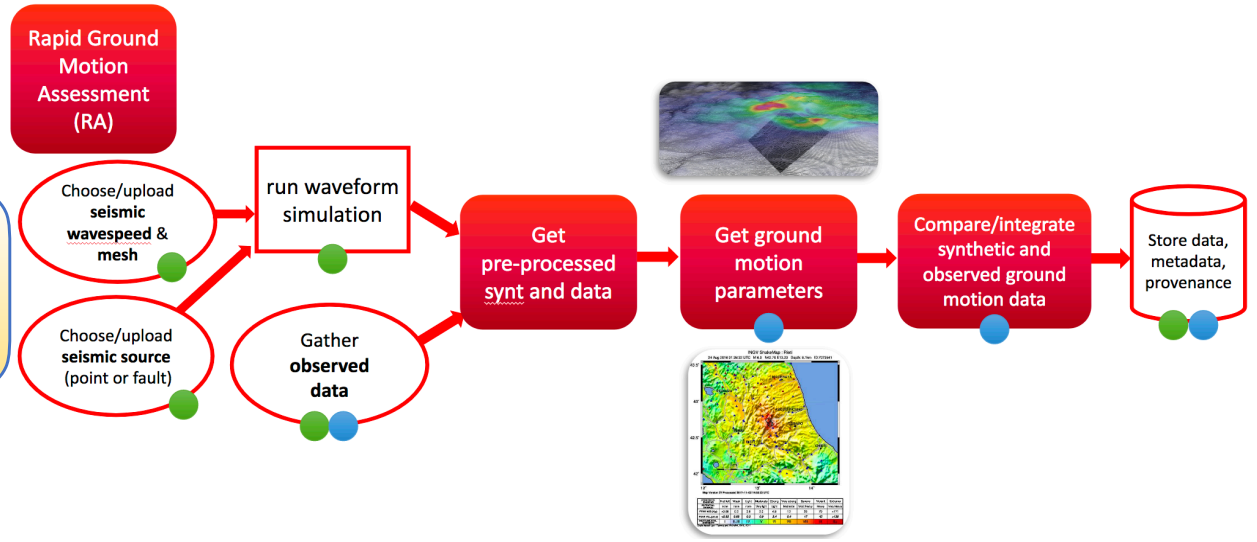

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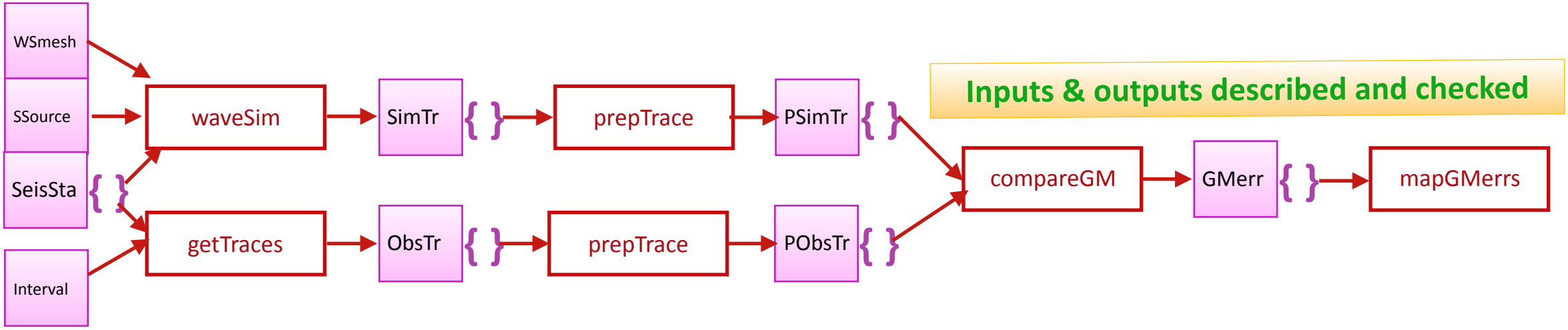

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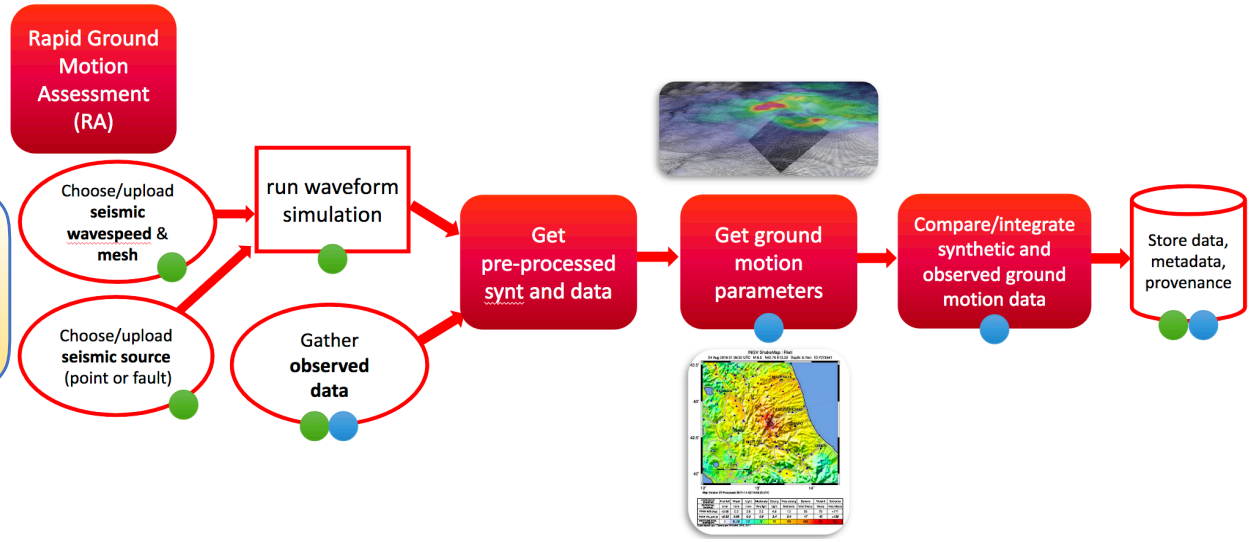

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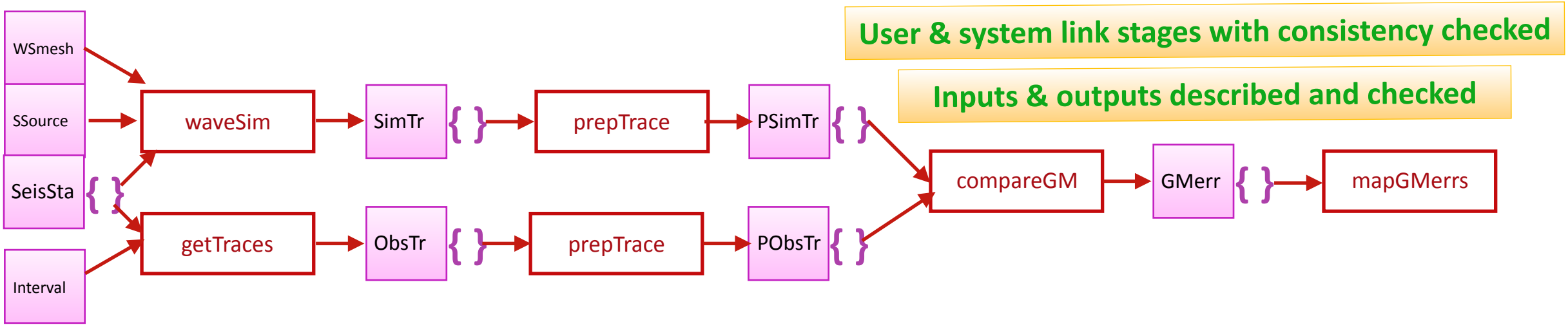

User & system link stages with consistency checked

Inputs & outputs described and checked

Whole seismic example

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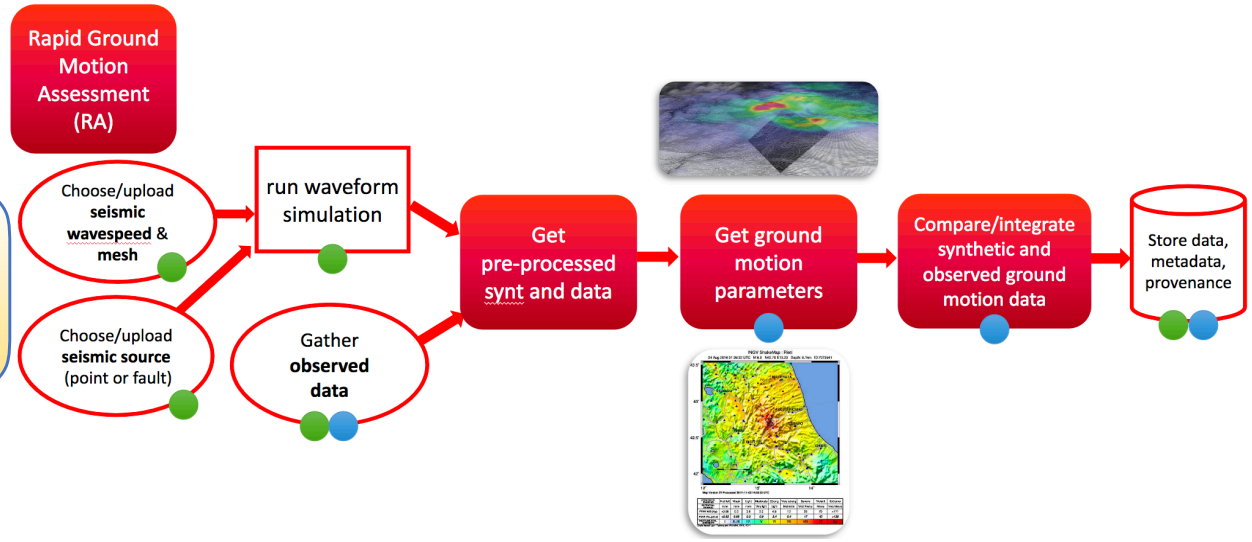

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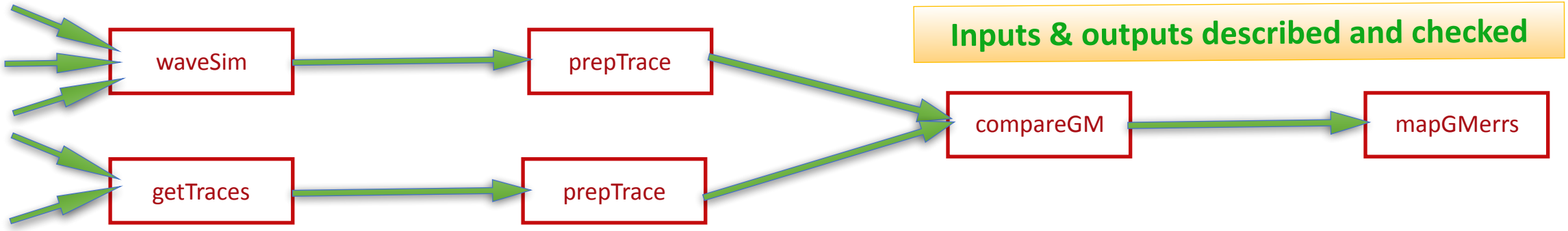

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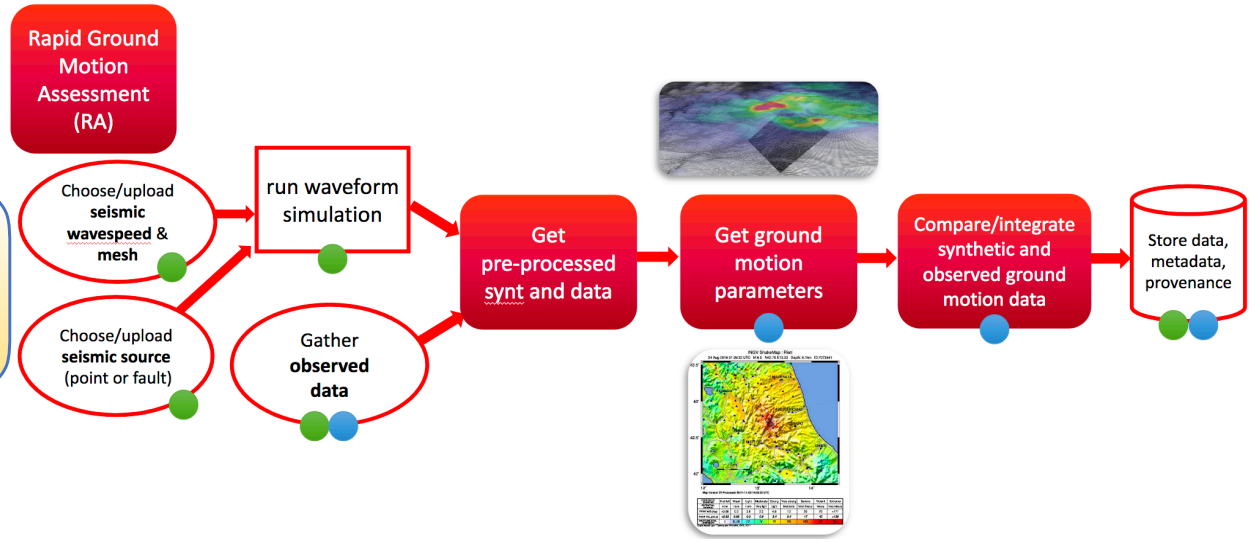
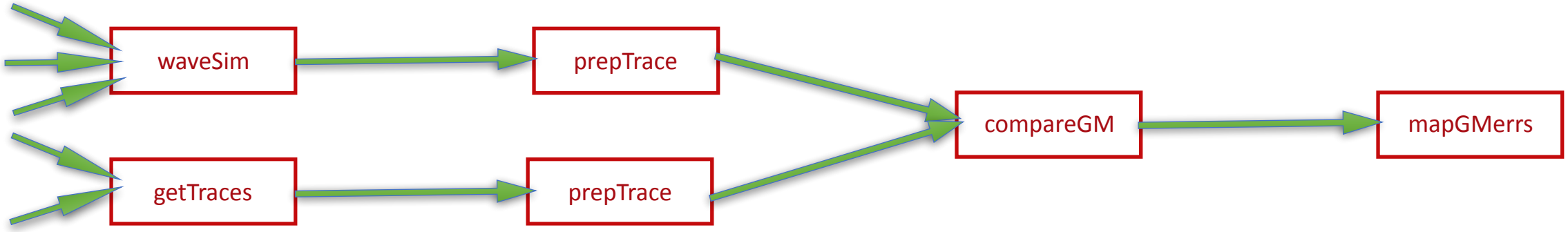
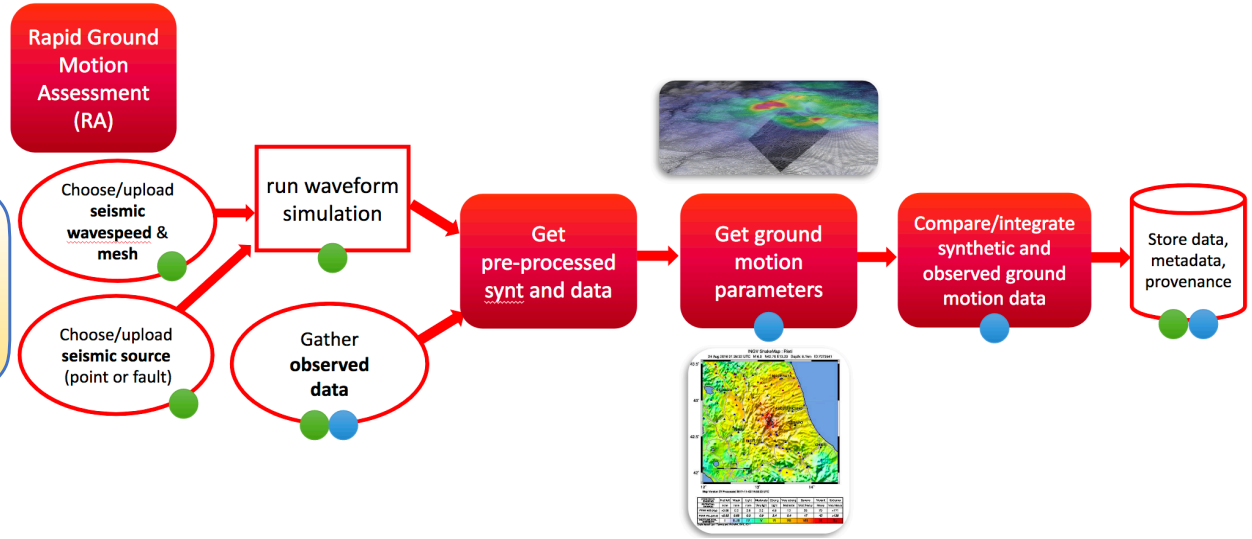


'Tomorrow' target selection, deployment, mapping and orchestrated enactment



Whole seismic example



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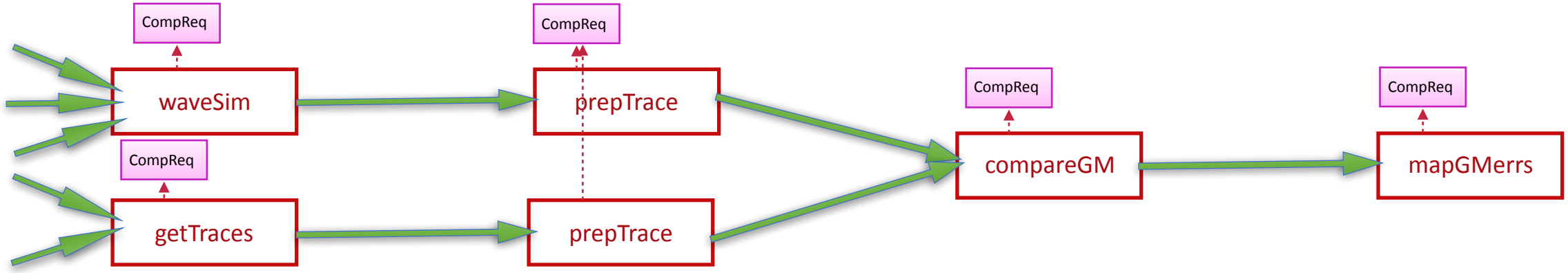

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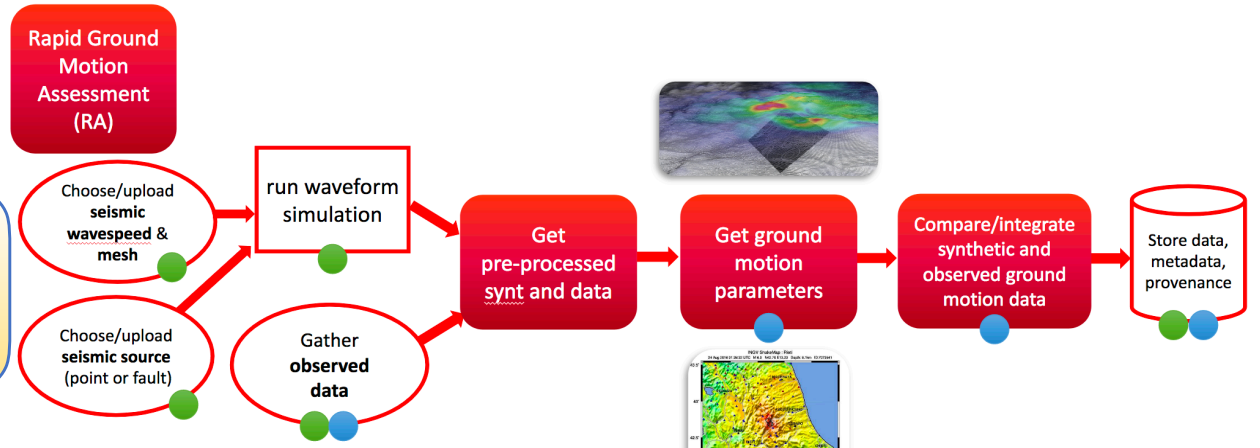

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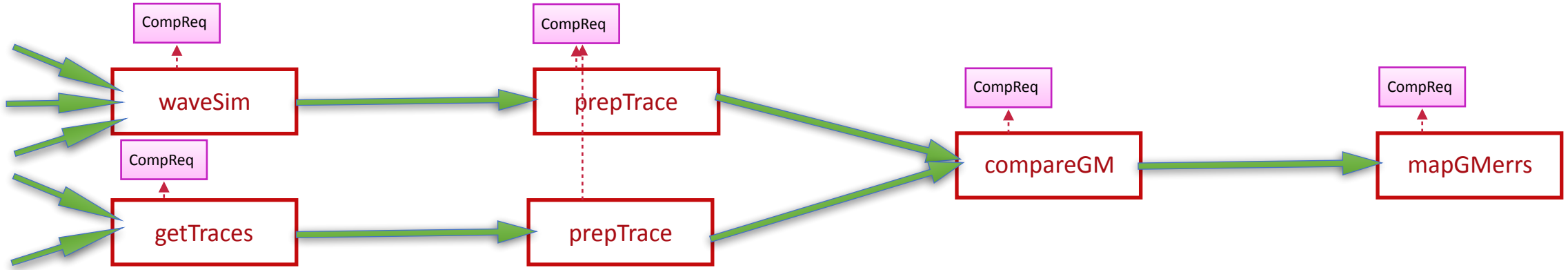

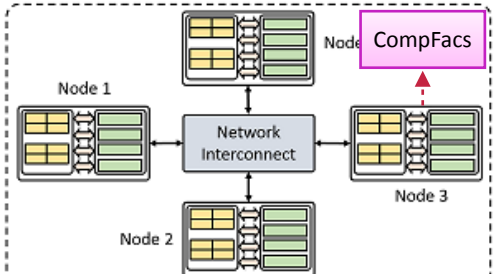

CompFacs

EUROPEAN OPEN SCIENCE CLOUD

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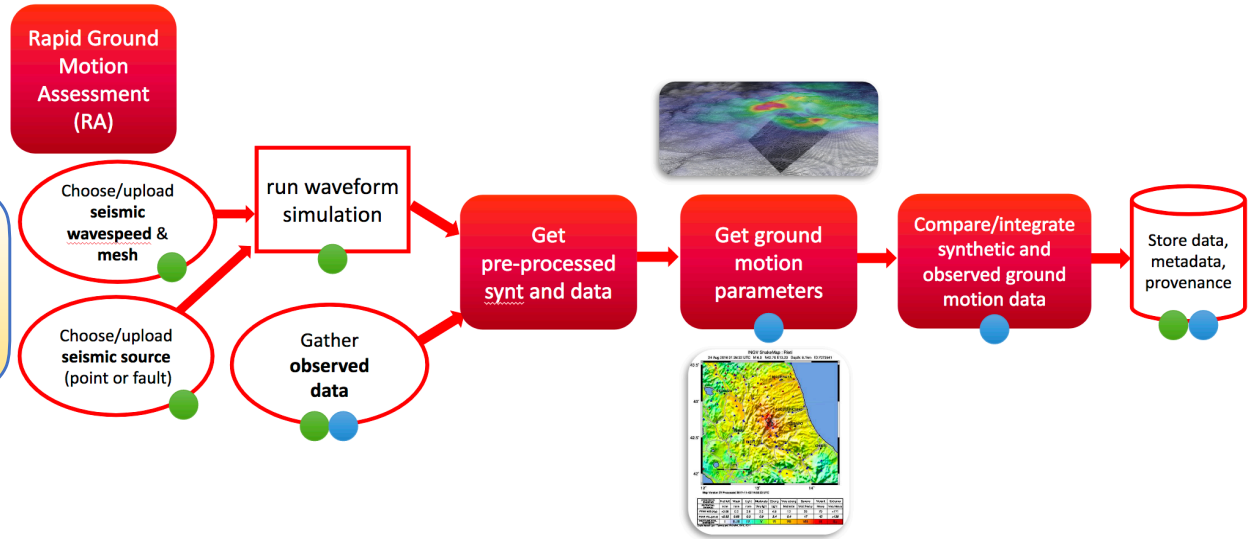
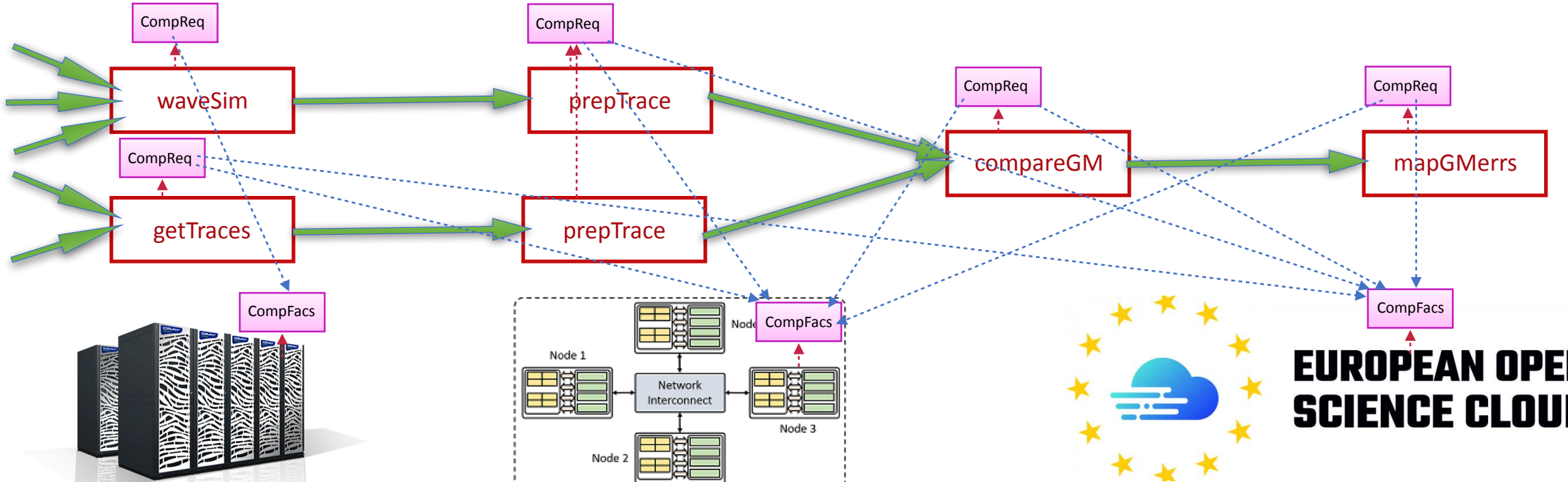


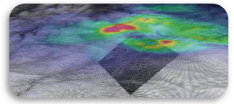
'Tomorrow' target selection, deployment, mapping and orchestrated enactment

target matching



Whole seismic example

Rapid Ground Motion Assessment (RA)



Choose/upload **seismic wavespeed & mesh**

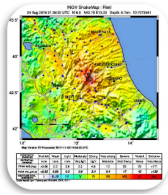
Choose/upload **seismic source** (point or fault)

run waveform simulation

Gather **observed data**

Get pre-processed synt and data

Get ground motion parameters



Compare/integrate synthetic and observed ground motion data

Store data, metadata, provenance

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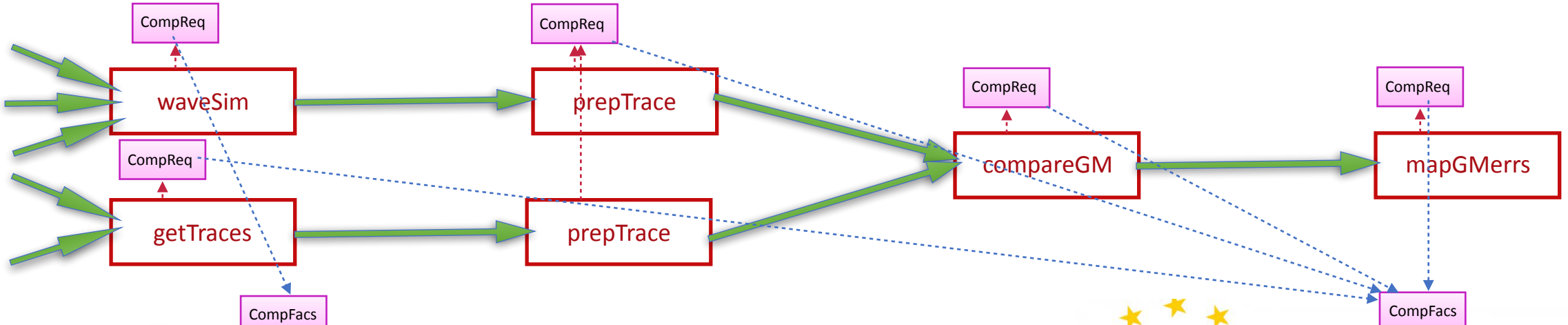
'Tomorrow' target selection, deployment, mapping and orchestrated enactment

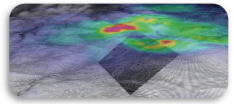
target matching target choice



EUROPEAN OPEN SCIENCE CLOUD

Whole seismic example

Rapid Ground Motion Assessment (RA)



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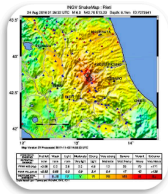

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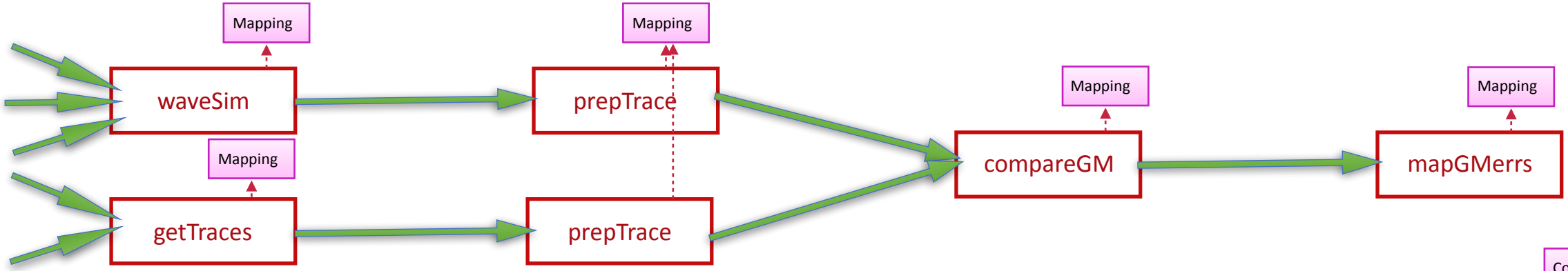
'Tomorrow' target selection, deployment, mapping and orchestrated enactment

target matching target choice target preparation



CompFacs

CompFacs

Distributed Connected Software Deployments

SCIENCE CLOUD

Whole seismic example

Today

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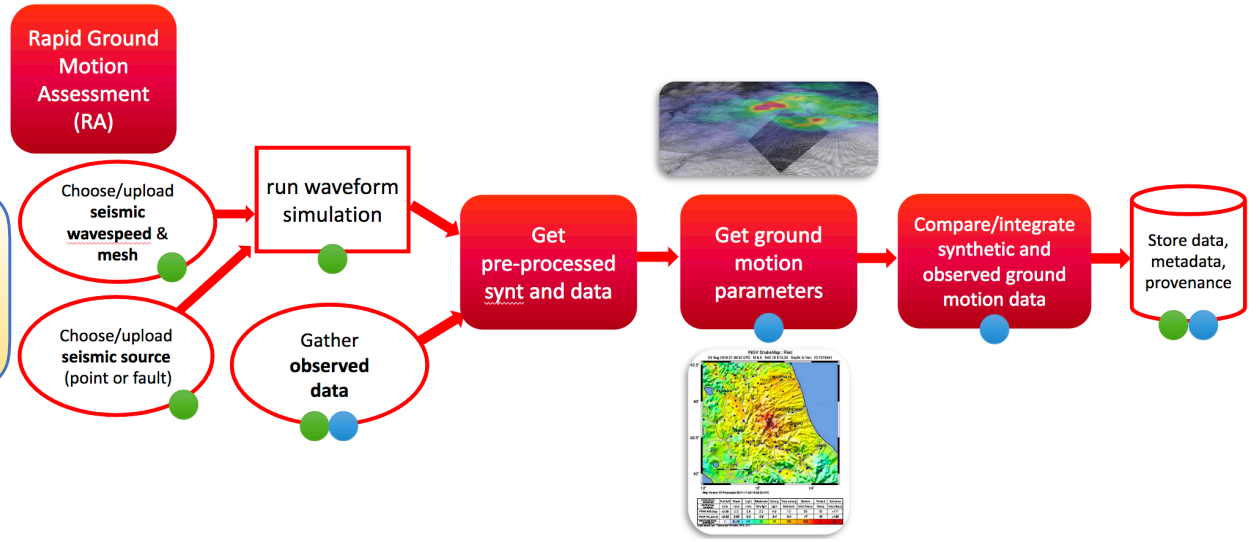
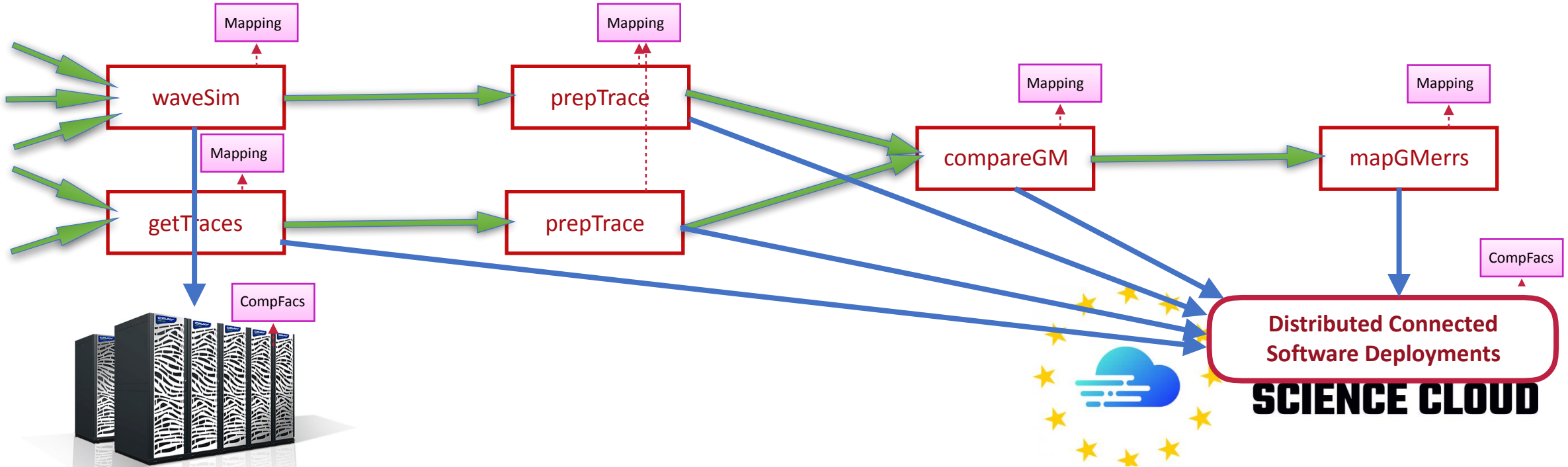
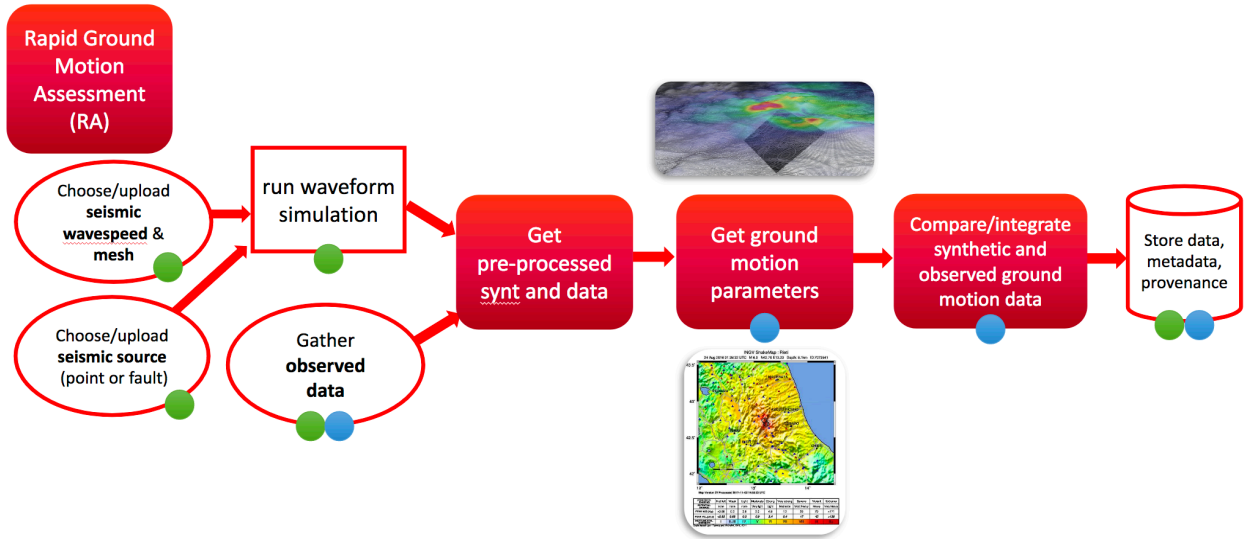


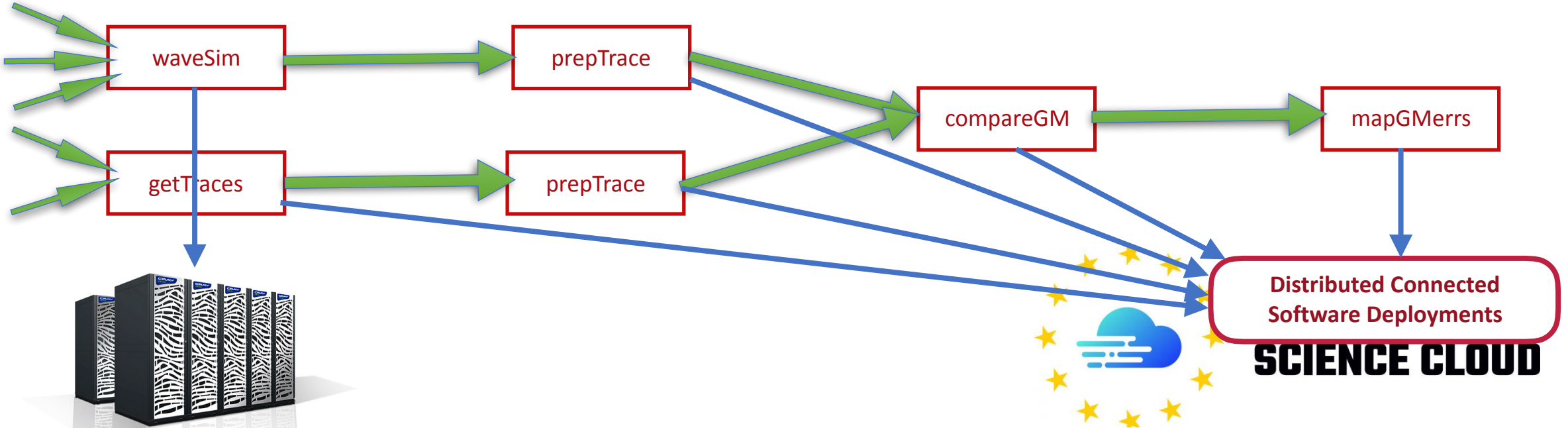
'Tomorrow' target selection, deployment, mapping and orchestrated enactment

target matching target choice target preparation map to targets



Seismic example summary

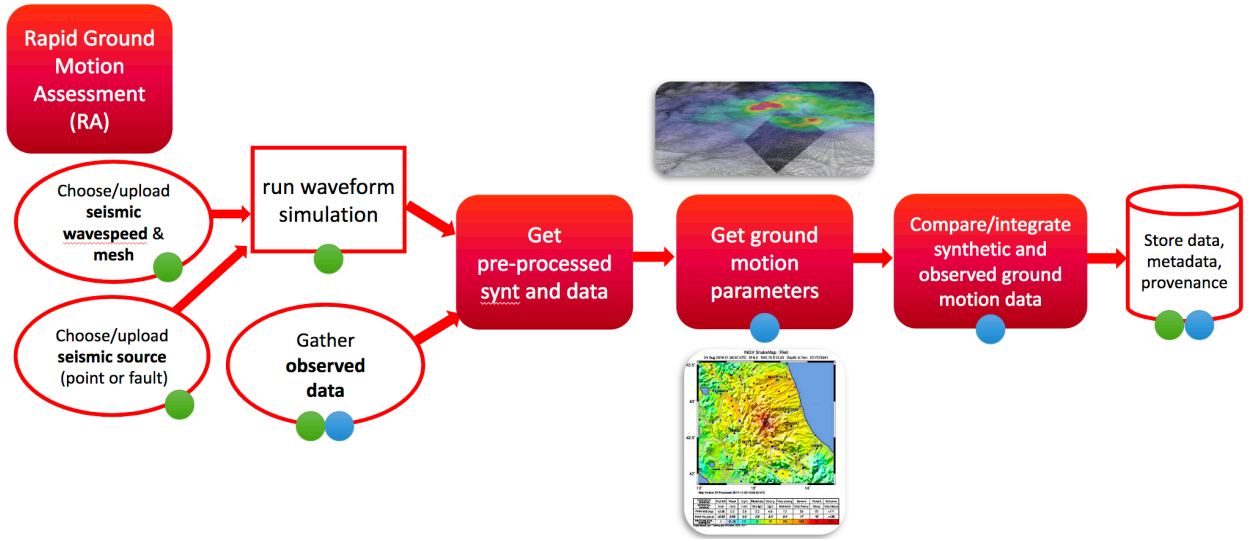


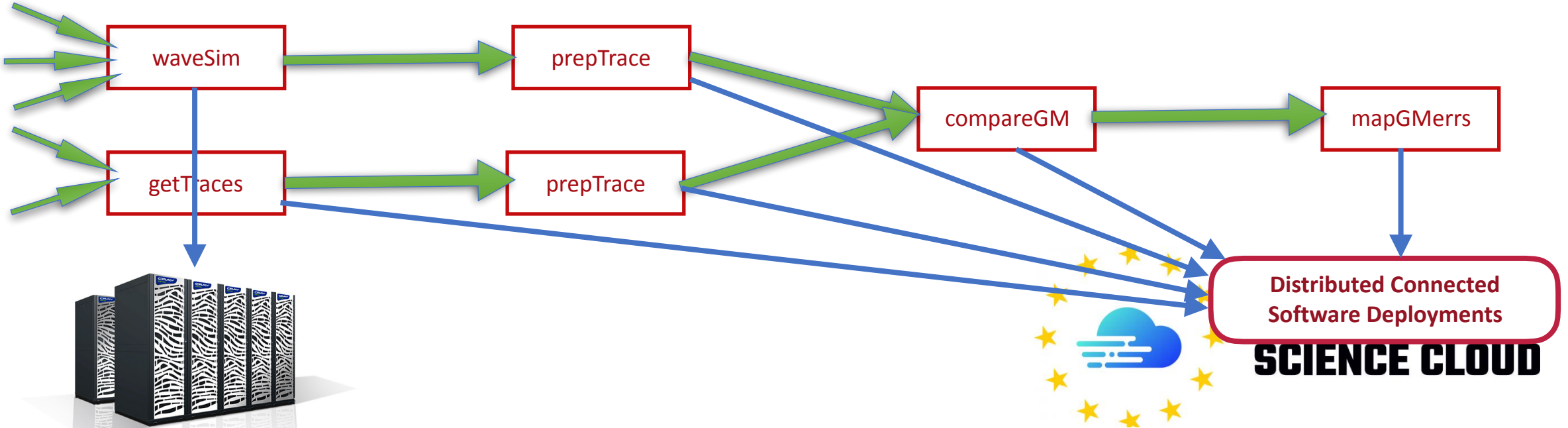


Seismic example summary

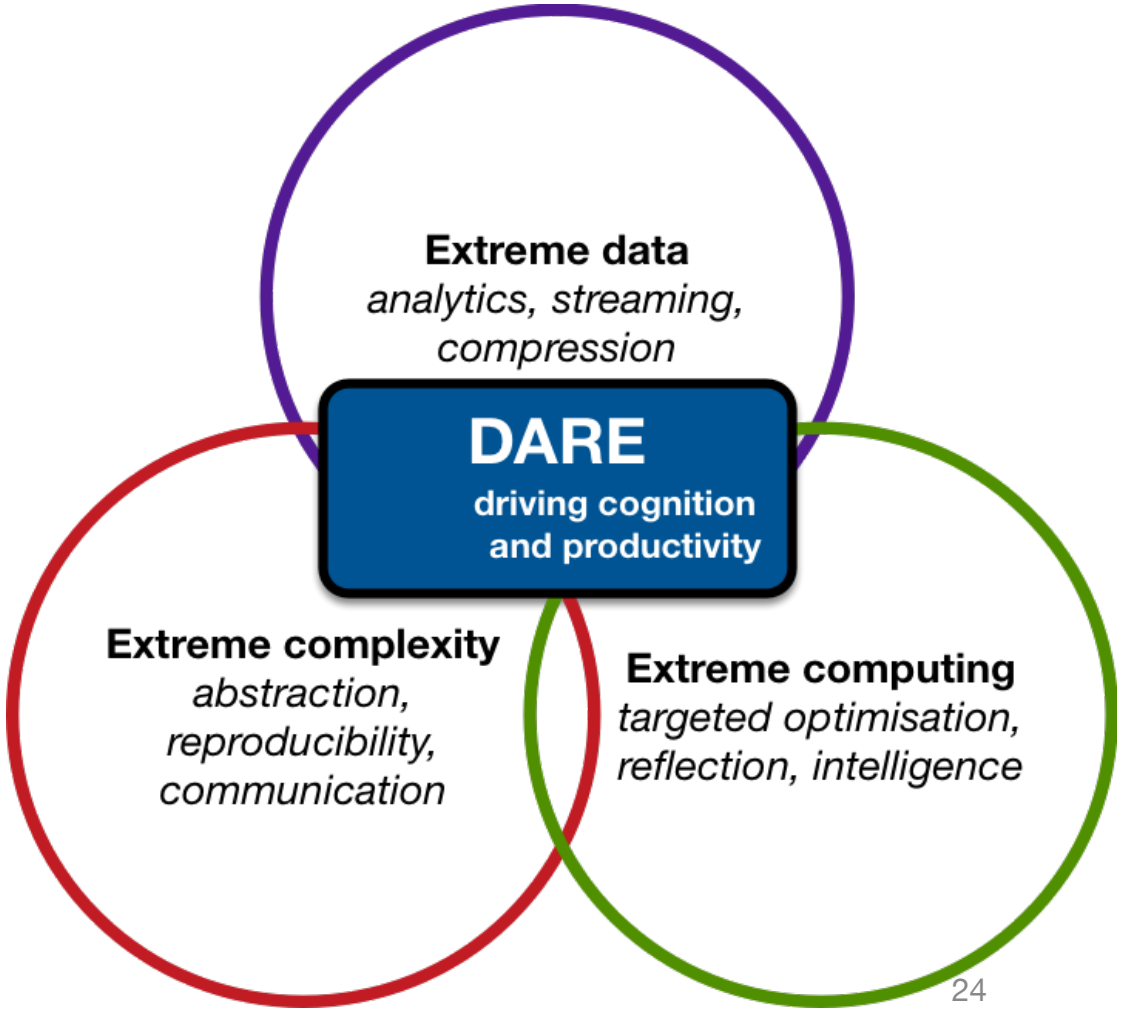
Key

- concept & representation input/output
- validated data flow
- linking an entity with a descriptive concept
- the target could enact the action
- action optimised and mapped to target
- action: action
- config: a distributed deployment of services and software stacks





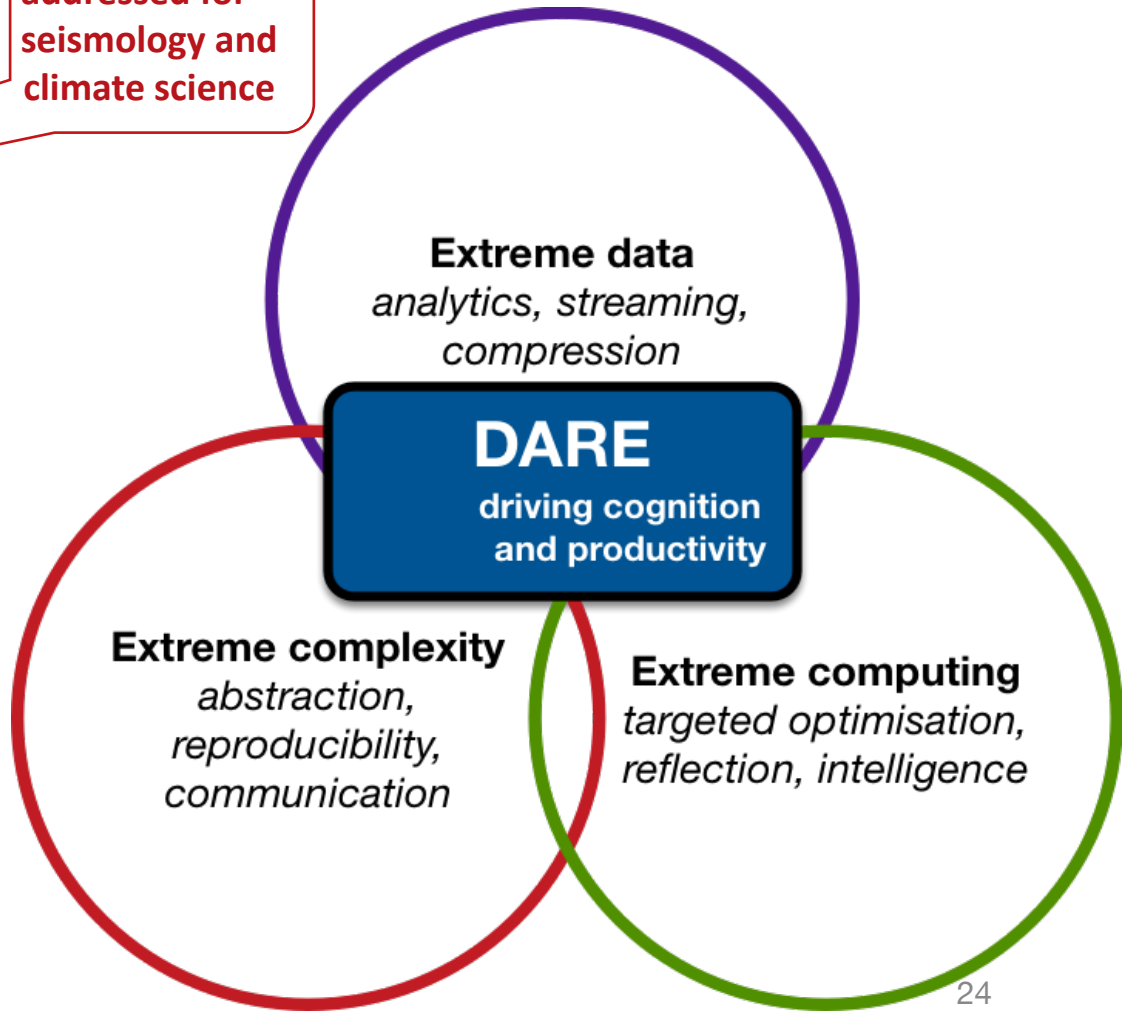
Summary to take home



Summary to take home

- Growth unlimited and sustained
  - Data
  - Computation
  - Complexity

Simultaneously addressed for seismology and climate science



Summary to take home

- Growth unlimited and sustained
  - Data
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  - Complexity
- Challenges demanding and urgent

Simultaneously addressed for seismology and climate science

Innovation and access to new capabilities via sustainable framework bridging from concepts to resources

Summary to take home

- Growth unlimited and sustained
  - Data
  - Computation
  - Complexity
- Challenges demanding and urgent
- Conserving scarce resources
  - Human intellectual effort
  - Willingness to collaborate
  - Energy / GHG emissions

Simultaneously addressed for seismology and climate science

Innovation and access to new capabilities via sustainable framework bridging from concepts to resources

Delivered via the CMDC quartet, work contexts, provenance-driven tools and optimisation

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Simultaneously addressed for seismology and climate science

DARE advances:
new API for developers
dispel4py + CWL workflows
SPECFEM3D on demand
Jupyter notebook sessions
Pervasive provenance + tools
imminent:
conceptualisation

Innovation and access to new capabilities via sustainable framework bridging from concepts to resources

Delivered via the CMDC quartet, work contexts, provenance-driven tools and optimisation

Thank you

Luca Trani, Malcolm Atkinson, Daniele Bailo, Rossana Paciello and Rosa Filgueira, *Establishing Core Concepts for Information-Powered Collaborations*, FGCS vol. 89, 421-437, 2018.

Malcolm Atkinson, Rosa Filgueira, Iraklis Klampanos, Antonis Koulourikos, Amrey Krause, Federica Magnoni, Christian Pagé, Andreas Rietbrock and Alessandro Spinuso *Comprehensible control for researchers and developers facing data challenges*, to appear in proceedings of IEEE eScience, 2019; https://drive.google.com/open?id=1JT6RdaFV0pTQ8aWx-8LY8etXlvd5mRag.

Thank you

L. Schubert, K. G. Jeffery, *New Software Engineering requirements in Clouds and large-scale systems*, IEEE Cloud Computing 2 (1) 48–58, 2015.

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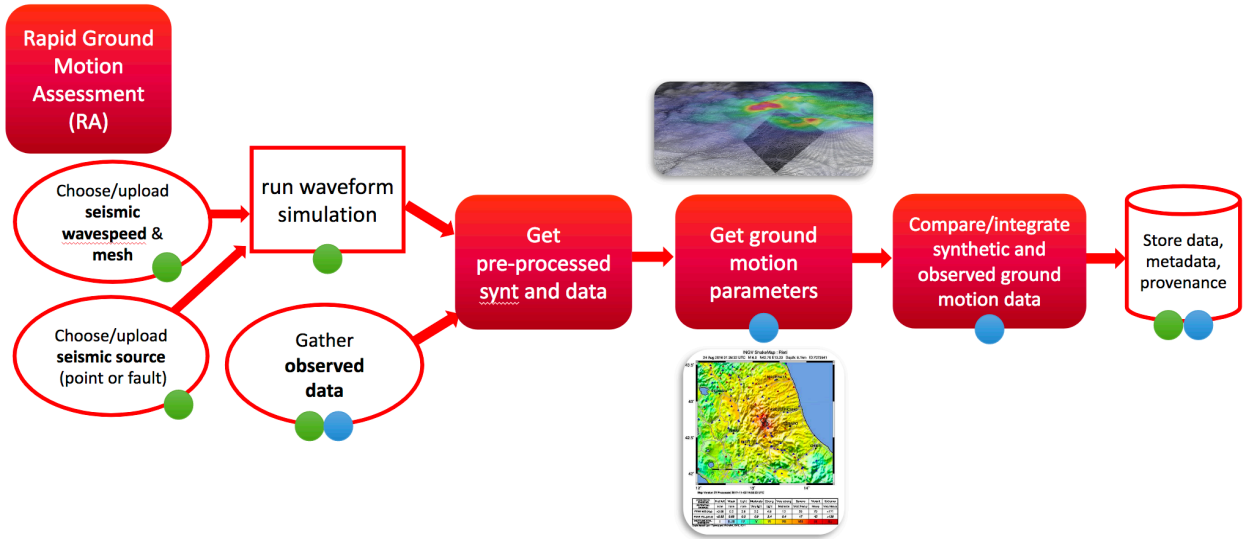
reserve material beyond here

Part seismic example



Part seismic example

Today

choose set of seismic stations

retrieve traces into local dir 1

prep or reject in local dir 2

start time & duration

prep parameters

user-driven actions forming collections in directories

Rapid Ground Motion Assessment (RA)

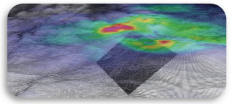
Choose/upload **seismic wavespeed & mesh**

Choose/upload **seismic source** (point or fault)

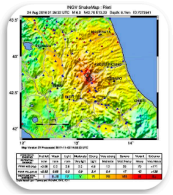
run waveform simulation

Gather **observed data**

Get pre-processed synt and data



Get ground motion parameters



Compare/integrate synthetic and observed ground motion data

Store data, metadata, provenance

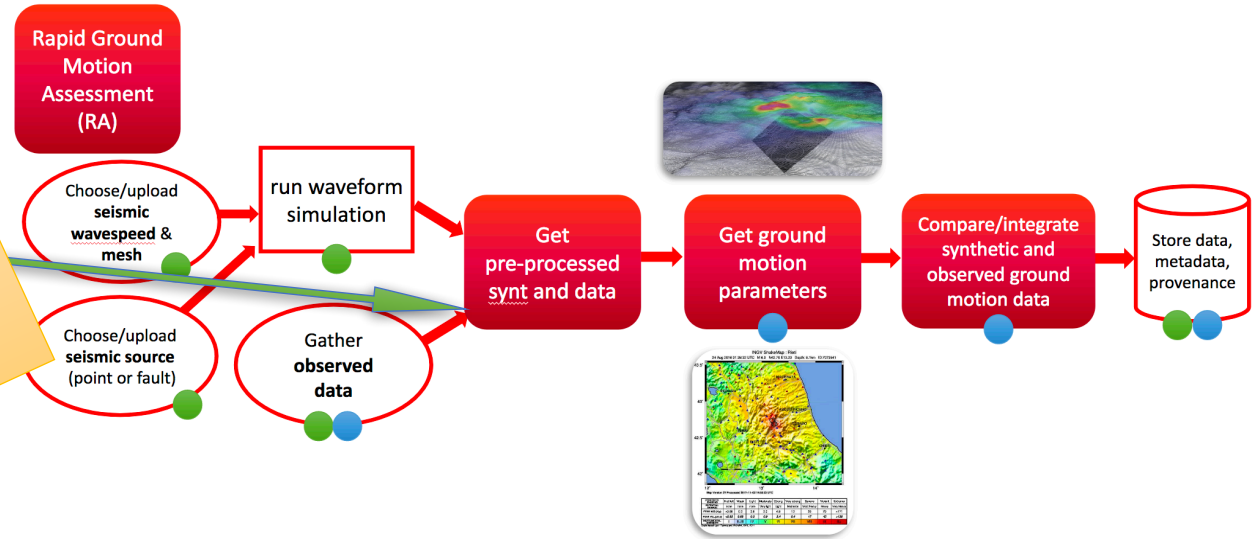
Part seismic example

User-driven consistency

Localised actions

Redundant data movement

Re-evaluate not re-use



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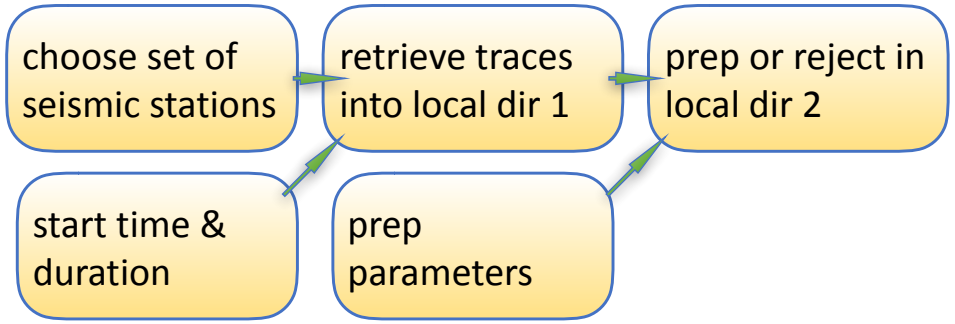
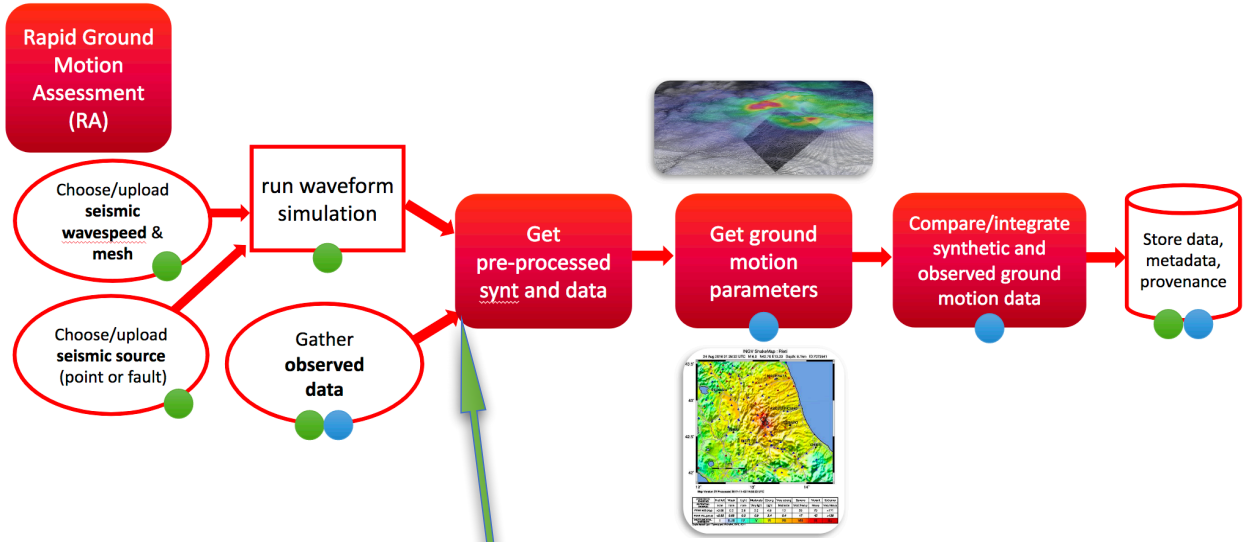




'Tomorrow'

wfcatalog SeisSta { } **setup in shared seismic work context**

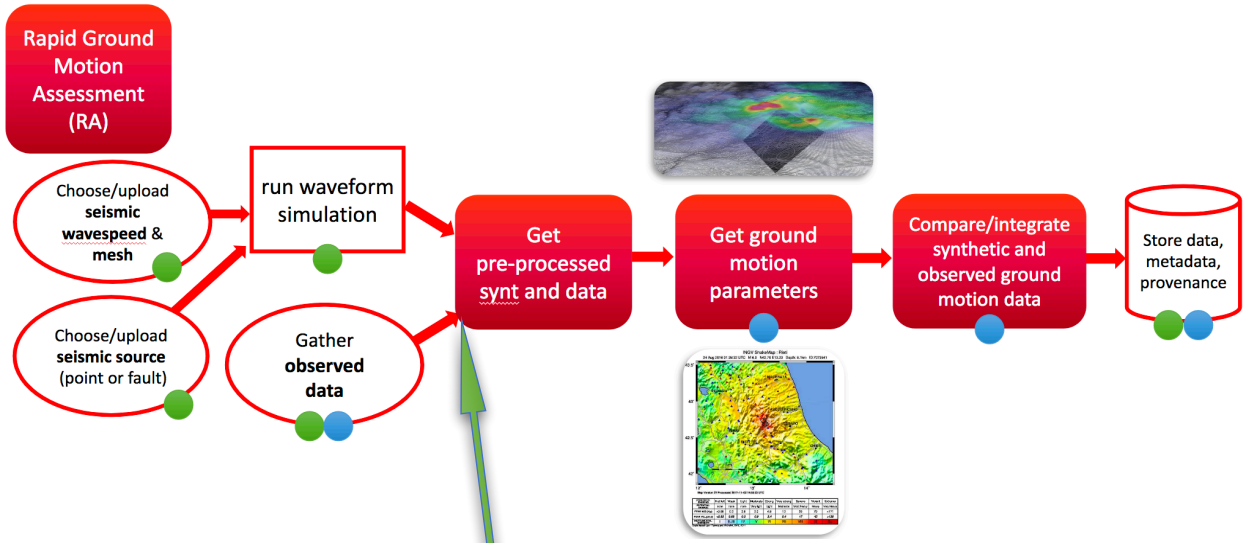
event = … user chooses

seisStations = query wfcatalog for zone(event) union ourDeployment excluding untrusted

traces = tracePrep(seisStations.getTraces(event.start, event.duration+delta, qualCheck))

co-developed by seismologist & developer

Part seismic example



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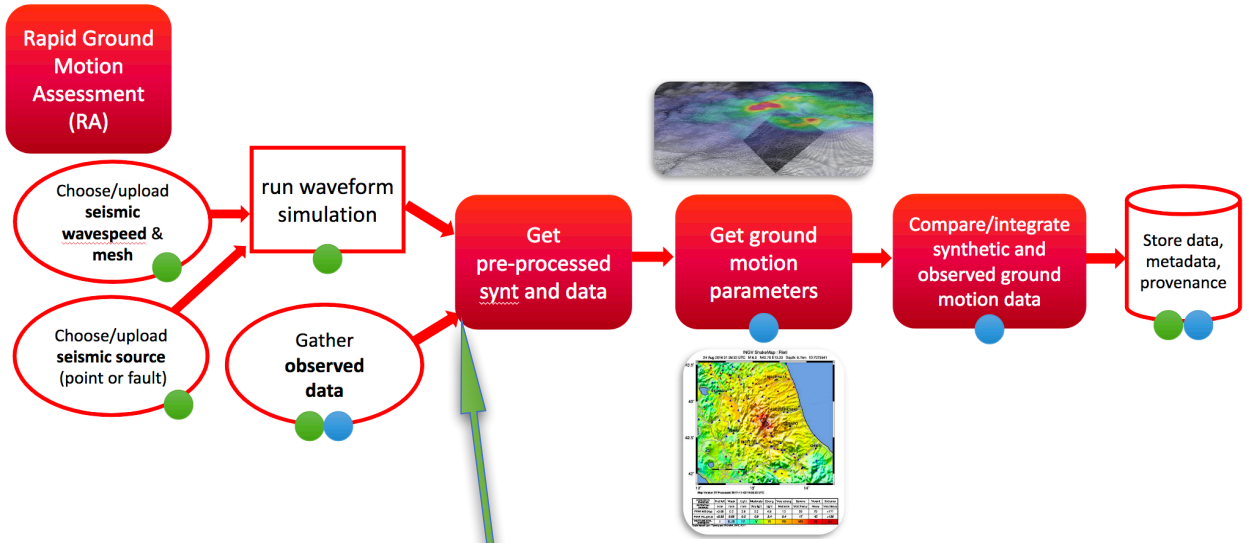

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DARE Dev. Kit makes it easy for developers to deliver to application experts in their preferred form

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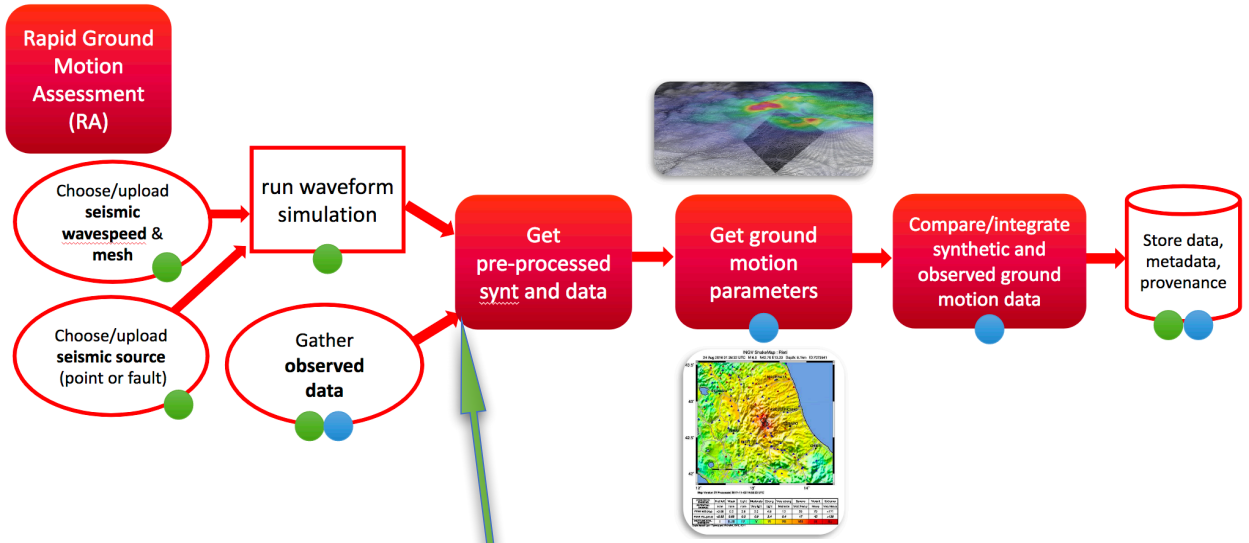

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co-developed by seismologist & developer

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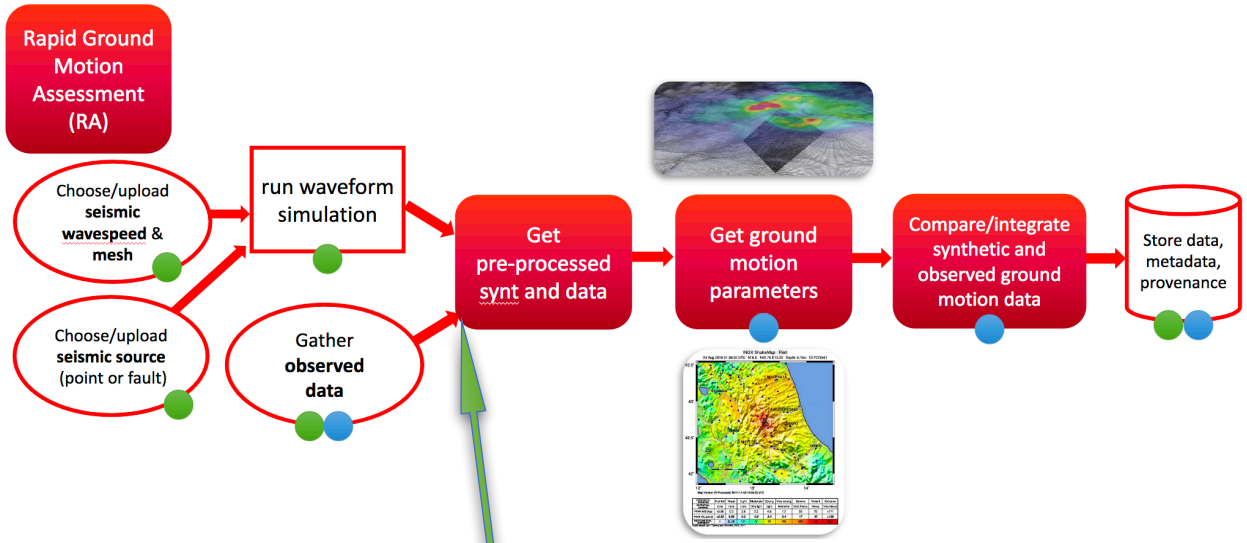
All terms consistently and correctly interpreted via the DKB

Part seismic example



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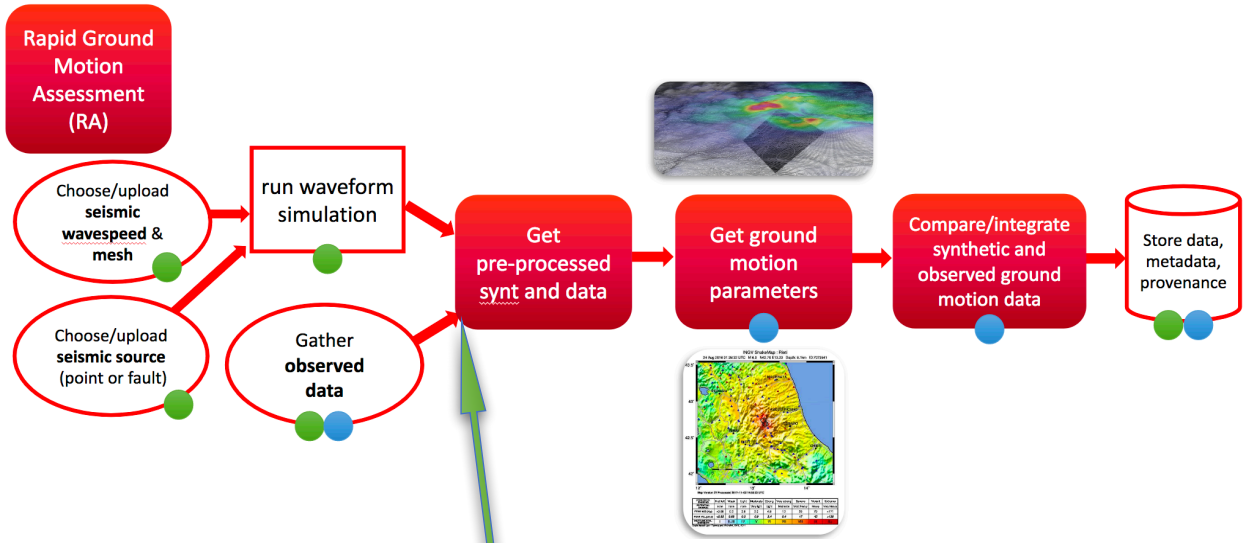

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traces — a virtual collection

seisStations — a virtual collection

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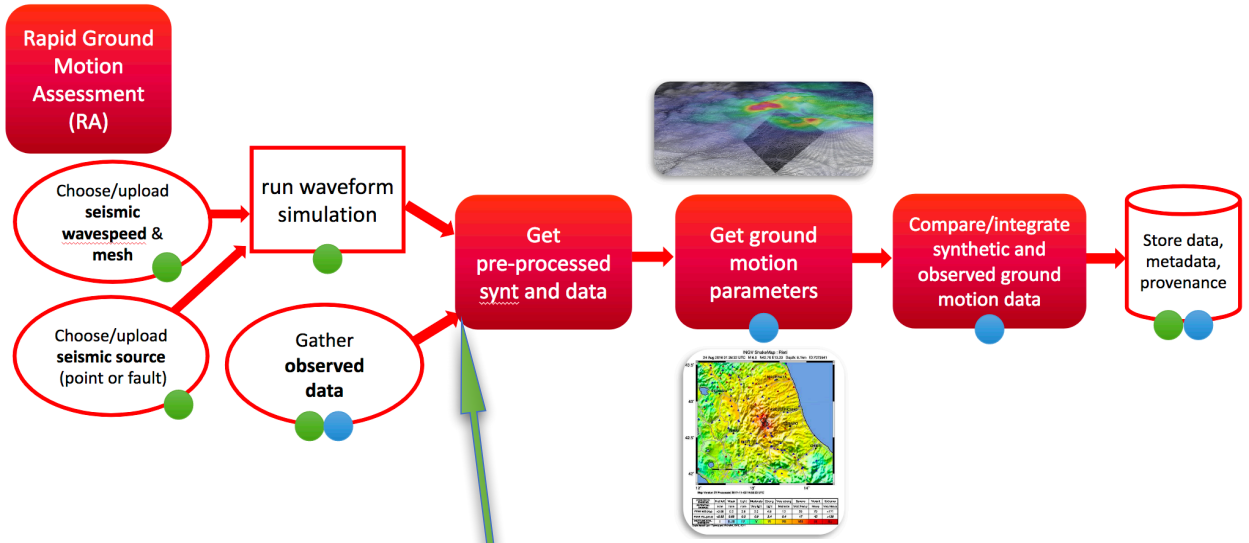

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Key

Concept — Concept

Concept {} — Collection

wfcatalog — Instance identifier

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  - tailored views
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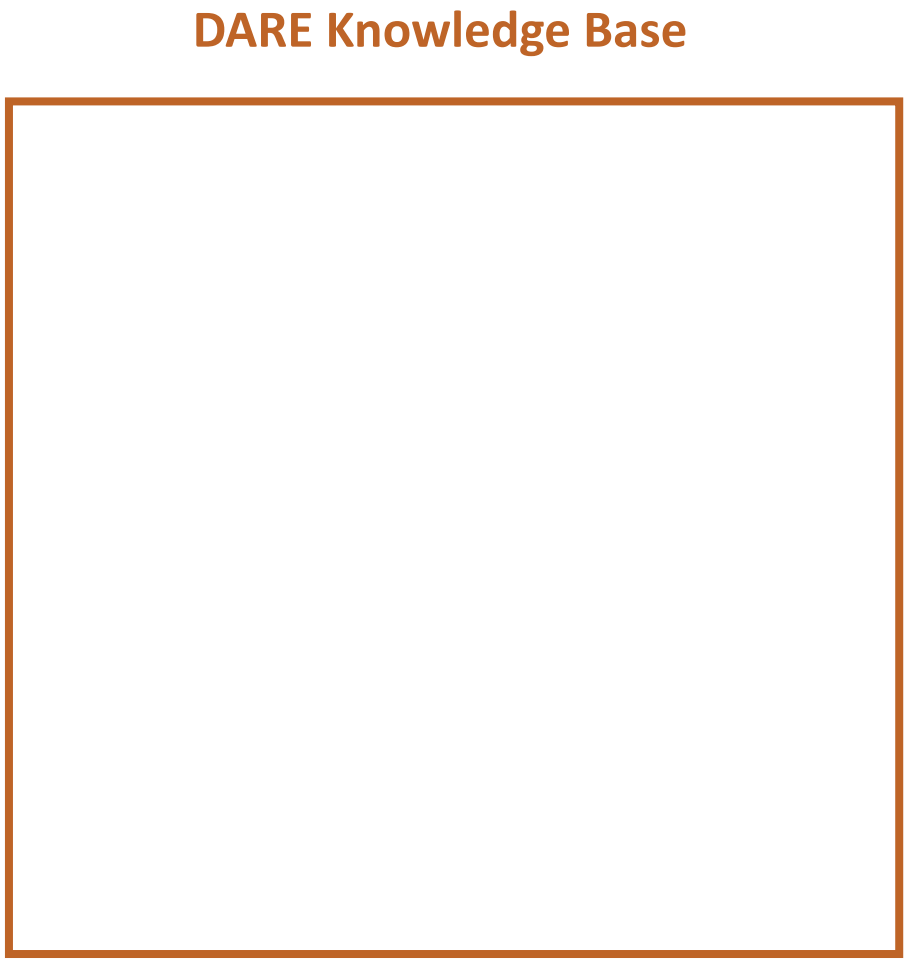

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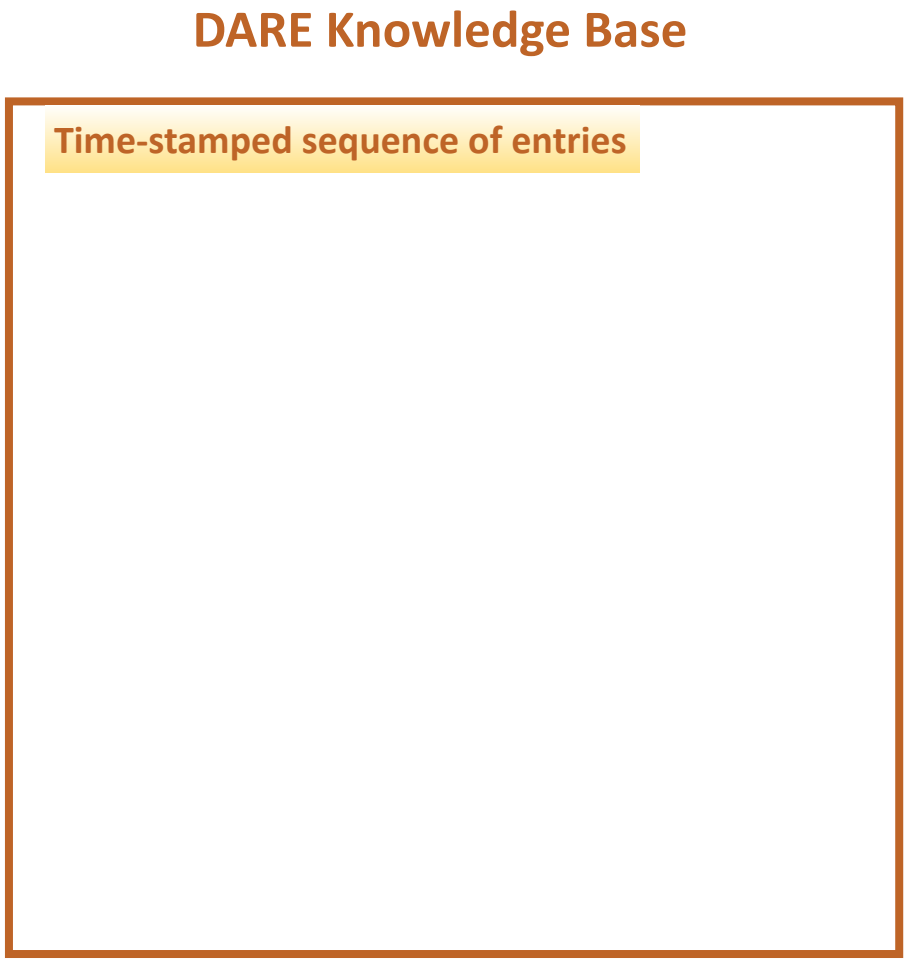

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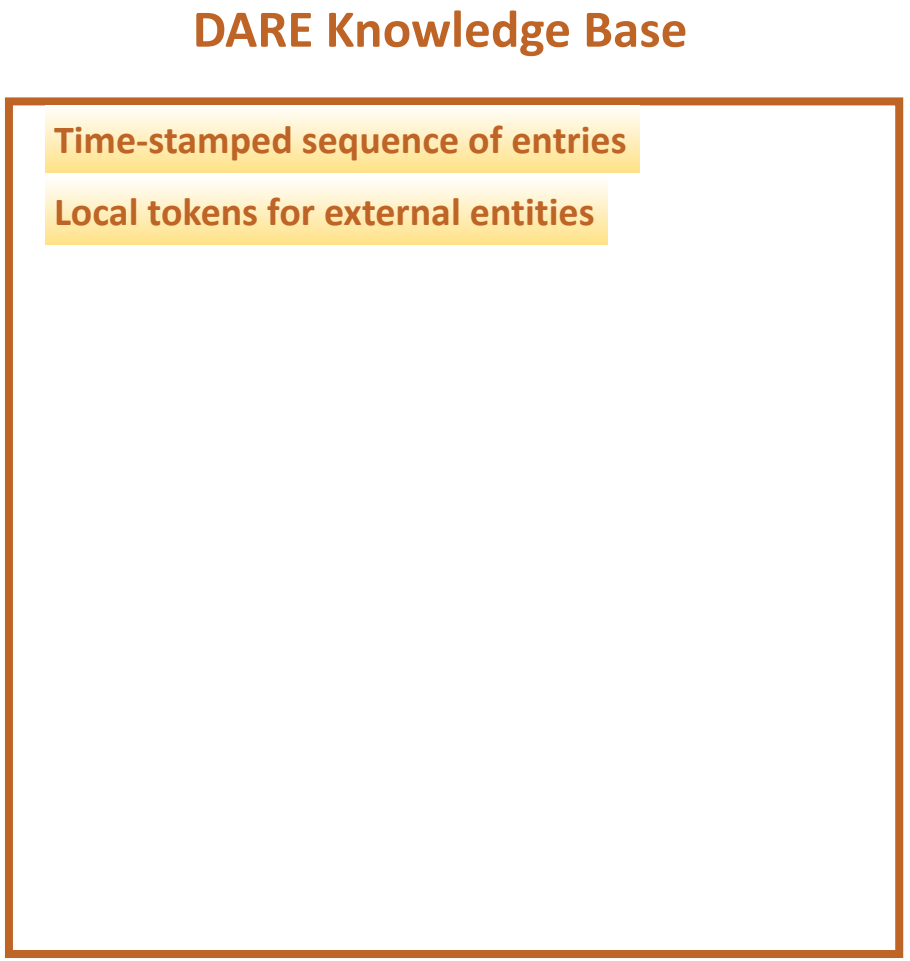

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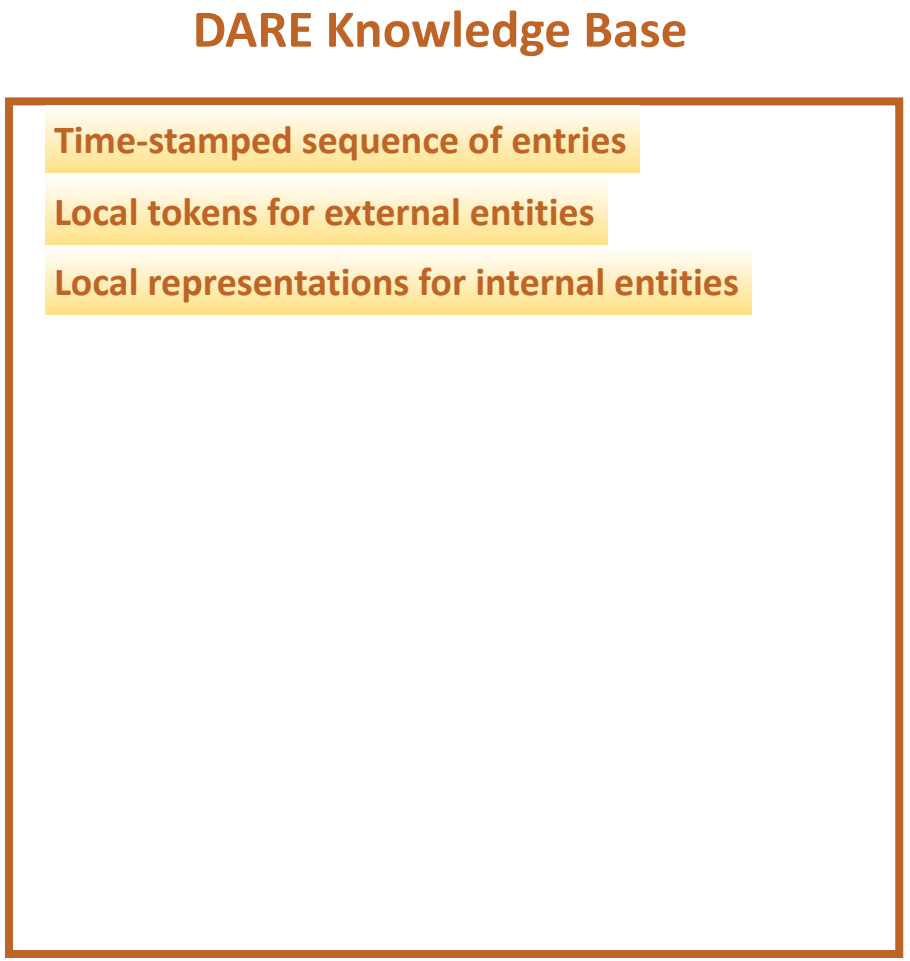

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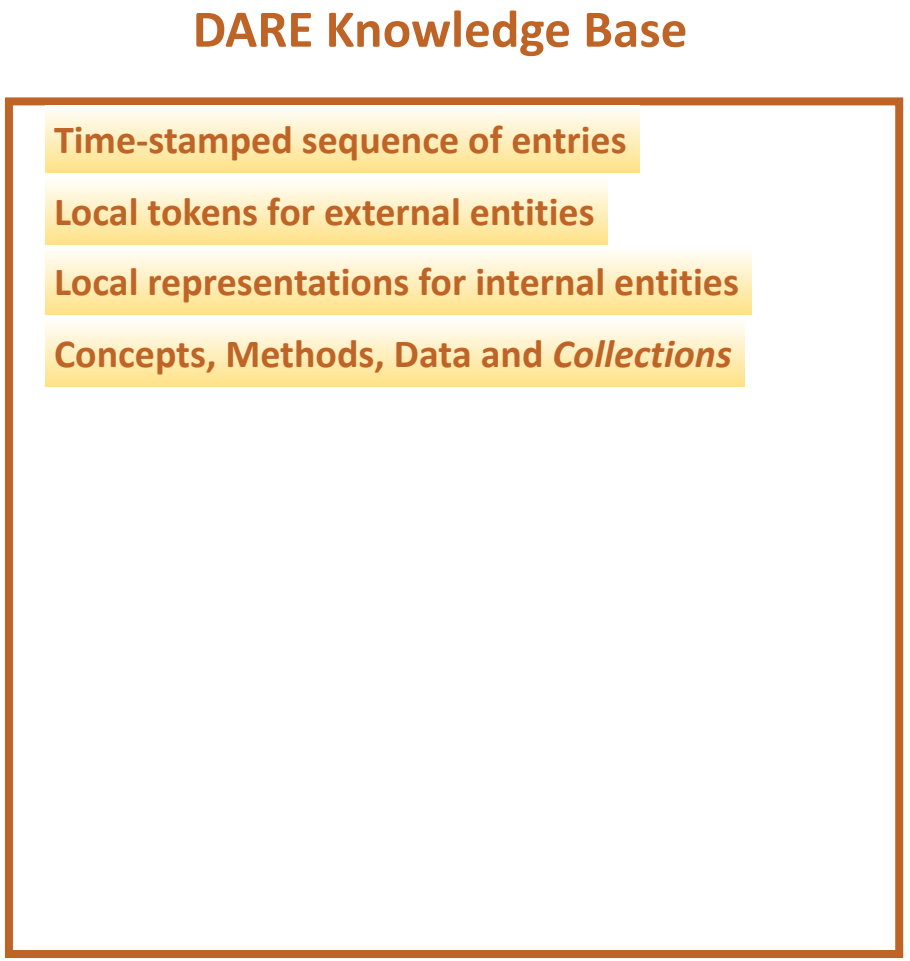

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DARE Knowledge Base

Time-stamped sequence of entries

Local tokens for external entities

Local representations for internal entities

Concepts, Methods, Data and *Collections*

Dynamic populations: create, update, use, discard

Virtual: local control external action + DKB delta

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One DKB per DARE platform deployment updated platform core releases