



Scientific Workflows for V&V of Codes

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Verification/Validation of a Family of Codes:
a scientific activity.

Use of Scientific Workflow Tools for V&V:

- Facilitation
- Repeatability
- Reproducibility
- Transparency
- Commonality
- Cross-checks (comparisons)
- Third party testing

Scientific Workflows for V&V of Codes

Characteristics of a Workflow:

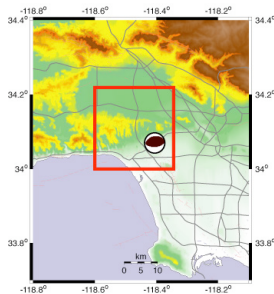
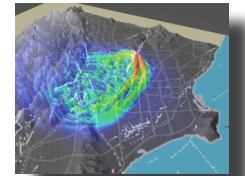
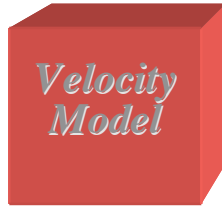
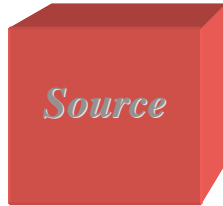
- Distributed computing ("Across-the-Internet").
- Use of existing scientific codes.
- Chain sequence of steps together:
Setup -> execution -> post-run analysis -> curation.
- Provides framework to choose among codes.

Functionality of Workflow Tools (bundle manual tasks using Workflow and Globus Grid tools):

- Submit a task Across-the-Internet for execution.
- Transfer files between platforms.
- Access digital libraries for storage or retrieval.
- Track provenance and scientific metadata.
- "Start" via web GUI or command line trigger.

CME-Earthworks: On Demand Synthetic Seismograms

SCEC, USC, ISI, SDSU, URScorp, CMU, SDSC



• Double-couple point EQ.

• kinematic fault rupture (*in develop.*).

• PEER-verification source.

• various source-time functions.

• Southern California
32.5-35.5°N
115-120°W

• Geographical Frame

• Local Frame (relative km)

- CVM 4.0
- CVM 3.0
- CVM 2.2
- Harvard VM.
- 1D Hadley-Kanamori.
- Constant velocity
- Top layer & halfspace.

- TeraShake2 @HPCC.usc
- TeraShake2 @Teragrid.sdsc
- Graves FD @HPCC.usc
- Graves FD @Teragrid.sdsc

- Carnegie-Mellon FE
- Caltech spectral element

- Intensity measures (PGA-PGV spectral accel.)
- wave processing (debias, filter, vel2accel.).
- PEER deconvol.
- archive (dig. libr.)
- PG map making.
- Viz SDSC
- Viz ISI

Use of Distributed Computing within *Earthworks*

1) define request

2) submit

3) prepare code
input files

4) prepare media
(V_p - V_s - ρ)

transfer

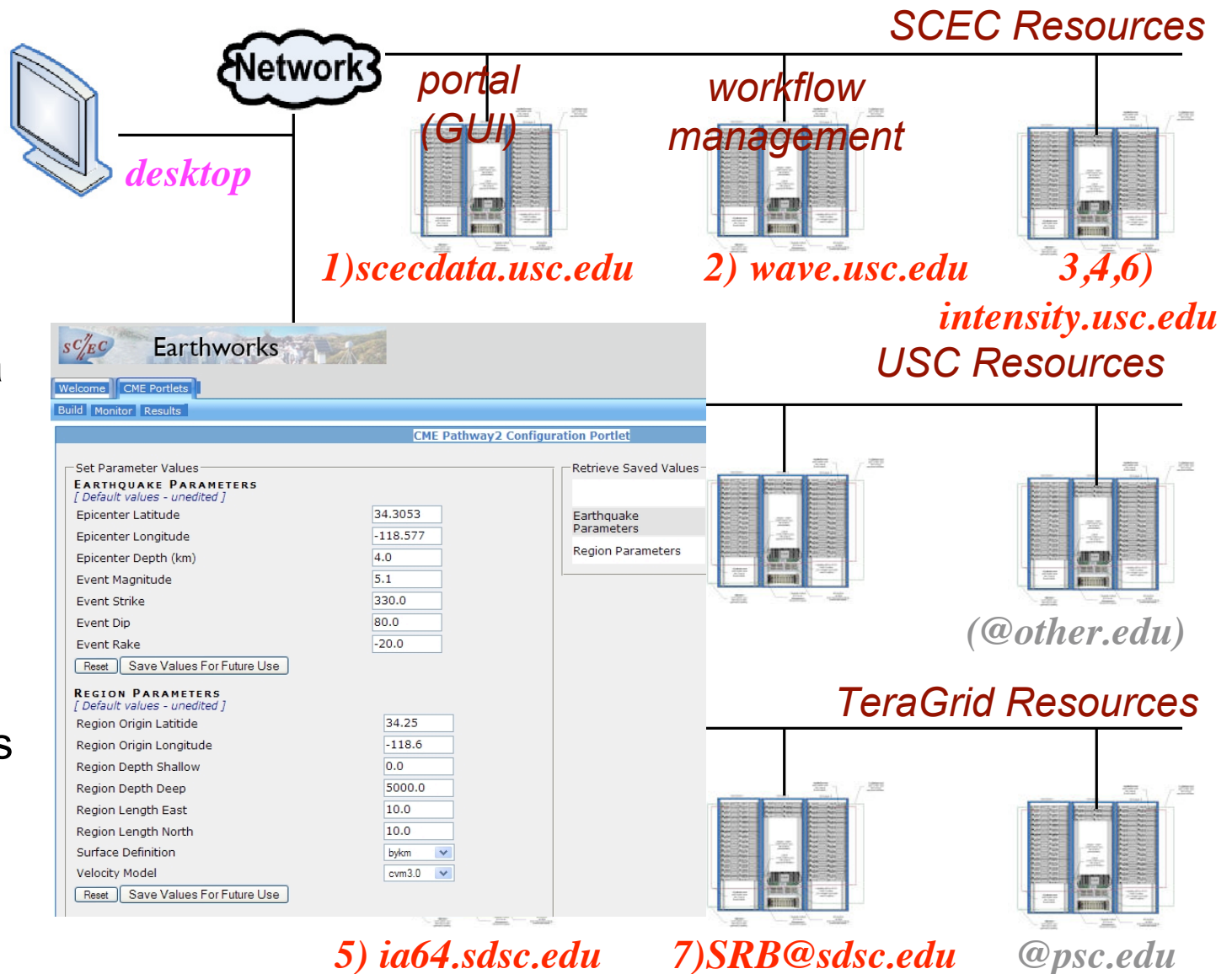
5) run code

transfer

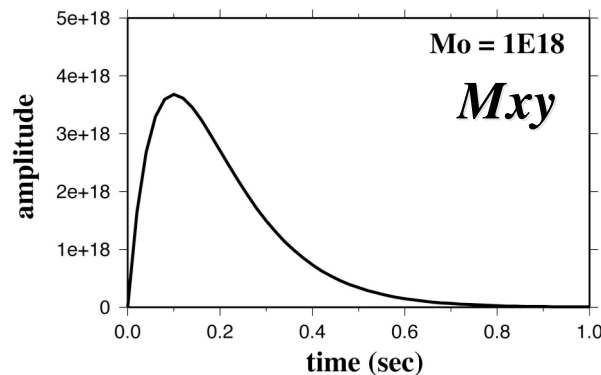
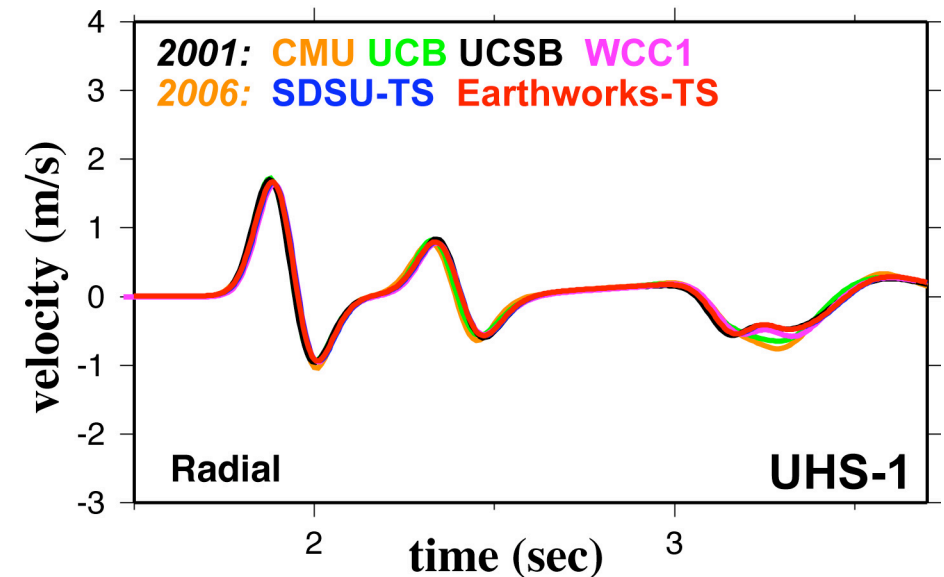
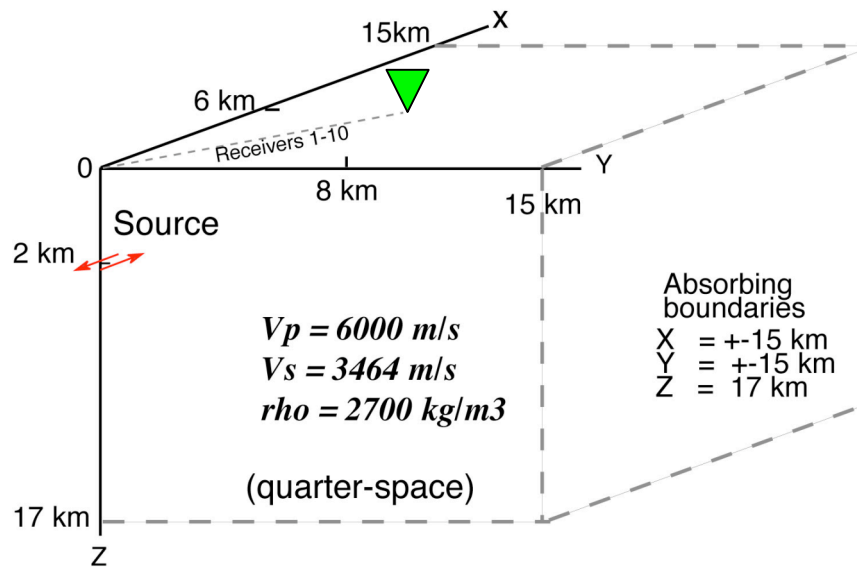
6) analyze results

transfer

7) digital library



SCEC Validation Group (2001): Verification Test #UHS-1 of Seismic Wave Prop. Codes



Suite of Tests:
(2001) set of analytical problems.
(2002) LA basin earthquakes

Considerations when using Workflows for Rupture Dynamics Code Validation

Construction of Benchmarks and Comparison Metrics:

- Community (scientific) activity.

Workflow Tools can be used for:

- End-to-end runs.
- Parsed into simulation, comparison workflows.
- Used just for computations which need distributed computing.

"Starting point" strategy:

- Common starting point vs. pre-made inputs.

Workflow-enabled codes:

- As is, with translator utilities.
- Or minor adjustments (removal of hard-codes, use of metadata).
- OK to bundle or wrap codes (shellscripts).



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