IN43B-1738: Using CyberShake Workflows to Manage Big Seismic Hazard Data on Large-Scale Open-Science HPC Resources

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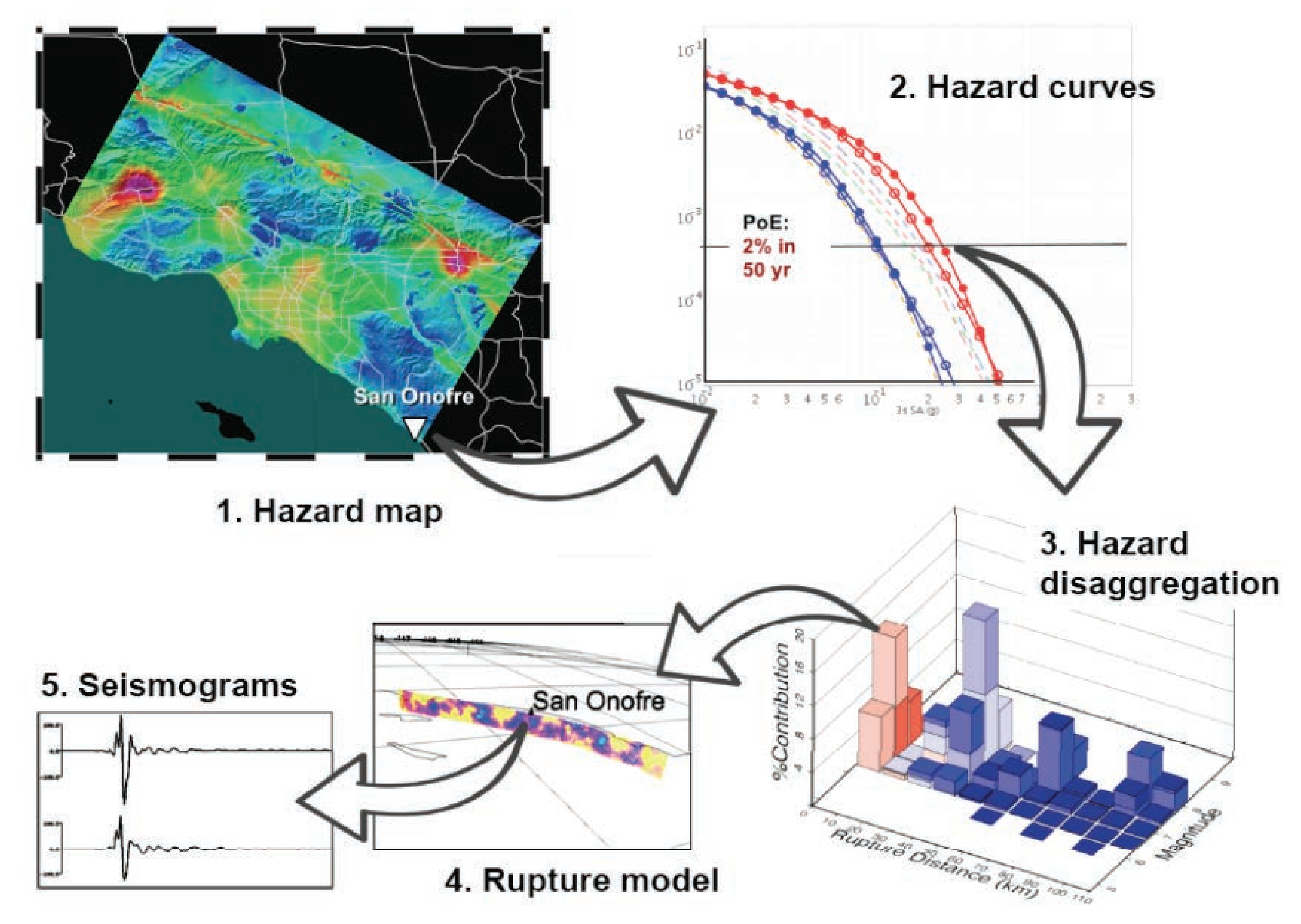
CyberShake Platform

The CyberShake computational platform is an integrated collection of scientific software and middleware that performs 3D physics-based probabilistic seismic hazard analysis (PSHA) for Southern California. The CyberShake platform generates a suite of Strain Green Tensors (SGTs), then uses seismic reciprocity to calculate synthetic seismograms for approximately 500,000 events per site. From these seismograms intensity measures, such as peak spectral acceleration and RotD100 are calculated, and combined with probabilities from the UCERF 2 ERF into a PSHA curve for the site of interest. Hazard curves from hundreds of sites are combined into a hazard map for a region.

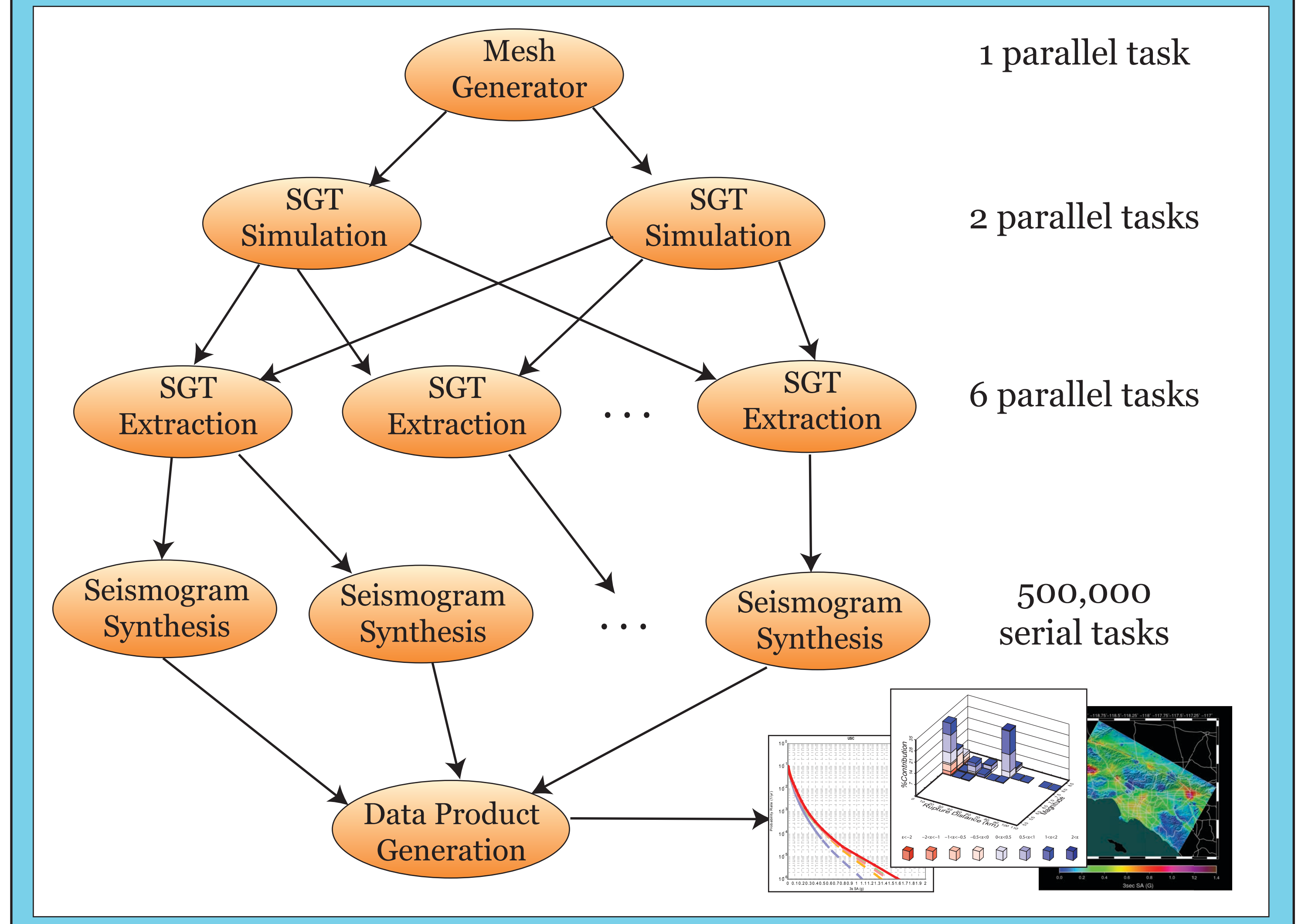
Each map has 336 sites; each site has 500,000 seismograms; and each seismogram has 120 intensity measures, meaning over 20 billion data products are calculated for each CyberShake model.



The CyberShake hazard model contains multiple layers of information, as illustrated by the image above.
(1) Hazard map for the LA region
(2) Hazard curves for a single site.
(3) Disaggregation of hazard in terms of magnitude and distance.
(4) Rupture with the highest hazard at the site (a nearby offshore fault)
(5) Seismograms simulated for this rupture.

CyberShake Computational Overview

CyberShake includes executables which range from single-core to GPU MPI jobs, and which require 100 ms - 1 hr of execution time. Below is an overview of the processing stages involved to calculate results for 1 location. Details of each stage are in the table below.


Mesh Generator
1 parallel task
SGT Simulation
SGT Simulation
2 parallel tasks
SGT Extraction
SGT Extraction
. . .
SGT Extraction
6 parallel tasks
Seismogram Synthesis
Seismogram Synthesis
. . .
Seismogram Synthesis
500,000 serial tasks
Data Product Generation

To manage these wide-ranging tasks and their data, CyberShake integrates large-scale parallel and high-throughput serial seismological research codes into a scientific workflow framework. We use a software stack including Pegasus-WMS, HTCondor, and Globus GRAM.

One big challenge for 2015 was migrating from 0.5 Hz to 1 Hz simulated seismic frequency. This resulted in the following increases in computational requirements:

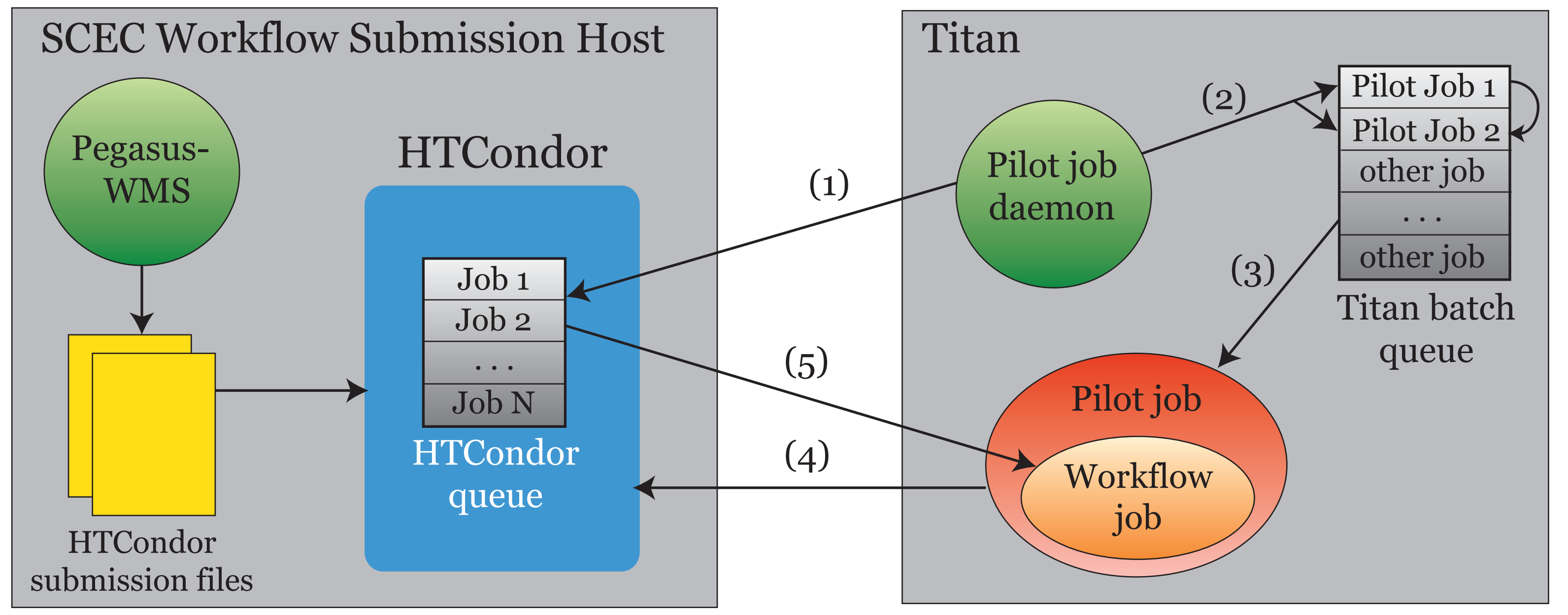
Component	0.5 Hz Data	1 Hz Data	Data Factor	0.5 Hz SUs	1 Hz SUs	Compute Factor
Mesh generation	15 GB	120 GB	8x	50 CPU-hrs	1400 CPU-hrs	28x
SGT Simulation	40 GB	1.5 TB	40x	200 GPU-hrs	1500 GPU-hrs	7.5x
SGT Extraction	690 GB	47 TB	70x	275 CPU-hrs	88,000 CPU-hrs	320x
Seismogram Synthesis	12 GB	32 GB	2.7x	2,300 CPU-hrs	101,000 CPU-hrs	43x
Data Product Generation	1 MB	1 MB	1x	1 CPU-hr	1 CPU-hr	1x

CyberShake Study 15.4

In 2015, we performed a large CyberShake study on NCSA Blue Waters and OLCF Titan. This calculation produced the first physics-based PSHA map for Southern California at 1.0 Hz, and calculated new intensity measures (RotD100) requested by engineers.

CyberShake Workflows

Our workflow tool stack (Pegasus-WMS, HTCondor) ran CyberShake workflows across multiple large-scale systems. On Blue Waters, we used Globus GRAM-based remote job submission. Titan does not support remote job submission, so we used pilot jobs, described below.

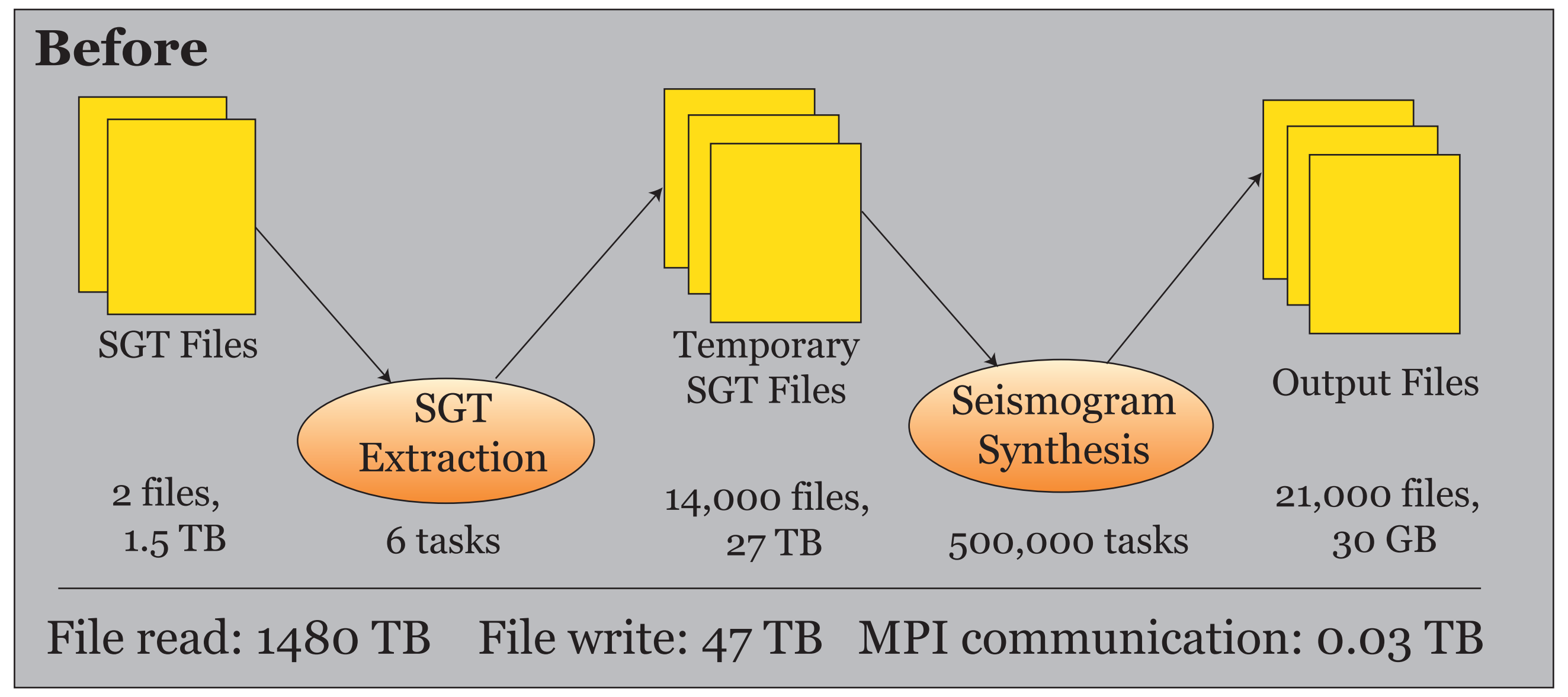

SCEC Workflow Submission Host
Pegasus-WMS
HTCondor
HTCondor submission files
Job 1
Job 2
. . .
Job N
HTCondor queue
Titan
Pilot job daemon
Pilot Job 1
Pilot Job 2
other job
. . .
other job
Titan batch queue
Pilot job
Workflow job
(1)
(2)
(3)
(4)
(5)

(1) Daemon on Titan login node monitors HTCondor queue on the SCEC submit host.
(2) When jobs are found, daemon submits pilot jobs to Titan queue
(3) Pilot job waits in queue, starts up
(4) Pilot job calls back to HTCondor collector, ready for work
(5) HTCondor negotiator assigns work to pilot job

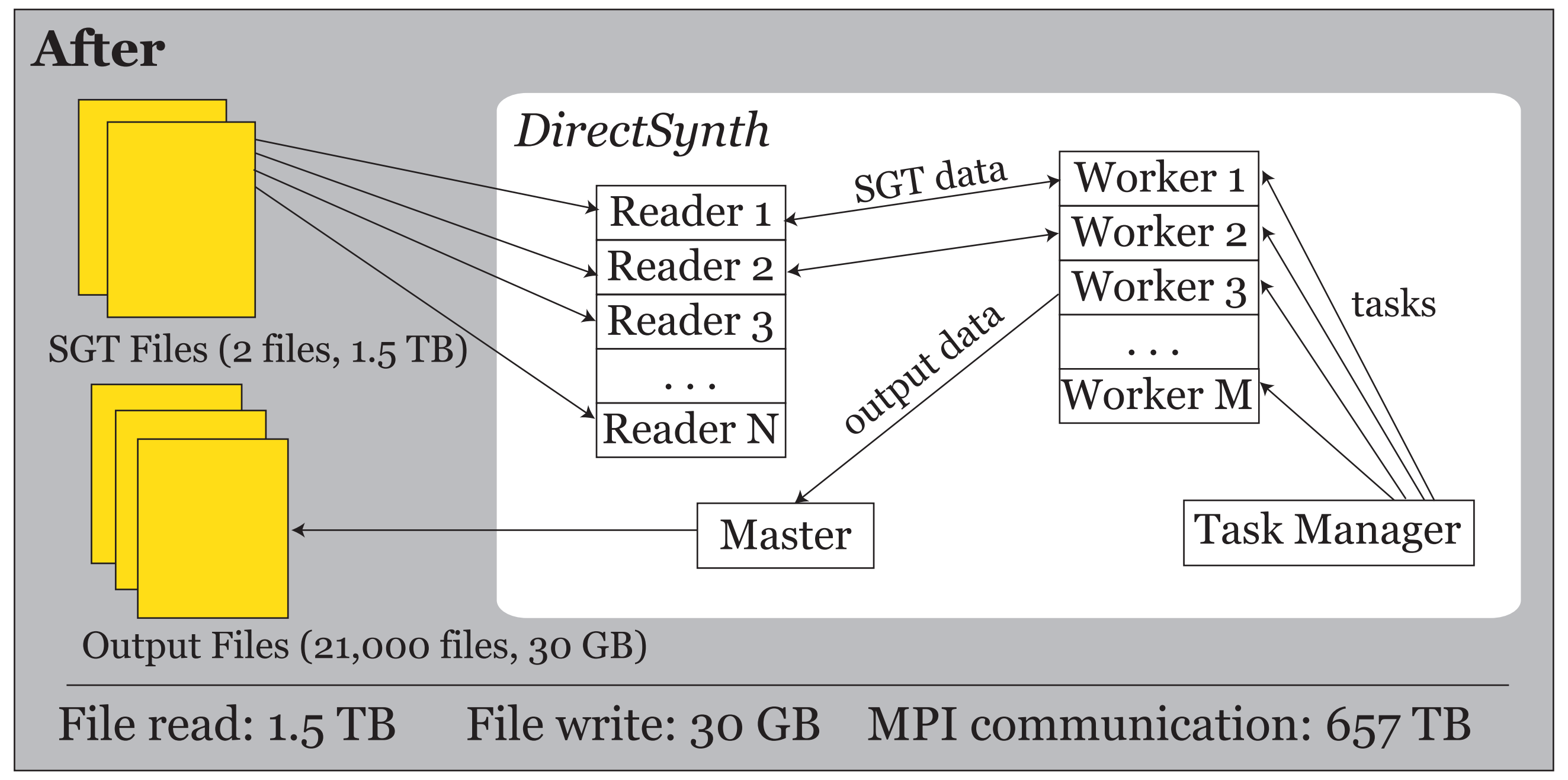
We used pilot jobs of different sizes for the mesh generation and SGT simulation jobs, and used qsub to enforce dependencies between them.

I/O Improvements

Moving from a seismic frequency of 0.5 Hz to 1 Hz resulted in a 40x increase in file I/O. To reduce this, we refactored the SGT Extraction and Seismogram Synthesis steps into a single job to no longer use intermediate files.


Before
SGT Files
2 files, 1.5 TB
SGT Extraction
6 tasks
Temporary SGT Files
14,000 files, 27 TB
Seismogram Synthesis
500,000 tasks
Output Files
21,000 files, 30 GB
File read: 1480 TB File write: 47 TB MPI communication: 0.03 TB

In the refactored code ("DirectSynth"), the input SGT files are read across multiple nodes, and served up to worker nodes on request. Seismogram synthesis jobs are assigned to worker nodes by the task manager. Output data is sent to the master and written centrally to streamline the output I/O and centralize checkpointing.


After
DirectSynth
SGT Files (2 files, 1.5 TB)
Reader 1
Reader 2
Reader 3
. . .
Reader N
SGT data
Worker 1
Worker 2
Worker 3
. . .
Worker M
tasks
output data
Master
Task Manager
Output Files (21,000 files, 30 GB)
File read: 1.5 TB File write: 30 GB MPI communication: 657 TB

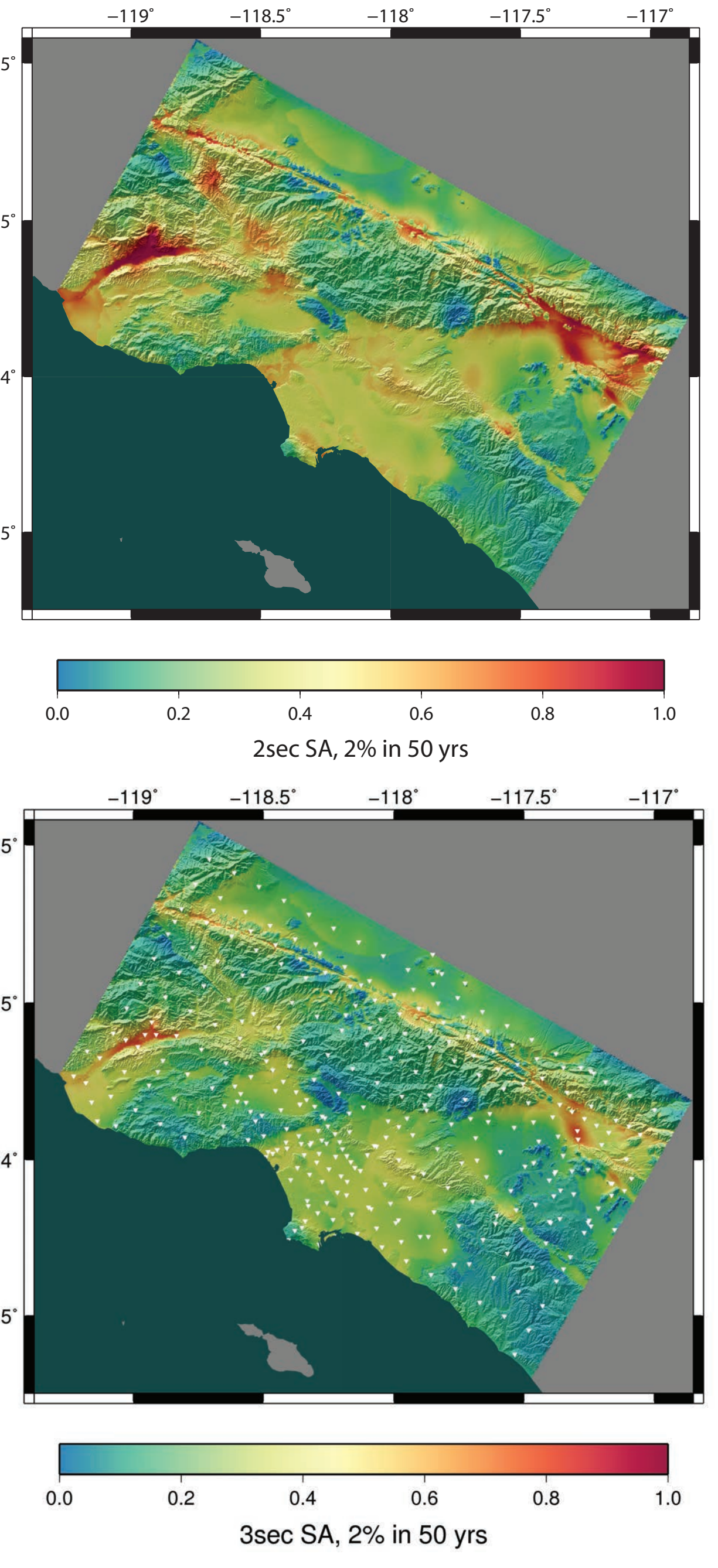
This results in a savings of 99.9% in file I/O and a reduction of 57% in filesystem and MPI communication.

Study 15.4 Technical Enhancements

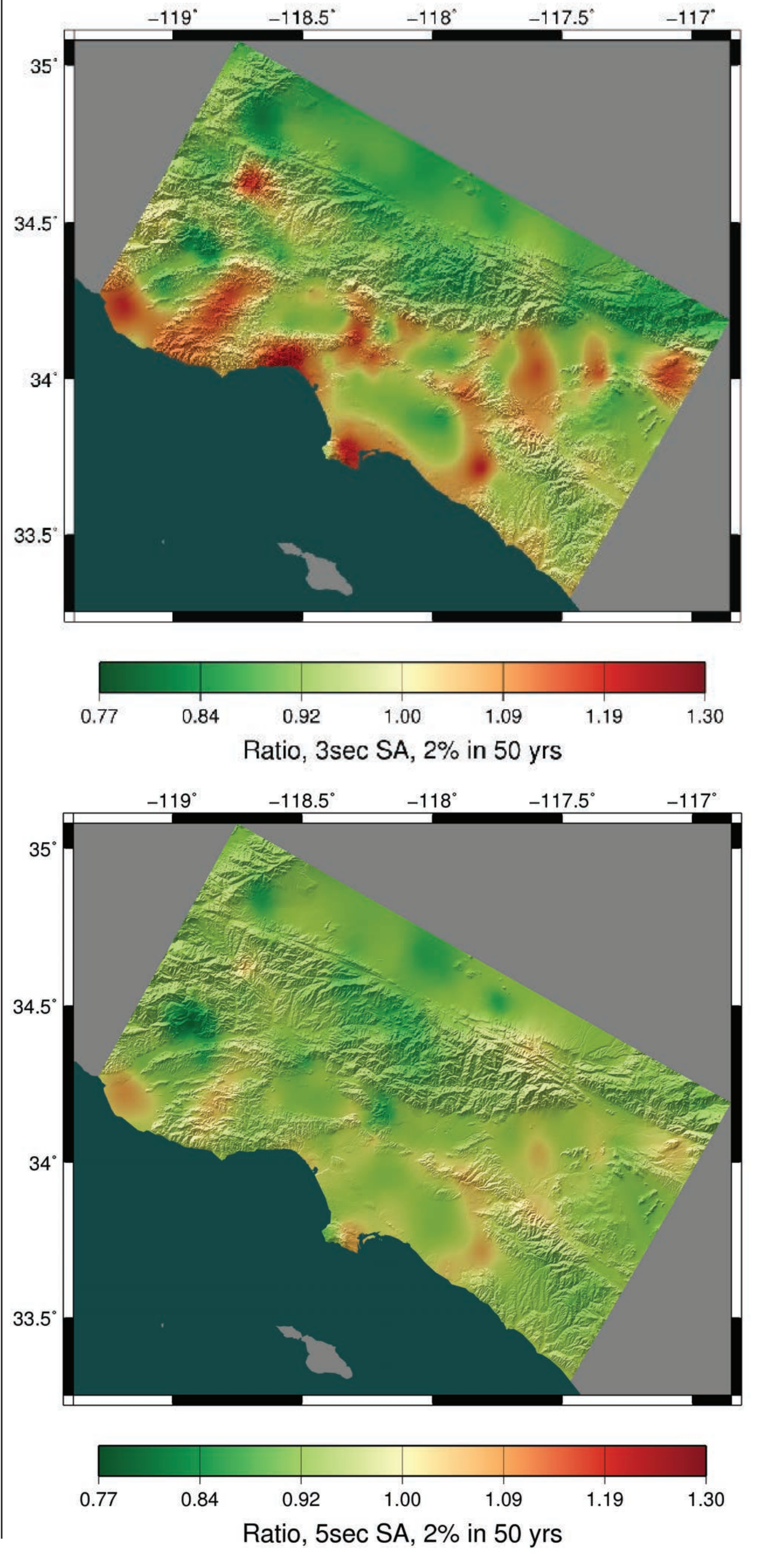
- Redesigned SGT Extraction/Seismogram Synthesis steps to reduce file I/O by 99.9% (see box at left).
- Only GPU software (AWP-ODC-SGT GPU) was used to produce the SGTs.
- Workflows were run on both NCSA Blue Waters and OLCF Titan.

Results

Study 15.4 hazard maps.
2 sec (top) and 3 sec (bottom).



Ratio maps, Study 15.4 (1 Hz) vs Study 14.2 (0.5 Hz).
3 sec (top), 5 sec (bottom).



Future Challenges

We plan to increase the scope of CyberShake to all of California, and to move to the UCERF 3 earthquake rupture forecast, which involves 25x as many earthquakes. Future challenges include:

- **Data management and access.**

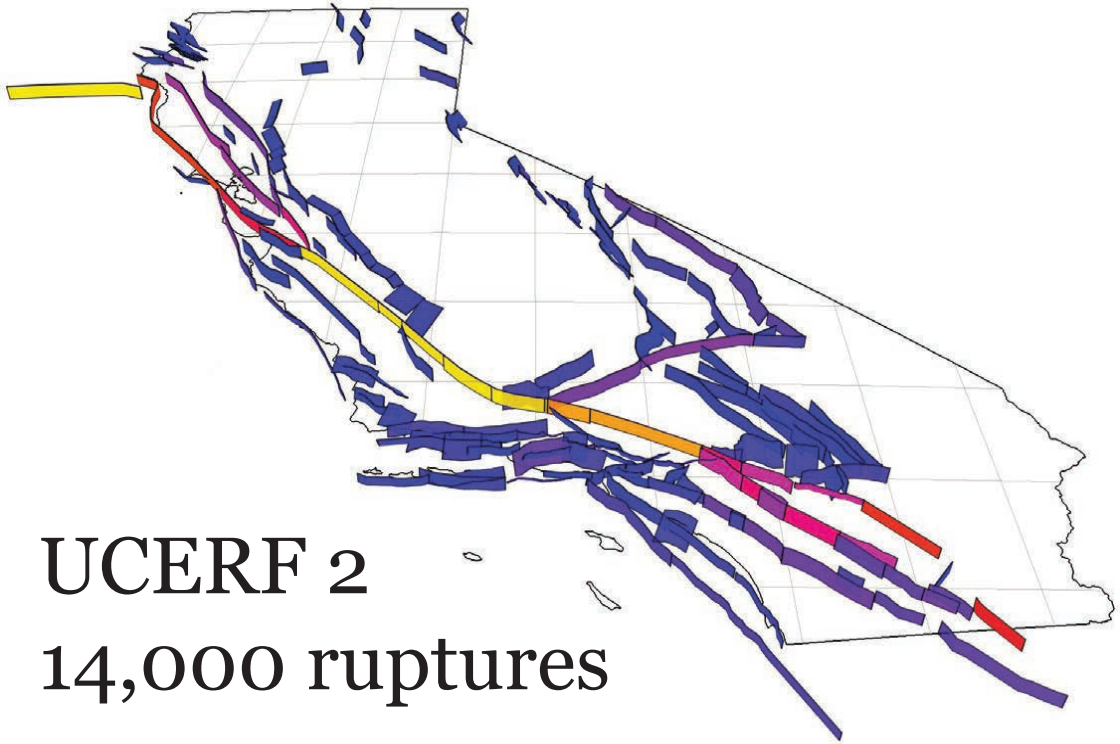
Since CyberShake is a layered model, how do we represent and provide context for users to discover and access desired data?

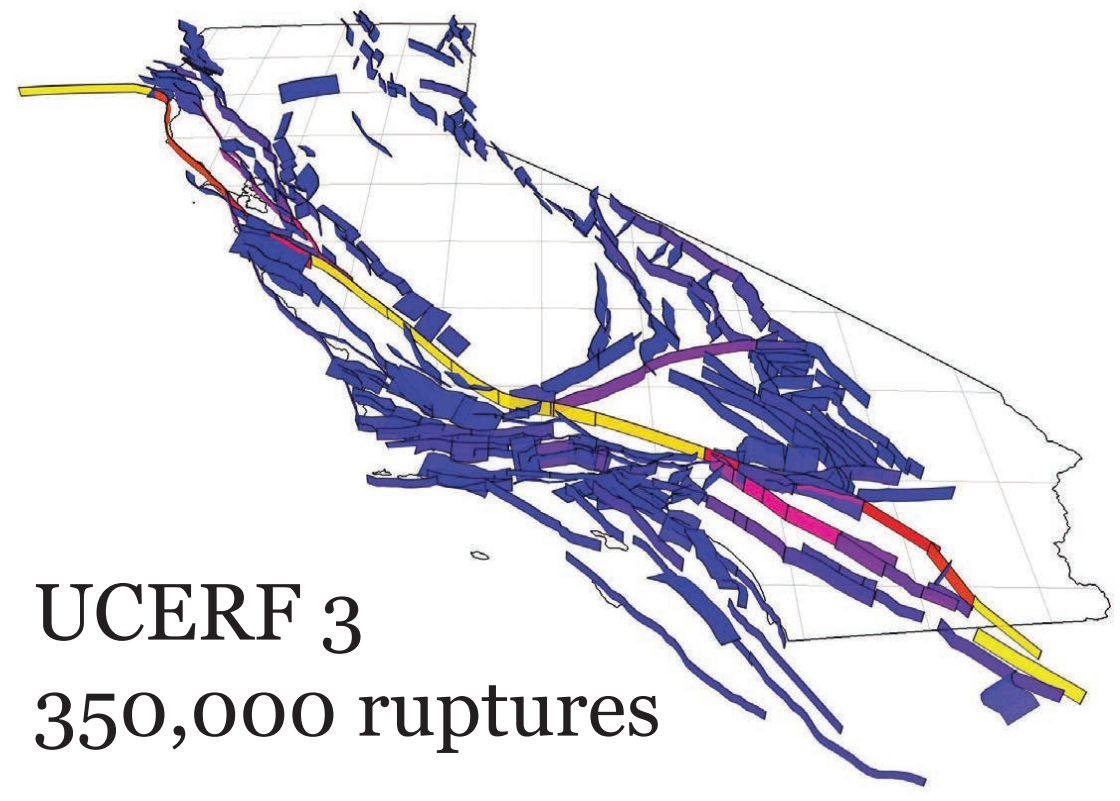
- **Data compression.**

Given that CyberShake data is used by a diverse audience, how do we define "good enough" with lossy compression?

- **Approximation.**

Some UCERF 3 ruptures run the entire state and are very expensive. Can we approximate them with regional ruptures?


UCERF 2
14,000 ruptures


UCERF 3
350,000 ruptures

Study 15.4 Performance Statistics

- 1 Hz PSHA calculations for **336 sites**
- Wallclock time: **914.2 hours** (38.1 days)
- **25,440 CPUs + 1,317 GPUs** used on average
- Peak of 20% of Blue Waters, **80% of Titan**
- **170 million** two-component seismograms generated (52/sec)
- **4332 jobs** submitted automatically to Titan and Blue Waters; 8.6 running, on average
- **510 TB of data** produced, 7.7 TB copied back to SCEC
- This study required 16x more computational work than previous CyberShake studies, but only 9x as much computer time due to code performance improvements.