SC/EC

Simplify Your Science with Workflow Tools

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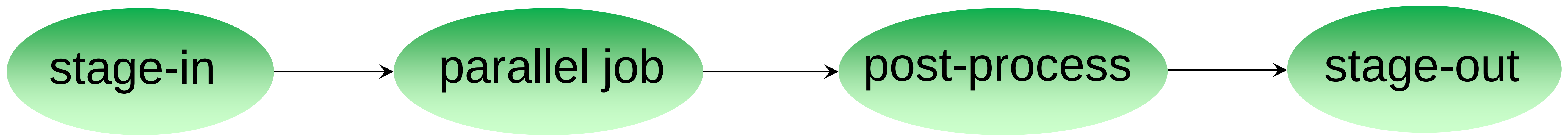
Overview

- What are scientific workflows?
- What problems do workflow tools solve?
- Overview of available workflow tools
- CyberShake (seismic hazard application)
  - Computational overview
  - Challenges and solutions
- Ways to simplify your work
- Goal: Help you figure out if this would be useful

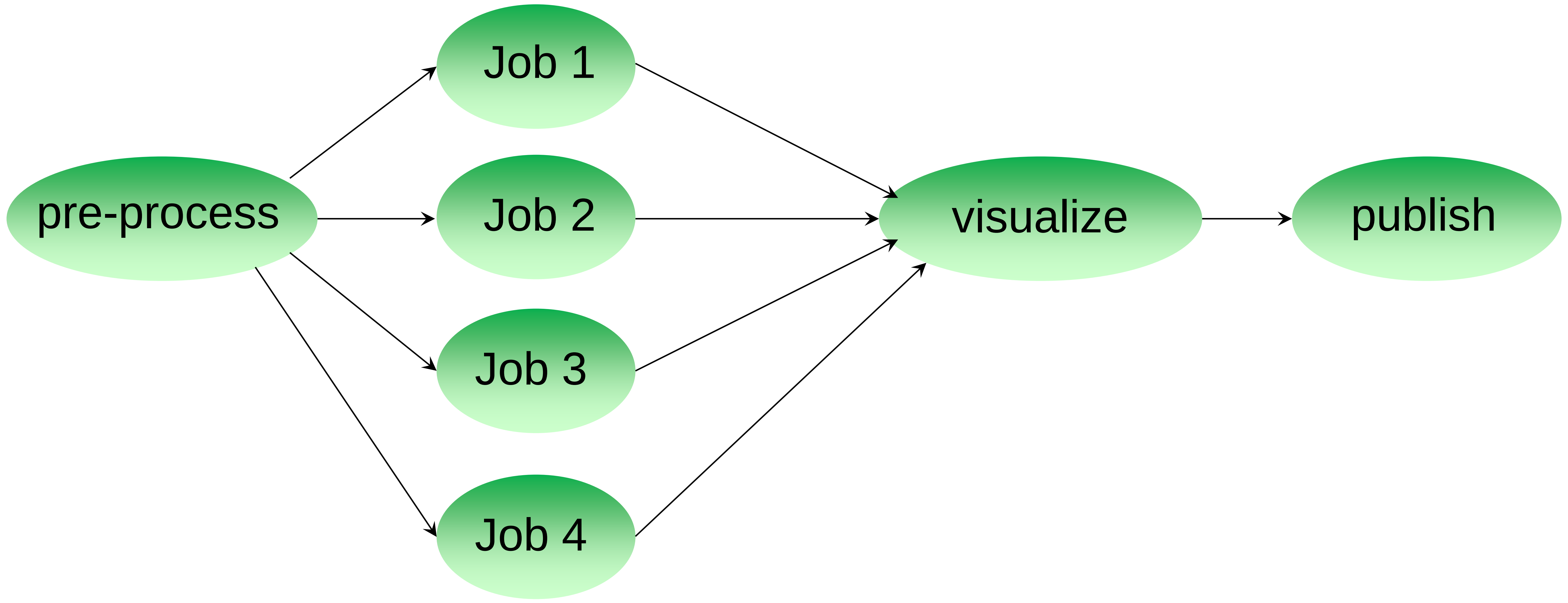
Scientific Workflows

- Formal way to express a scientific calculation
- Multiple tasks with dependencies between them
- No limitations on tasks
- Capture task parameters, input, output
- Independence of workflow process and data
  - Often, run same workflow with different data
- You use workflows all the time…

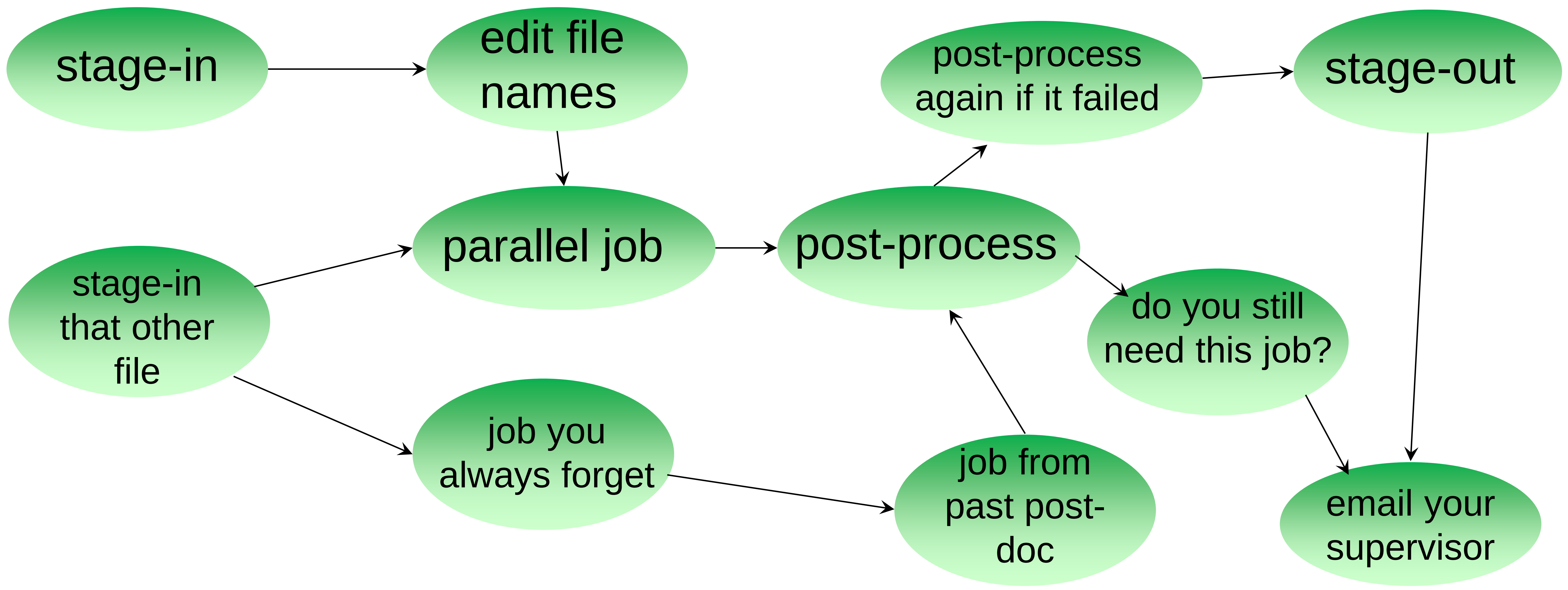
Perhaps your workflow is simple…



…or maybe a bit more complicated…



…or maybe just confusing



Workflow Components

- Task executions
  - Specify a series of tasks to run
- Data and control dependencies between tasks
  - Outputs from one task may be inputs for another
- Task scheduling
  - Some tasks may be able to run in parallel with other tasks
- File and metadata management
  - Track when a task was run, key parameters
- Resource provisioning (getting cores)
  - Computational resources are needed to run jobs

What do we need help with?

- Task executions
  - What if something fails in the middle?
- Data and control dependencies
  - Make sure inputs are available for tasks
- Task scheduling
  - Minimize execution time while preserving dependencies
- Metadata
  - Automatically capture and track
- Getting cores

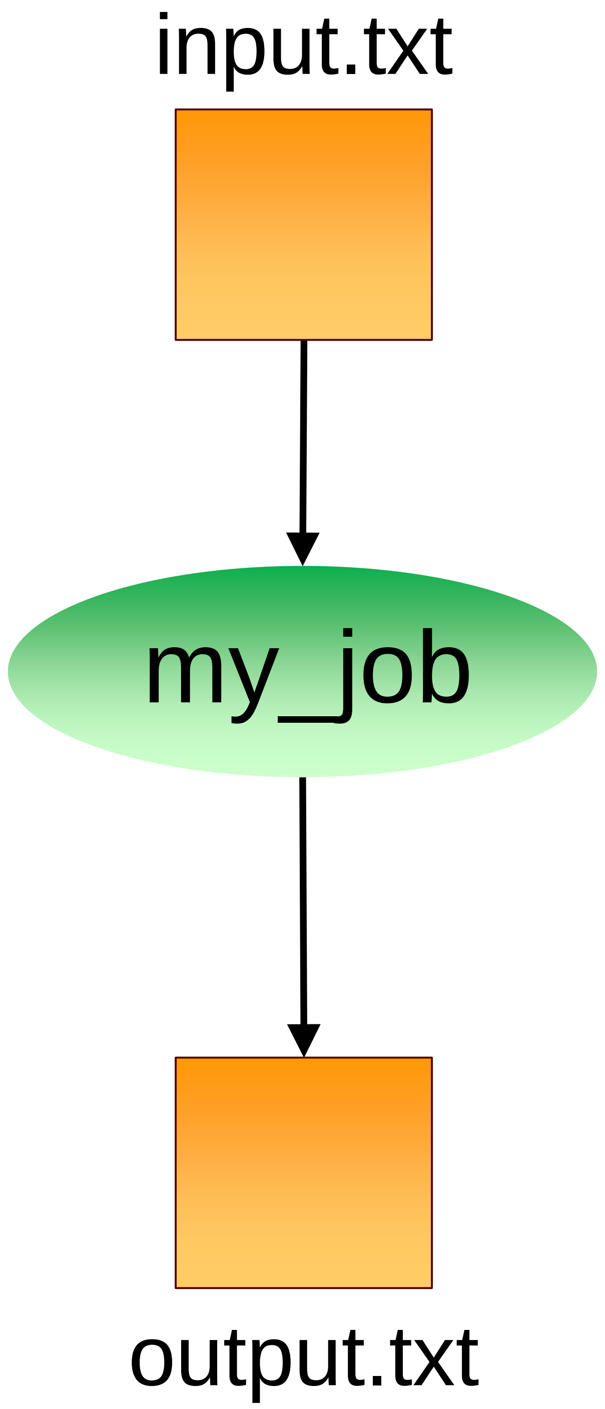
Workflow tools can help!

- Automate your pipeline
- Define your workflow via programming or GUI
- Run workflow on local or remote system
- Can support all kinds of workflows
- Use existing code (no changes)
- Provide many kinds of fancy features and capabilities
  - Flexible but can be complex
- Will discuss one set of tools (Pegasus) as example, but concepts are shared

Pegasus-WMS

- Developed at USC’s Information Sciences Institute
- Used in many domains, including LIGO project
- Workflows are executed from local machine
  - Jobs can run on local machine or on distributed resources
- You use API to write code describing workflow (“create”)
  - Python, Java, Perl
  - Tasks with parent / child relationships
  - Files and their roles
- Pegasus creates XML file of workflow called a DAX
- Workflow represented by directed acyclic graph

Sample Workflow Creation

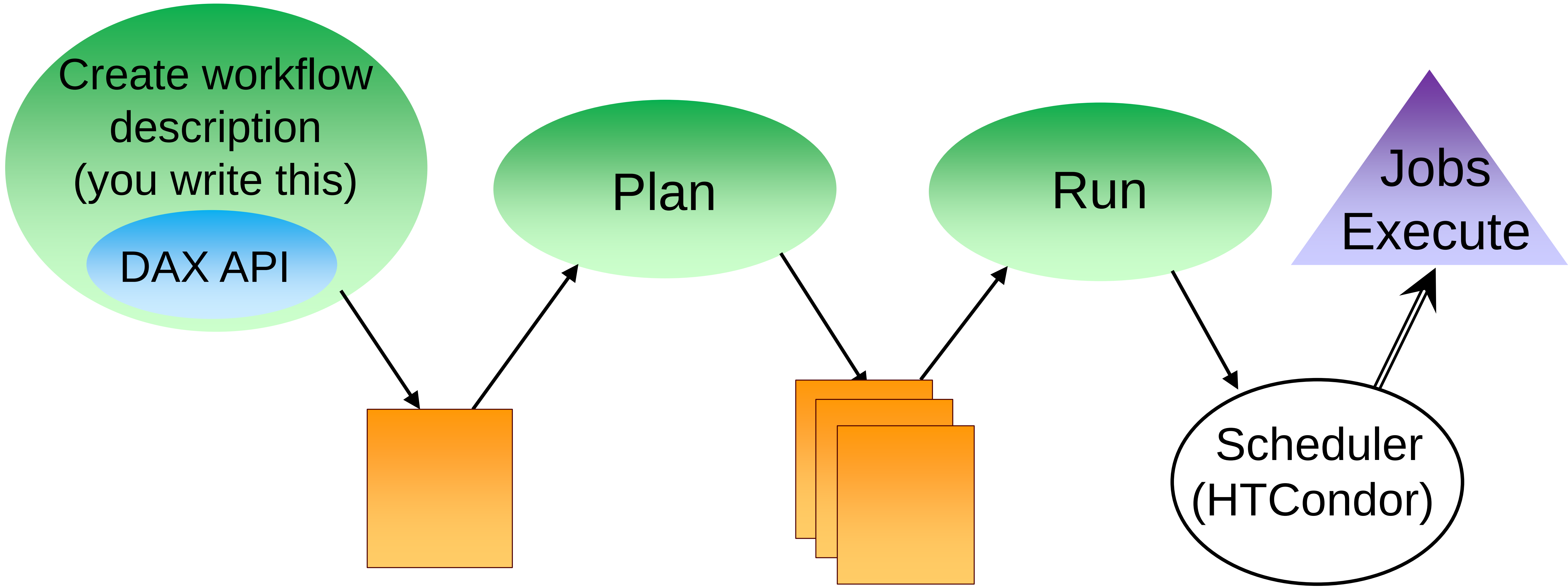


```
//Create DAX object
dax = ADAG("test_dax")
//Define my job
myJob = Job(name="my_job")
//Input and output files to my job
inputFile = File("input.txt")
outputFile = File("output.txt")
//Arguments to my_job (./my_job input=input.txt output=output.txt)
myJob.addArgument("input=input.txt", "output=output.txt")
//Role of the files for the job
myJob.uses(inputFile, link=Link.INPUT)
myJob.uses(outputFile, link=Link.OUTPUT)
//Add the job to the workflow
dax.addJob(myJob)
//Write to file
fp = open("test.dax", "w")
dax.writeXML(fp)
fp.close()
```

Getting ready to run ("Planning")

- DAX is "abstract workflow"
  - Logical filenames and executables
  - Algorithm description
- Use Pegasus to "plan" workflow for execution
  - Uses catalogs to resolve logical names, compute info
  - Pegasus automatically augments workflow
    - Staging jobs (if needed) with Globus Online
    - Registers output files in a catalog to find later
    - Wraps jobs in pegasus-kickstart for detailed statistics
  - Generates a DAG
    - Top-level workflow description (tasks and dependencies)
    - Submission file for each job

Pegasus Workflow Path



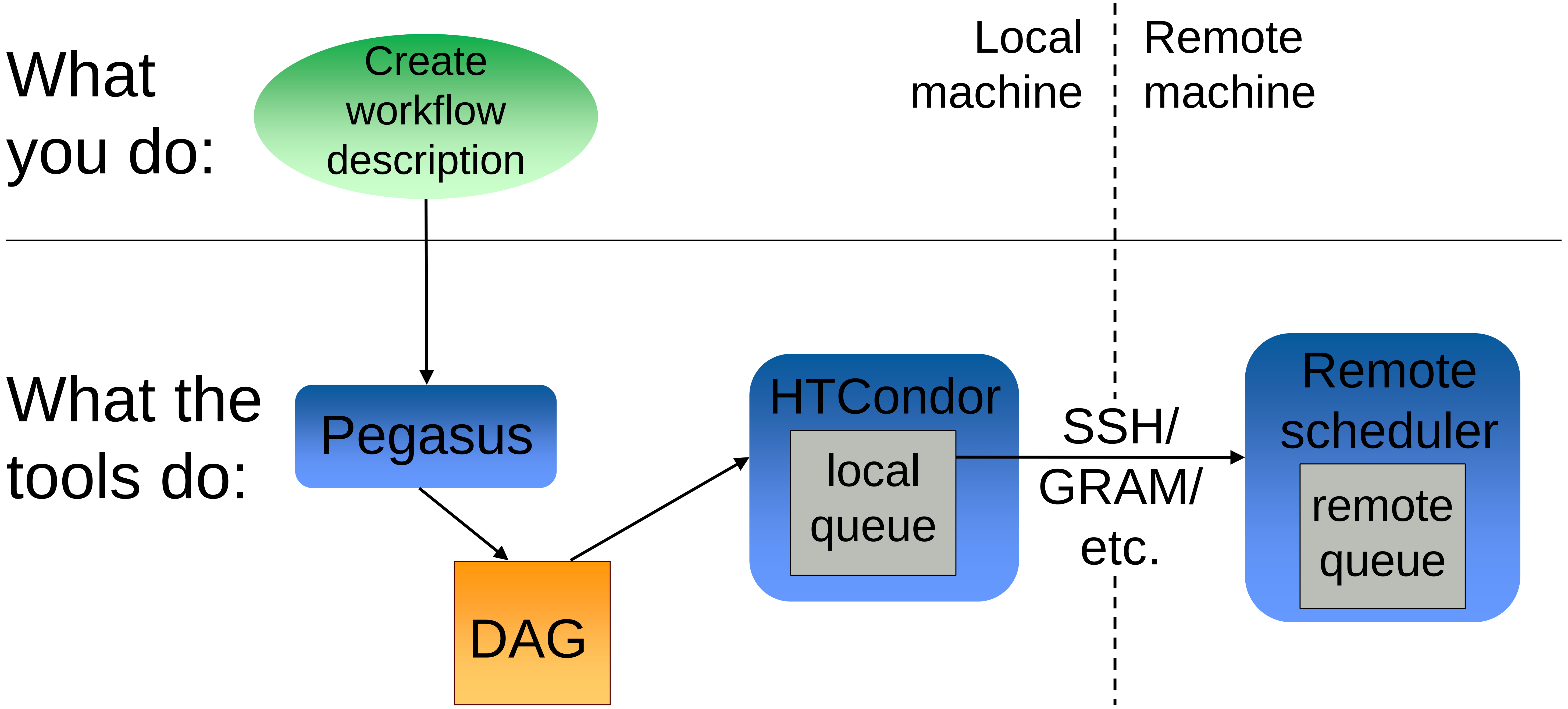
Abstract workflow (DAX)
Logical names, algorithm

Concrete workflow (DAG)
Physical paths, job scripts

Other tools in stack

- HTCondor (UW Madison)
  - Pegasus ‘submits’ workflow to HTCondor
  - Supervises runtime execution of DAG files
    - Maintains job queue
    - Monitors dependencies
    - Schedules jobs
    - Retries failures
    - Writes checkpoint
- Tools for remote job submission to clusters and clouds
  - GRAM, SSH, BOSCO, CREAMCE, glideins/pilot jobs, …
  - Condor uses tool to match jobs to resources

Full workflow stack



Other Workflow Tools

- Regardless of the tool, same basic stages
  - Describe your workflow (Pegasus “Create”)
  - Prepare your workflow for the execution environment (Pegasus “Plan”)
  - Send jobs to resources (HTCondor, SSH, GRAM)
  - Monitor the execution of the jobs (HTCondor DAGMan)
- Brief overview of some other available tools

Other Workflow Tools

- Swift (U of Chicago)
  - Workflow defined via scripting language

```
//Create new type
type messagefile;
//Create app definition, returns messagefile
app (messagefile t) greeting() {
    //Print and pipe stdout to t
    echo “Hello, world!” stdout=@filename(t);
}
//Create a new messagefile, linked to hello.txt
messagefile outfile <“hello.txt”>
//Run greeting() and store results
outfile = greeting();
```

  - Workflow compiled internally and executed
  - Focus on large data, many tasks

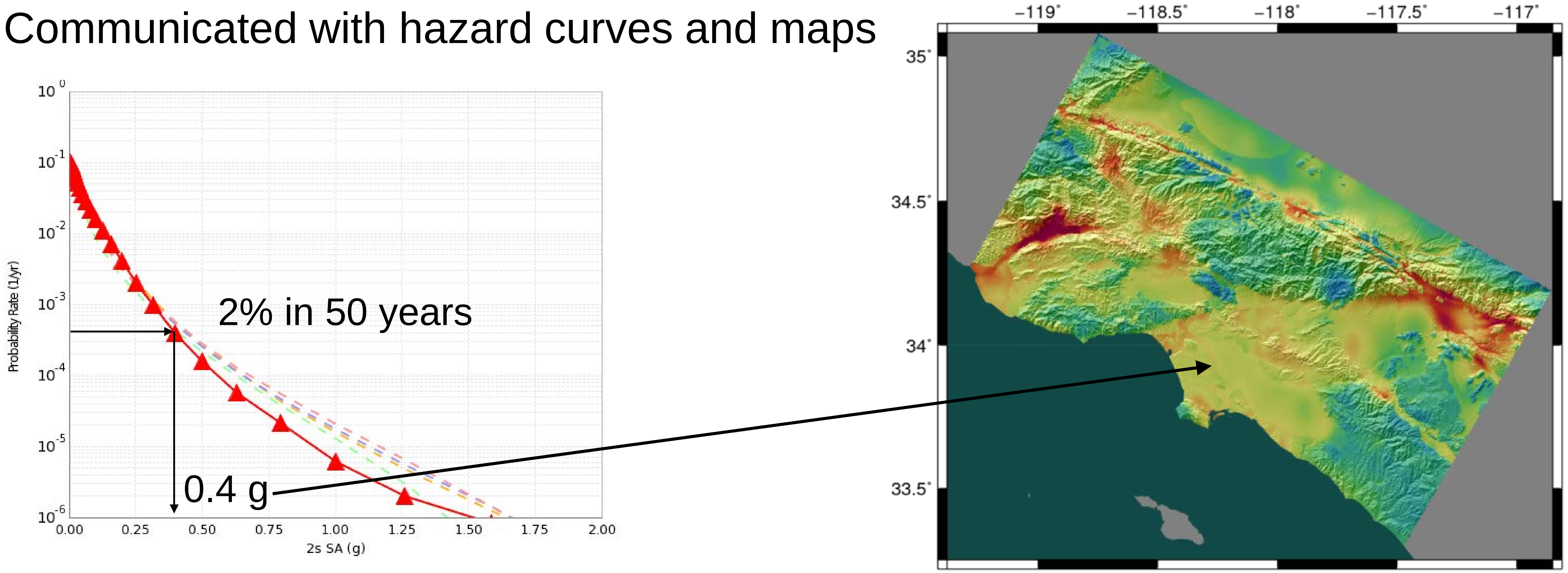
- Askalon (U of Innsbruck)
  - Create workflow description
    - Use workflow language
    - Or use UML editor to graphically create
  - Conversion: like planning, to prep for execution
  - Submit jobs to Enactment Engine, which distributes jobs for execution at remote grid or cloud sites
  - Provides monitoring tools

More Workflow Tools

- Kepler (diverse US collaboration)
  - GUI interface
  - Many models of computation (‘actors’) with built-in components (tasks)
- RADICAL Cybertools (international)
  - Sits atop SAGA, a Python API for submitting remote jobs
  - Uses pilot jobs to provision resources
- UNICORE (Jülich Supercomputing Center)
  - GUI interface to describe workflow
  - Branches, loops, parallel loops
- Many more: ask me about specific use cases
- NCSA Blue Waters has webinars online on several tools

Workflow Application: CyberShake

- What will peak ground motion be over the next 50 years?
  - Used in building codes, insurance rates, disaster planning
  - Answered via Probabilistic Seismic Hazard Analysis (PSHA)
  - Communicated with hazard curves and maps



CyberShake Computational Requirements

- Determine shaking of ~500,000 earthquakes per site
- Large parallel jobs
  - 2 GPU wave propagation jobs, 800 nodes x 1 hr, 1.5 TB output
- Small serial jobs
  - 500,000 seismogram calculation jobs, 1 core x 4.7 min, 30 GB
- Need ~300 sites for hazard map
- Decided to use scientific workflows
  - Automation
  - Data management
  - Error recovery

Challenge: Resource Provisioning

- For large parallel jobs, submit to remote scheduler
  - GRAM (or other tool) puts jobs in remote queue
  - Runs like a normal batch job
  - Can specify either CPU or GPU nodes
- For small serial jobs, need high throughput
  - Putting lots of jobs in the batch queue is ill-advised
    - Scheduler isn’t designed for heavy job load
    - Scheduler cycle is ~5 minutes
    - Policy limits number of job submissions
- Solution: Pegasus-mpi-cluster (PMC)

Pegasus-mpi-cluster

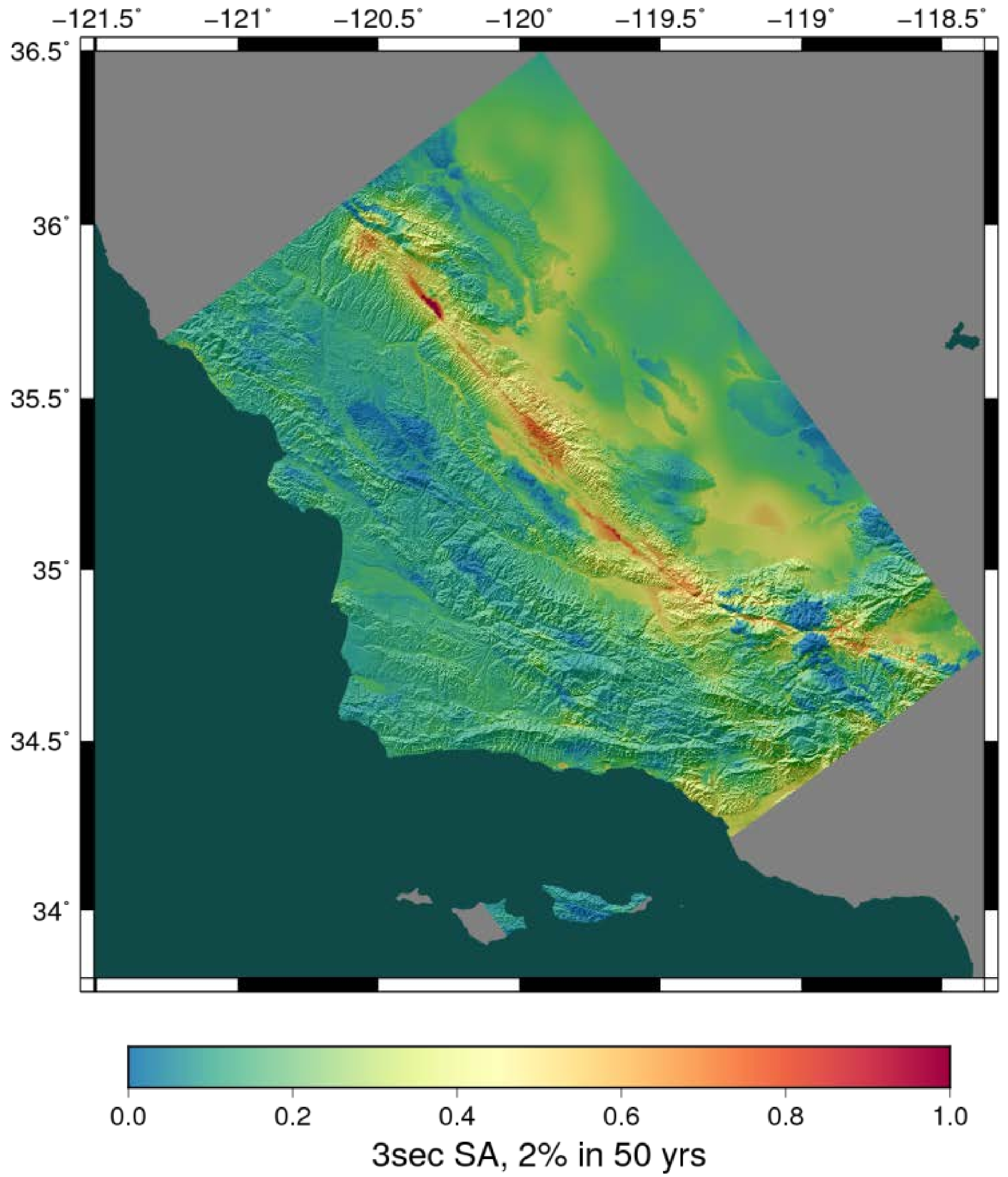
- MPI wrapper around serial or thread-parallel jobs
  - Master-worker paradigm
  - Preserves dependencies
  - HTCondor submits job to multiple nodes, starts PMC
  - Specify jobs as usual, Pegasus does wrapping
- Uses intelligent scheduling
  - Core counts
  - Memory requirements
- Can combine writes
  - Workers write to master, master aggregates to fewer files

Challenge: Data Management

- Millions of data files
  - Pegasus provides staging
    - Symlinks files if possible, transfers files if needed
    - Transfers output back to local archival disk
    - Supports running parts of workflows on separate machines
  - Cleans up temporary files when no longer needed
  - Directory hierarchy to reduce files per directory
- We added automated checks to check integrity
  - Correct number of files, NaN, zero-value checks, correct size
  - Included as new jobs in workflow

CyberShake Study 17.3

- Hazard curves for 876 sites
- Used OLCF Titan and NCSA Blue Waters
- Averaged 1295 nodes (CPUs and GPUs) for 31 days
  - Workflow tools scheduled 15,581 jobs
  - 23.9 workflows running concurrently
- Generated 285 million seismograms
- Workflow tools managed 777 TB of data
  - 308 TB of intermediate data transferred
  - 10.7 TB (~17M files) staged back to local disk
- Workflow tools scale!



Problems Workflows Solve

- Task executions
  - Workflow tools will retry and checkpoint if needed
- Data management
  - Stage-in and stage-out data for jobs automatically
- Task scheduling
  - Optimal execution on available resources
- Metadata
  - Automatically track runtime, environment, arguments, inputs
- Getting cores
  - Whether large parallel jobs or high throughput

Should you use workflow tools?

- Probably using a workflow already
  - Replaces manual hand-offs and polling to monitor
- Provides framework to assemble community codes
  - Also useful for training new teammates
- Scales from local computer to large clusters
- Provide portable algorithm description independent of data
  - CyberShake has run on 9 systems since 2007 with same workflow
- Does add additional software layers and complexity
  - Some development time is required

Final Thoughts

- Automation is vital, even without workflow tools
  - Eliminate human polling
  - Get everything to run automatically if successful
  - Be able to recover from common errors
- Put ALL processing steps in the workflow
  - Include validation, visualization, publishing, notifications
- Avoid premature optimization
- Consider new compute environments (dream big!)
  - Larger clusters, XSEDE/PRACE/RIKEN/SciNet, Amazon EC2
- Tool developers want to help you!

Links

- SCEC: http://www.scec.org
- Pegasus: http://pegasus.isi.edu
- Pegasus-mpi-cluster: http://pegasus.isi.edu/wms/docs/latest/cli-pegasus-mpi-cluster.php
- HTCondor: http://www.cs.wisc.edu/htcondor/
- Globus: http://www.globus.org/
- Swift: http://swift-lang.org
- Askalon: http://www.dps.uibk.ac.at/projects/askalon/
- Kepler: https://kepler-project.org/
- RADICAL Cybertools: https://radical-cybertools.github.io/
- UNICORE: http://www.unicore.eu/
- CyberShake: http://scec.usc.edu/scecpedia/CyberShake

Questions?