Swift Parallel Scripting for Science, Engineering and Data Analysis

Globus World – April 14, 2015

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http://swift-lang.org

Swift gratefully acknowledges support from:

NSF

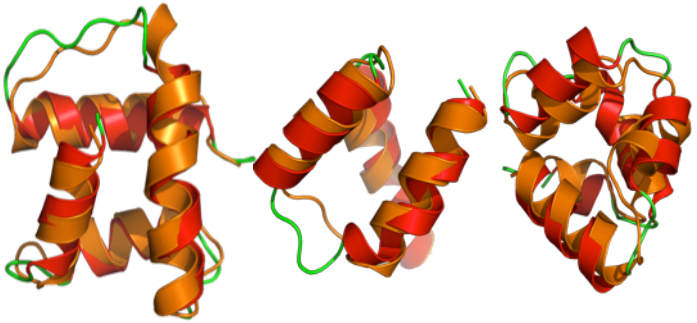
U.S. DEPARTMENT OF ENERGY

THE UNIVERSITY OF CHICAGO Argonne NATIONAL LABORATORY

When do you need high-performance workflow?

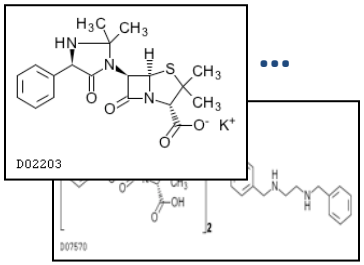
example: protein-ligand docking for drug screening

O(10) proteins implicated in a disease



X

O(100K) drug candidates



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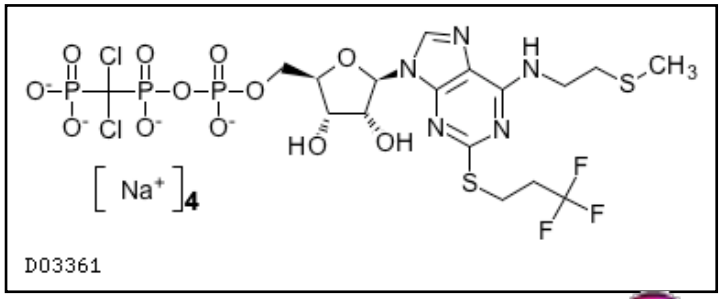
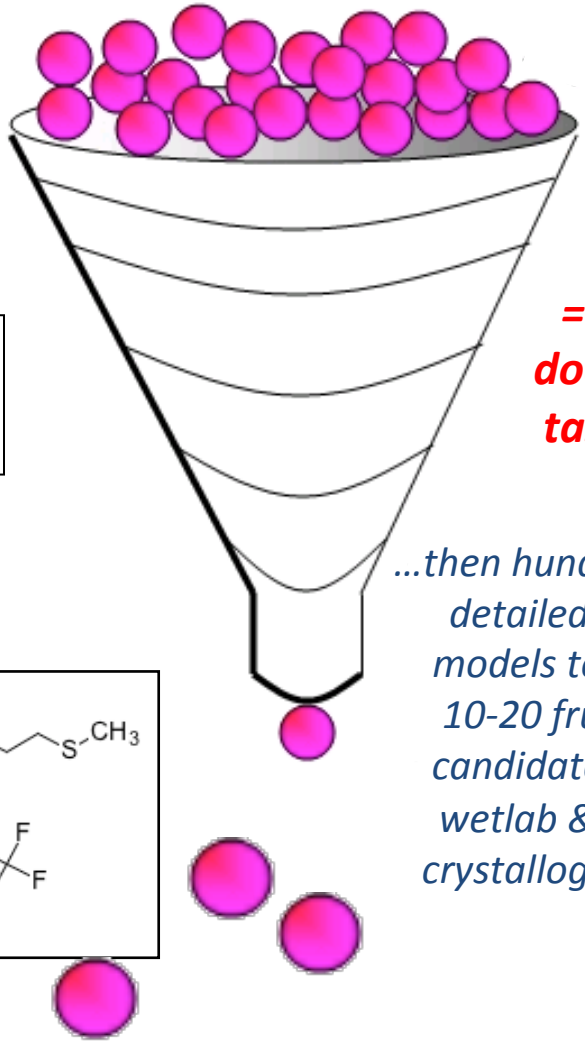




= 1M docking tasks…

…then hundreds of detailed MD models to find 10-20 fruitful candidates for wetlab & APS crystallography

Expressing this workflow in Swift

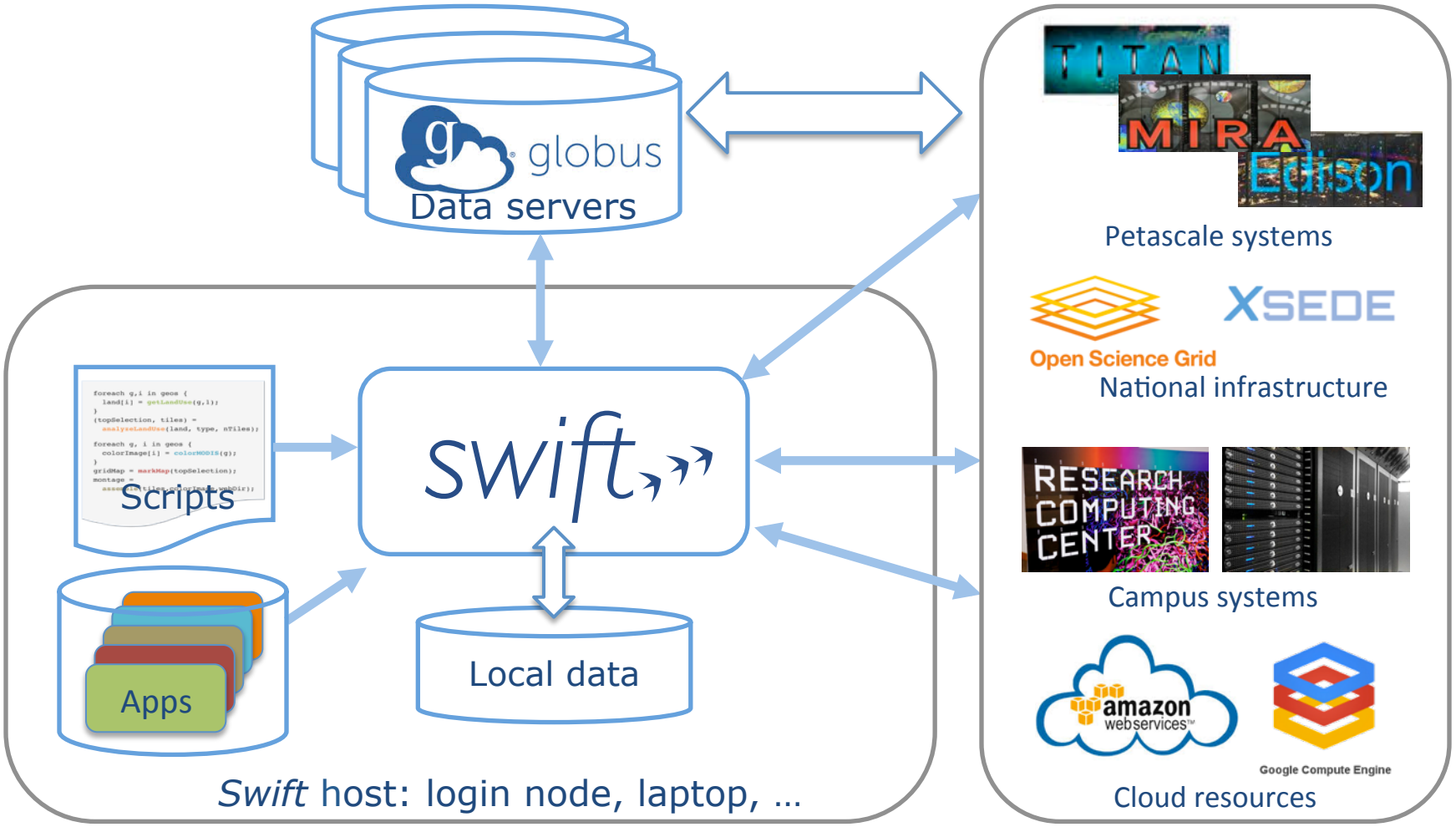
For protein docking workflow:

```
foreach p, i in proteins {
   foreach c, j in ligands {
      (structure[i,j], log[i,j]) =
       dock(p, c, minRad, maxRad);
}
scatter_plot = analyze(structure)
```

To run:

```
swift –site tukey,blues dock.swift
```

Swift enables execution of simulation campaigns across multiple HPC and cloud resources



Swift runtime drivers support and aggregate diverse runtime environments

Swift provides 4 important benefits:

Makes parallelism more transparent

Implicitly parallel functional dataflow programming

Makes computing location more transparent

Runs your script on multiple distributed sites and diverse computing resources (desktop to petascale)

Makes basic failure recovery transparent

Retries/relocates failing tasks

Can restart failing runs from point of failure

Enables provenance capture

Tasks have recordable inputs and outputs

Example of Swift's implicit parallelism: Processing MODIS land-use data

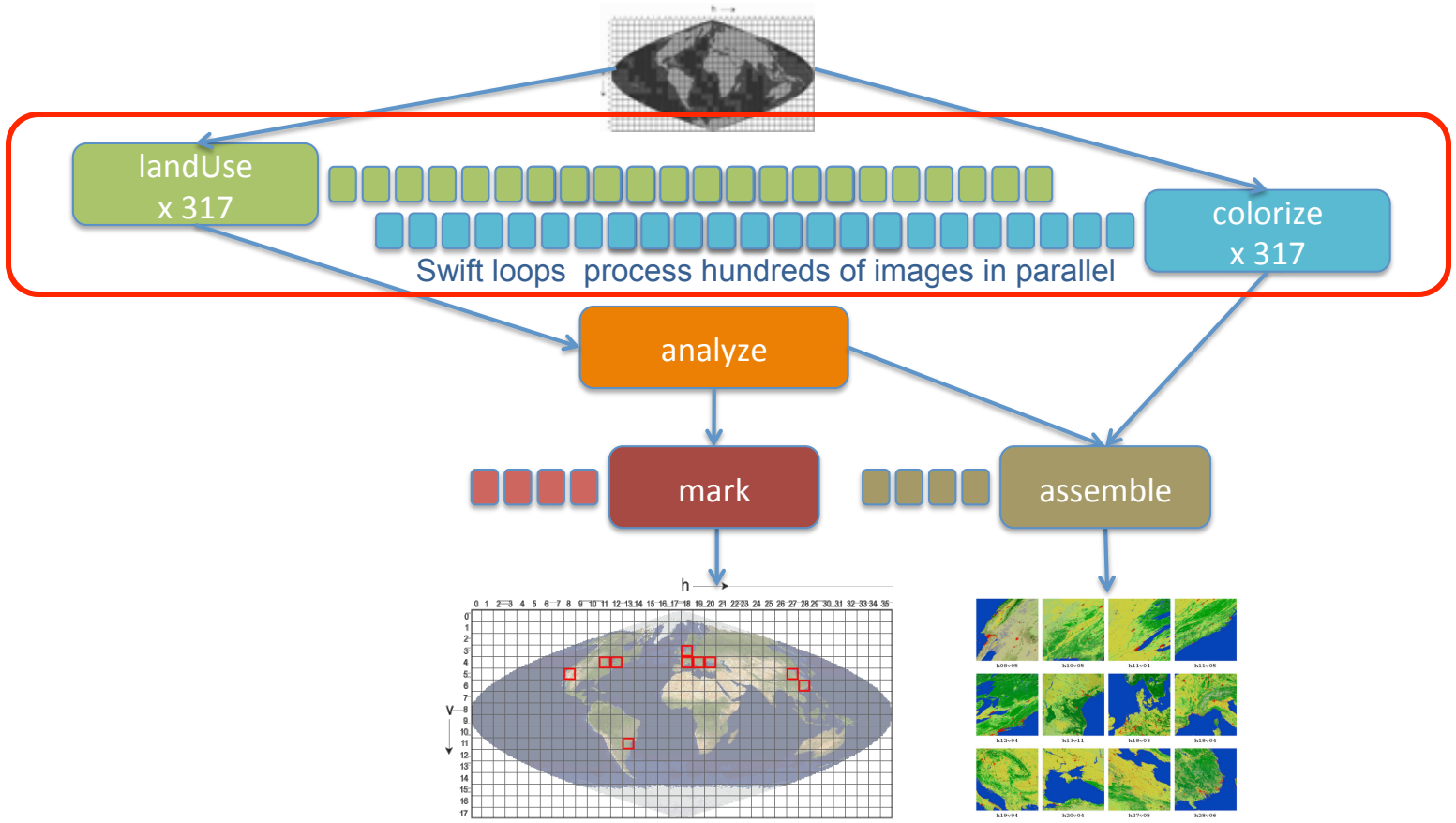
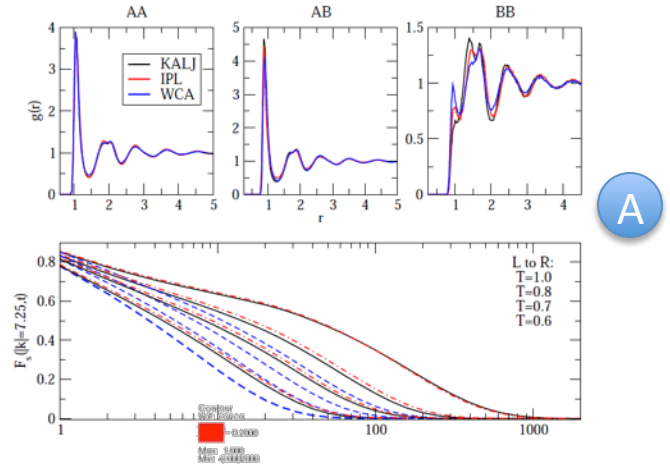


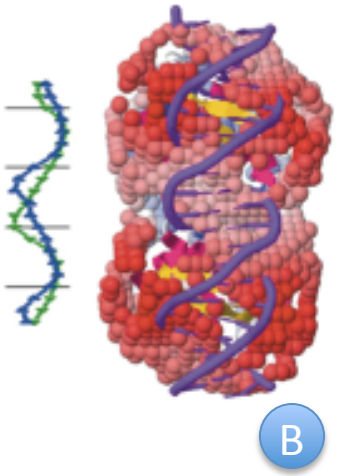
Image processing pipeline for land-use data from the MODIS satellite instrument…

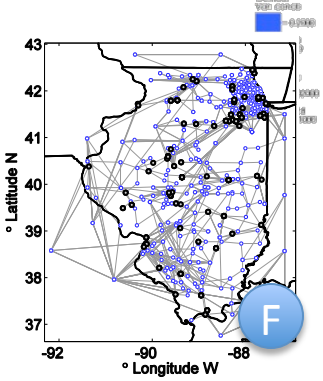
Large-scale applications using Swift

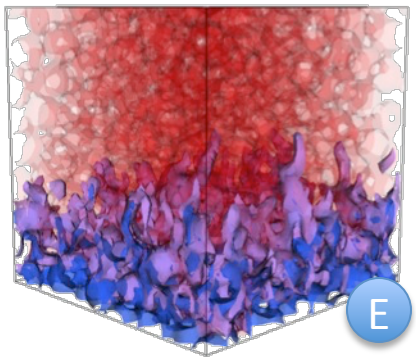
- **A** Simulation of super-cooled glass materials
- **B** Protein and biomolecule structure and interaction
- **C** Climate model analysis and decision making for global food production & supply
- **D** Materials science at the Advanced Photon Source
- **E** Multiscale subsurface flow modeling
- **F** Modeling of power grid for OE applications

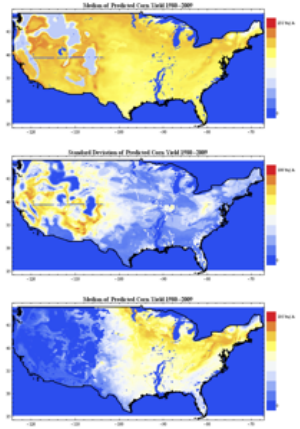
All have published science results obtained using Swift

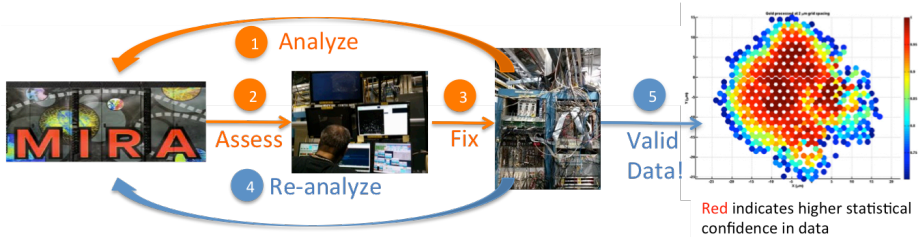


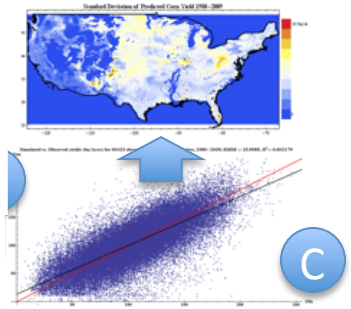








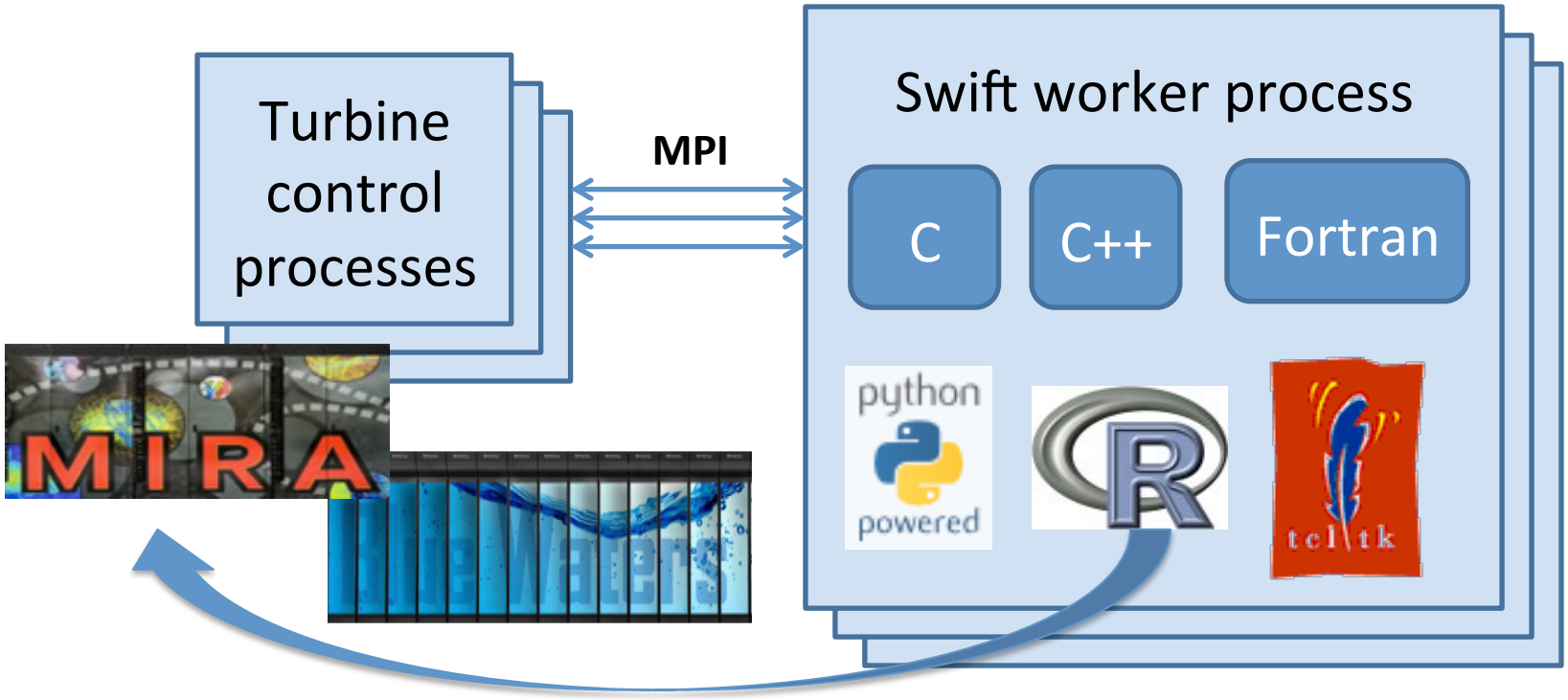




swift

http://swift-lang.org

Swift/T: productive extreme-scale scripting



- Script-like global-view programming with "leaf" tasks
  - function calls in C, C++, Fortran, Python, R, Julia or Tcl
- Leaf tasks can be MPI programs, etc. Can be separate processes if OS permits.
- Distributed, scalable runtime manages tasks, load balancing, data movement
- User function calls to external code run on thousands of worker nodes
- More expressive than master-worker for "programming in the large"

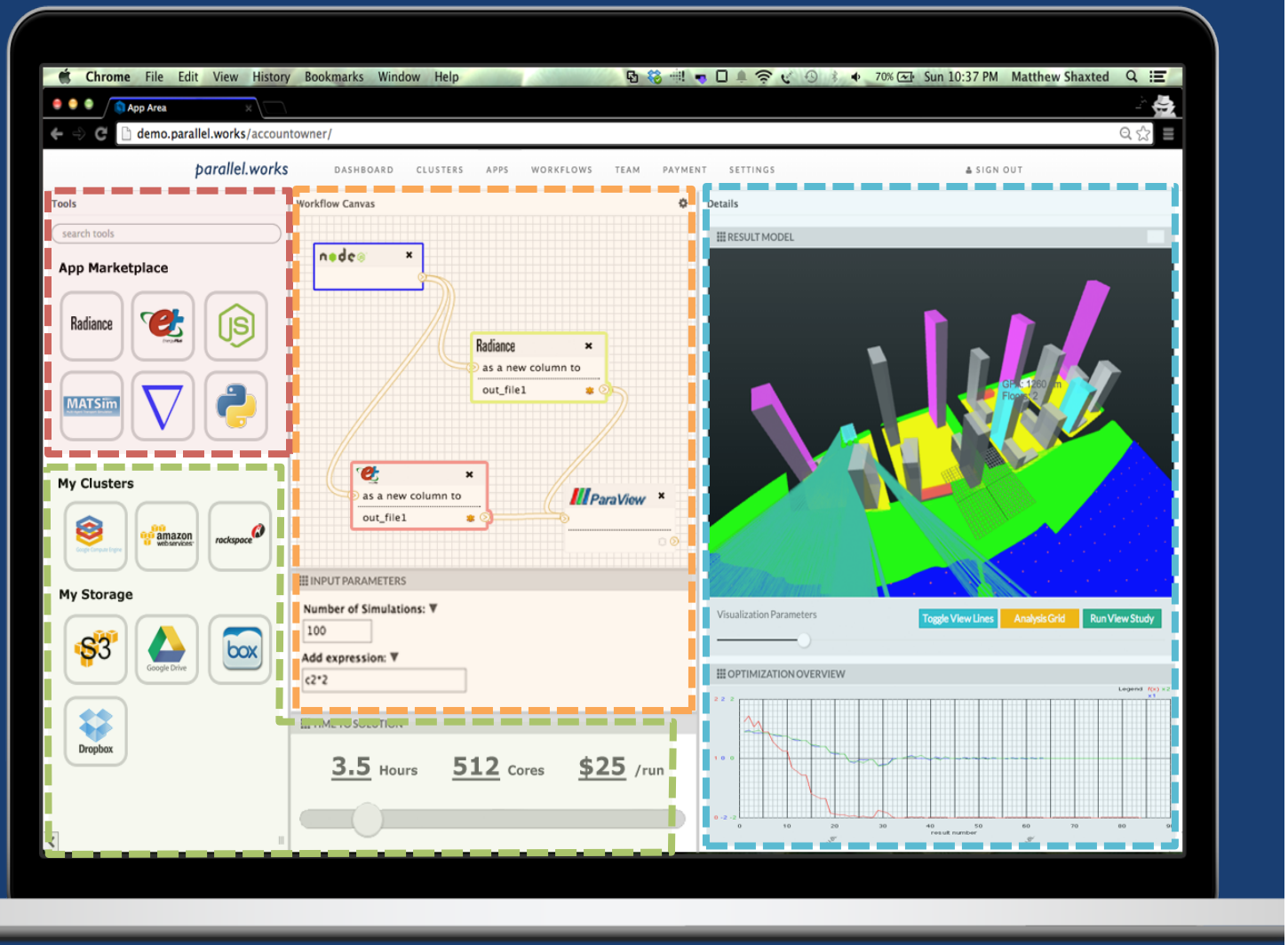
The *parallel.works* solution

Select third-party and open-source applications

Link apps together to create a workflow

Select compute and storage resources and desired time to solution

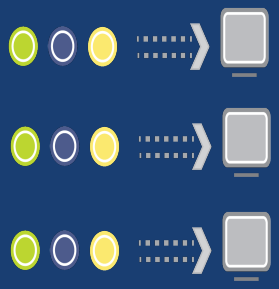
Run simulation workflow and visualize results



The *parallel.works* Paradigm Shift

Early experience at leading architecture firm SOM

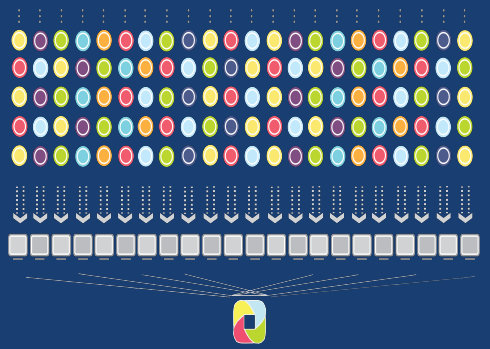
Current Practice



130 days

time-to-solution on a typical
desktop computer (8 CPU cores)

***parallel.works* Solution**



5 hours

time-to-solution using 5,000 CPU cores
on a remote supercomputing facility

625 X faster simulation gives a monetizable time advantage by creating more innovative designs that reduce cost for clients.

parallel.works

What's Inside?

swift

Scalable workflow language & engine

Automates parallelization, data movement, failure recovery, and provenance capture.

Fast, secure, reliable data transfer

Moves and shares data robustly and securely at gigabytes/second

Galaxy

Easy to use web workflow interface

Create, run, view, manage, discover & share workflows

parallel.works' competitive advantage derives from the integration of – and expertise in – three powerful technologies

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