Swift Parallel Scripting: Workflows for Simulations and Data Analytics at Extreme Scale

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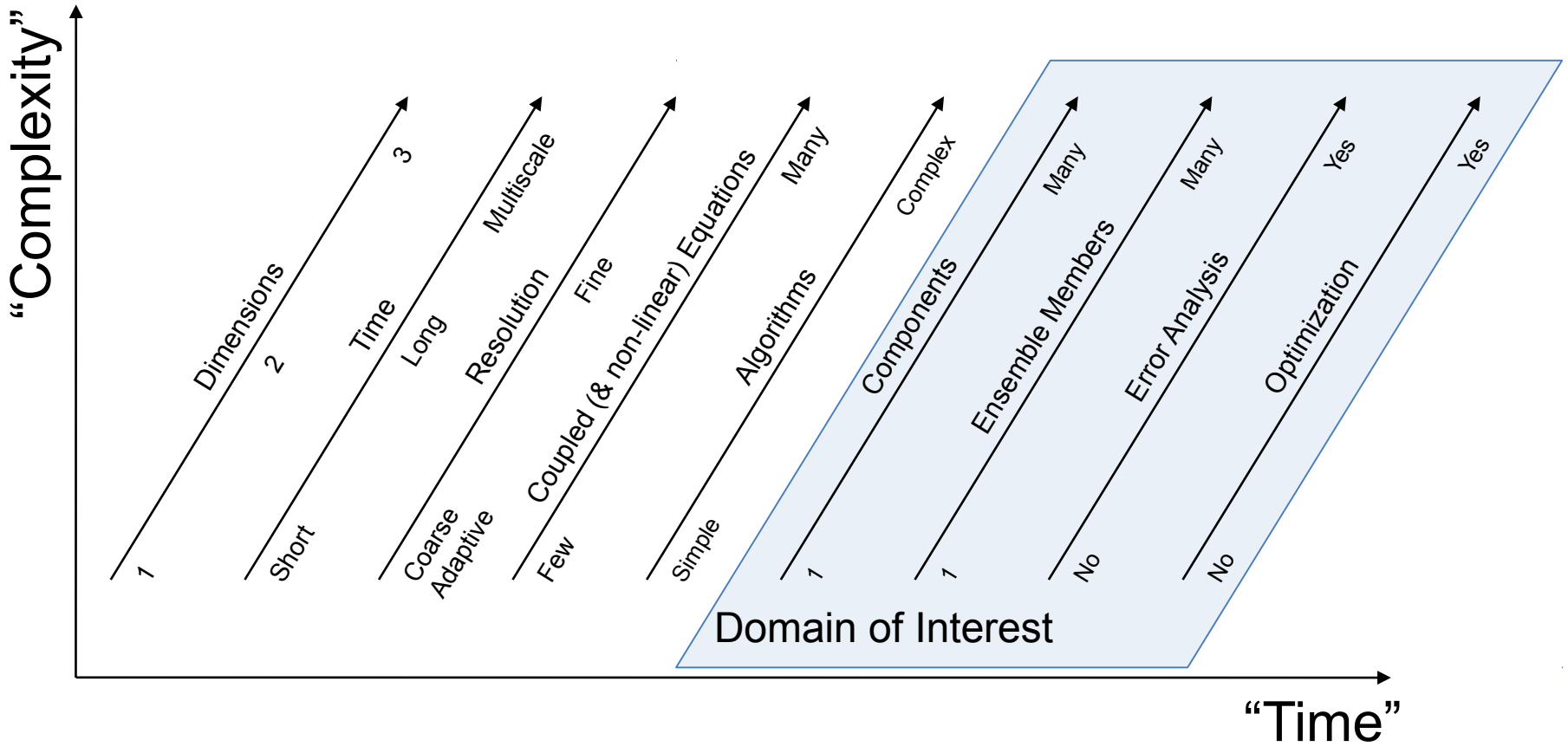
http://swift-lang.org

Increasing capabilities in computational science



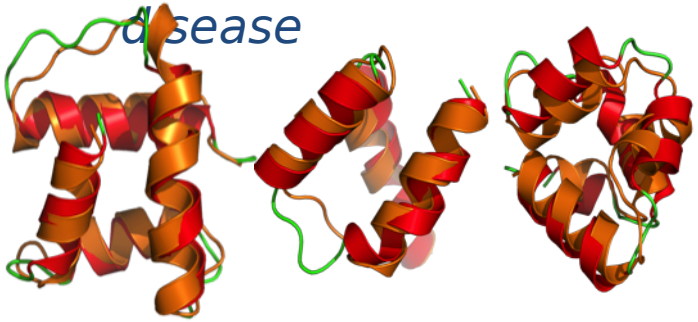
Workflow needs

- Application Drivers
  - Applications that are many-task in nature: parameters sweeps, UQ, inverse modeling, *and data-driven applications*
  - Analysis of capability application outputs
  - Analysis of stored or collected data
  - Increase productivity at major research instrumentation
  - Urgent computing
  - These applications are all *many-task* in nature
- Requirements
  - Usability and ease of workflow expression
  - Ability to leverage complex architecture of HPC and HTC systems (fabric, scheduler, hybrid node and programming models), individually and collectively
  - Ability to integrate high-performance data services and volumes
  - Make use of the system task rate capabilities from clusters to extreme-scale systems
- Approach
  - A programming model for *programming in the large*

When do you need HPC workflow?

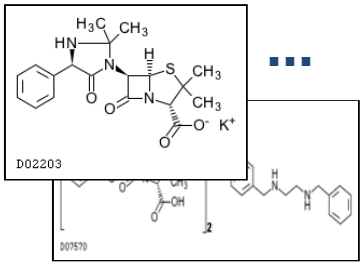
Example application: protein-ligand docking for drug screening

O(10) proteins implicated in a disease



x

O(100K) drug candidates



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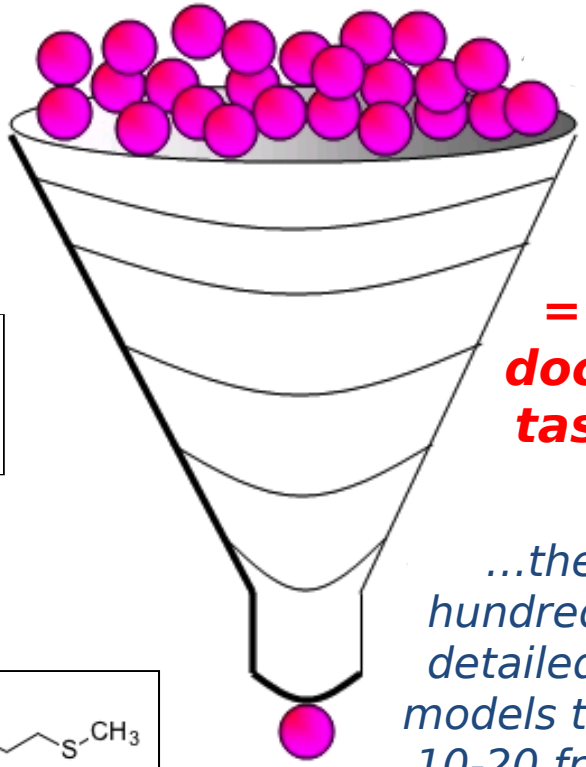
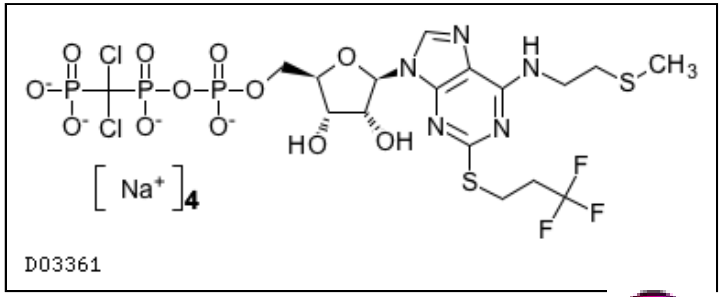


= 1M docking tasks…



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

Expressing this many task workflow in Swift

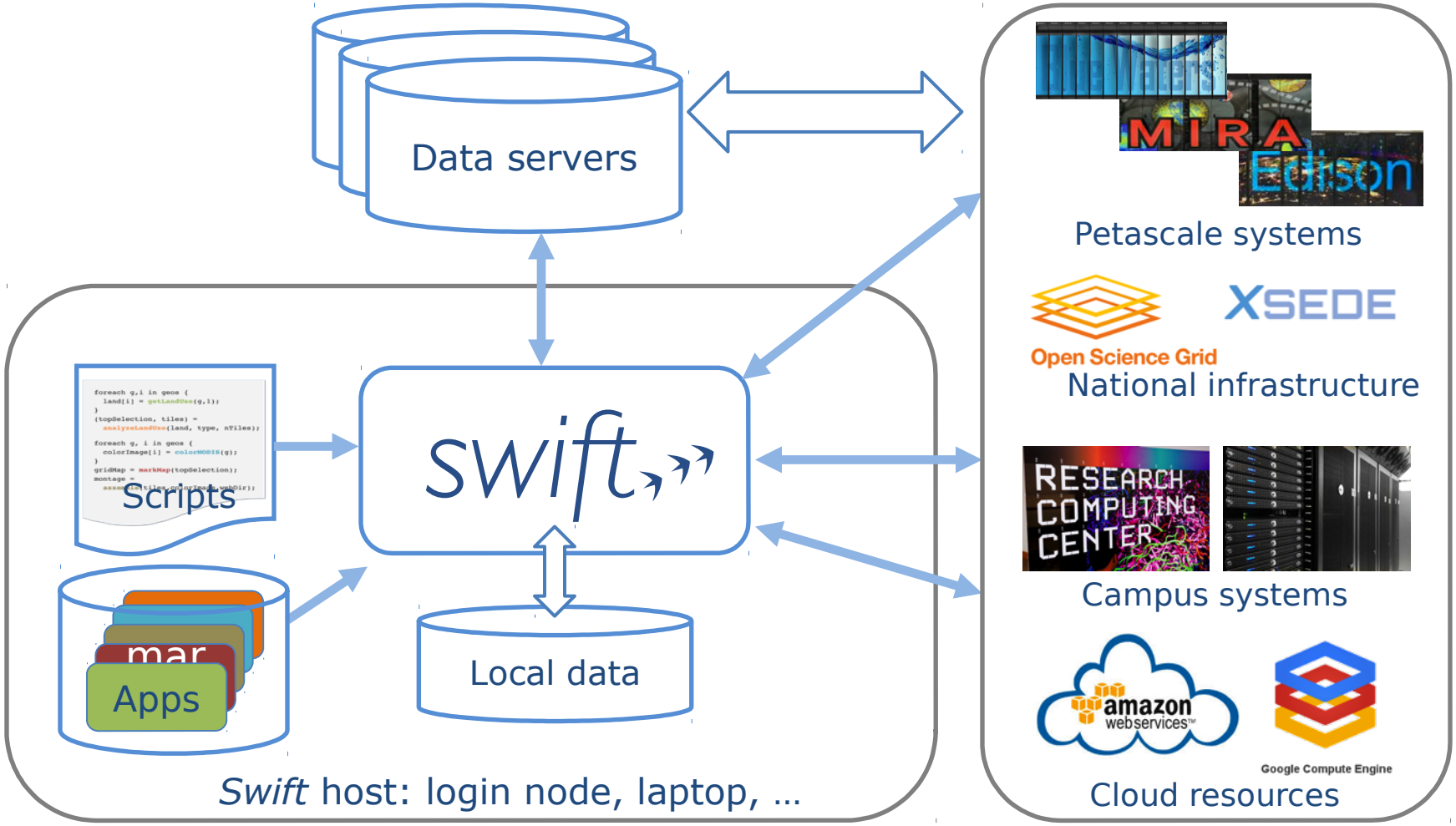
For protein docking workflow:

```
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:

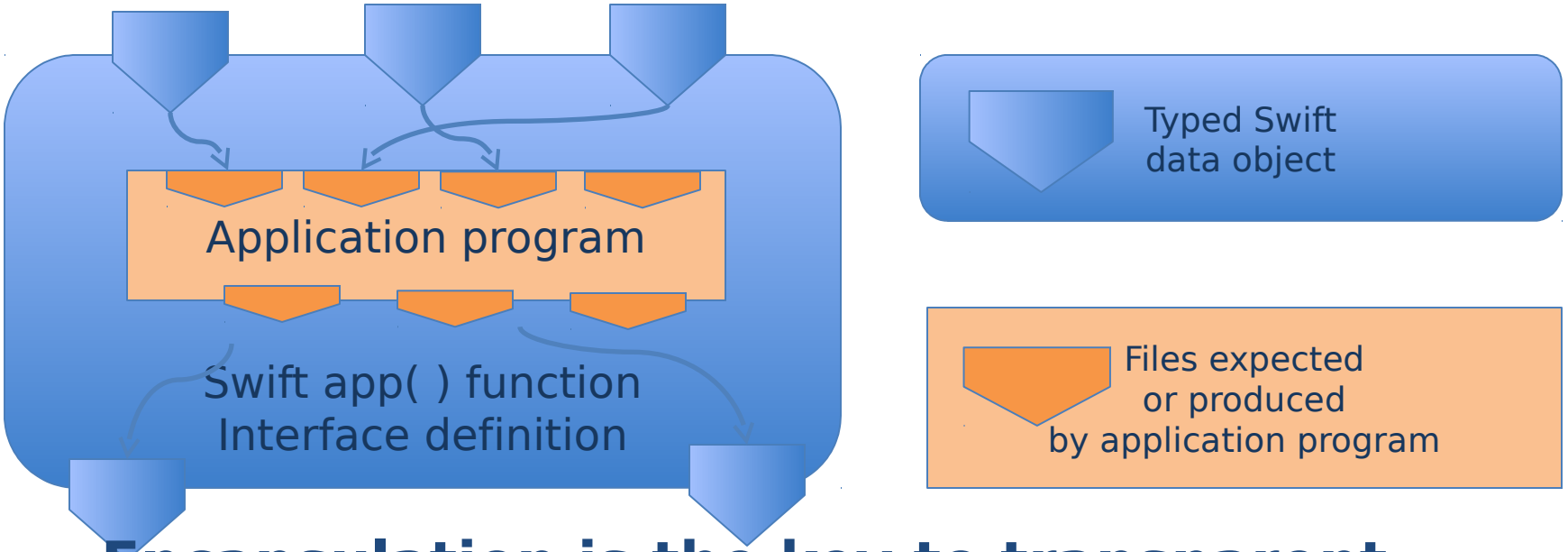
```
swift –site tukey,blues dock.swift
```

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



The Swift runtime system has drivers and algorithms to efficiently support and aggregate diverse runtime environments

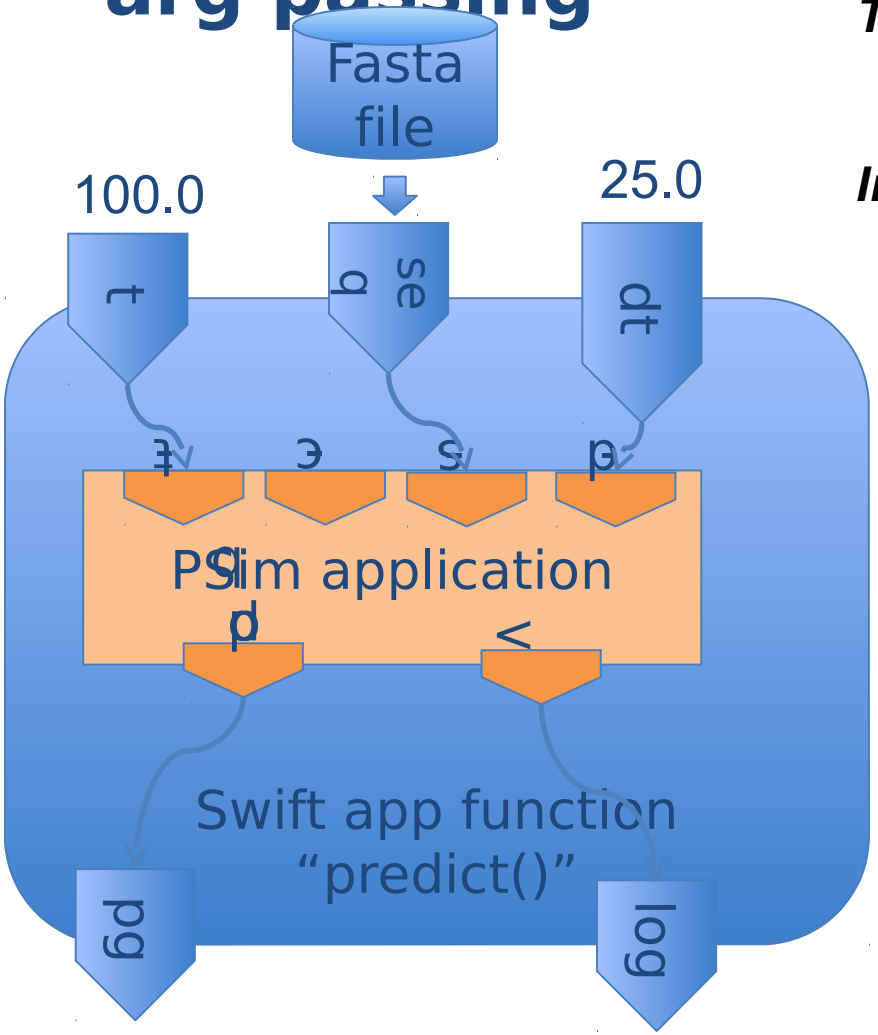
Encapsulation enables distributed parallelism



Encapsulation is the key to transparent distribution, parallelization, and automatic provenance capture

Critical in a world of scientific, engineering, technical and analytical applications

app( ) functions specify command line arg passing



To run:

psim -s 1ubq.fas -pdb p -t 100.0 -d 25.0 >log

In Swift code:

```
app (PDB pg, Text log) predict (Protein seq,
                                Float t, Float dt)
{
   psim "-c" "-s" @pseq.fasta "-pdb" @pg
        "–t" temp "-d" dt;
}
```

```
Protein p <ext; exec="Pmap", id="1ubq">;
PDB structure;
Text log;
```

```
(structure, log) = predict(p, 100., 25.);
```

Swift in a nutshell

- Data types

```
string s = "hello world";
int i = 4;
int A[];
```

- Mapped data types

```
type image;
image file1<"snapshot.jpg">;
```

- Mapped functions

```
app (file o) myapp(file f, int i)
{ mysim  "-s" i @f @o; }
```

- Conventional expressions

```
if (x == 3) {
    y = x+2;
    s = @strcat("y: ", y);
}
```

- Structured data

```
image  A[]<array_mapper…>;
```

- Loops

```
foreach f,i in A {
    B[i] = convert(A[i]);
}
```

- Data flow

```
analyze(B[0], B[1]);
analyze(B[2], B[3]);
```

Swift: A language for distributed parallel scripting, J. Parallel Computing, 2011

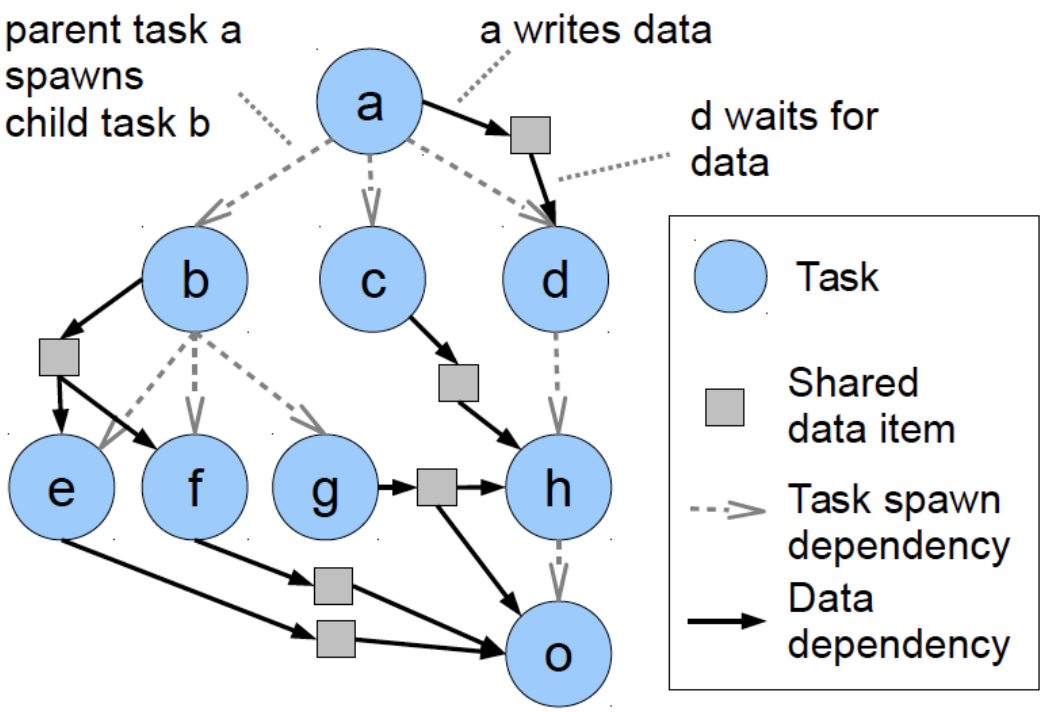
Implicitly parallel

- Swift is an implicitly parallel functional programming language for clusters, grids, clouds and supercomputers
- All expressions evaluate when their data inputs are “ready”

```
(int r) myproc (int i)
{
    int f = F(i);
    int g = G(i);
    r = f + g;
}
```

- F() and G() are computed in parallel
  - Can be Swift functions, or leaf tasks (executables or scripts in shell, python, R, Octave, MATLAB, ...)
- r computed when they are done
- This parallelism is *automatic*
- Works recursively throughout the program’s call graph

Pervasive parallel data flow



Functional composition in *Swift* – *enables powerful parallel loops*

```
1.  Sweep(Protein pSet[ ])
2.  {
3.    int nSim = 1000;
4.    int maxRounds = 3;
5.    float startTemp[ ] = [ 100.0, 200.0 ];
6.    float delT[ ] = [ 1.0, 1.5, 2.0, 5.0, 10.0 ];
7.    foreach p, pn in pSet {
8.      foreach t in startTemp {
9.        foreach d in delT {
10.         IterativeFixing(p, nSim, maxRounds, t, d);
11.       }
12.     }
13.   }
14. }
```

10 proteins x 1000 simulations x 3 rounds x 2 temps x 5 deltas = 300K tasks

Data-intensive example: Processing MODIS land-use data

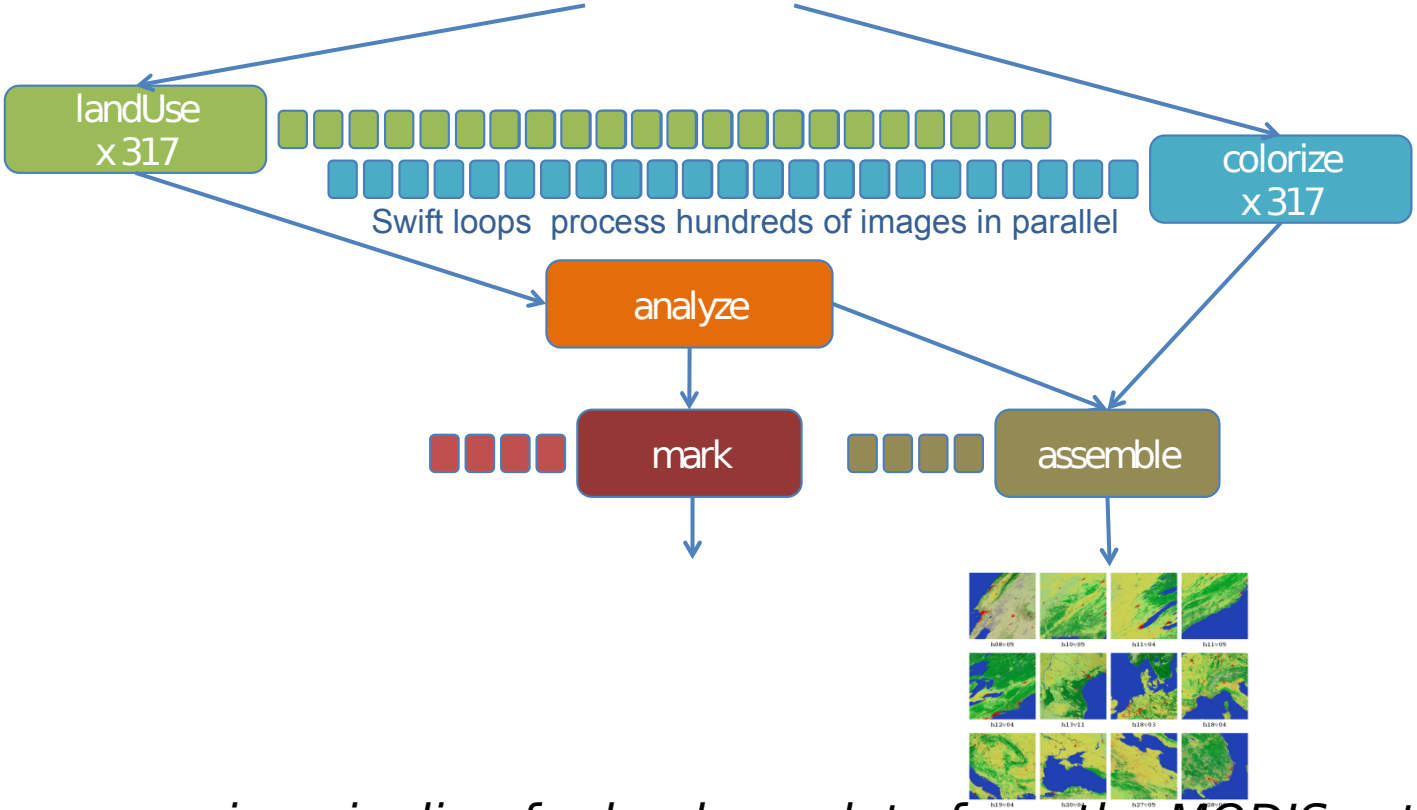


Image processing pipeline for land-use data from the MODIS satellite instrument...

Processing MODIS land-use data

```
foreach raw,i in rawFiles {
    land[i] = landUse(raw,1);
    colorFiles[i] = colorize(raw);
}
(topTiles, topFiles, topColors) =
    analyze(land, landType, nSelect);

gridMap = mark(topTiles);
montage =
  assemble(topFiles,colorFiles,webDir);
```

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

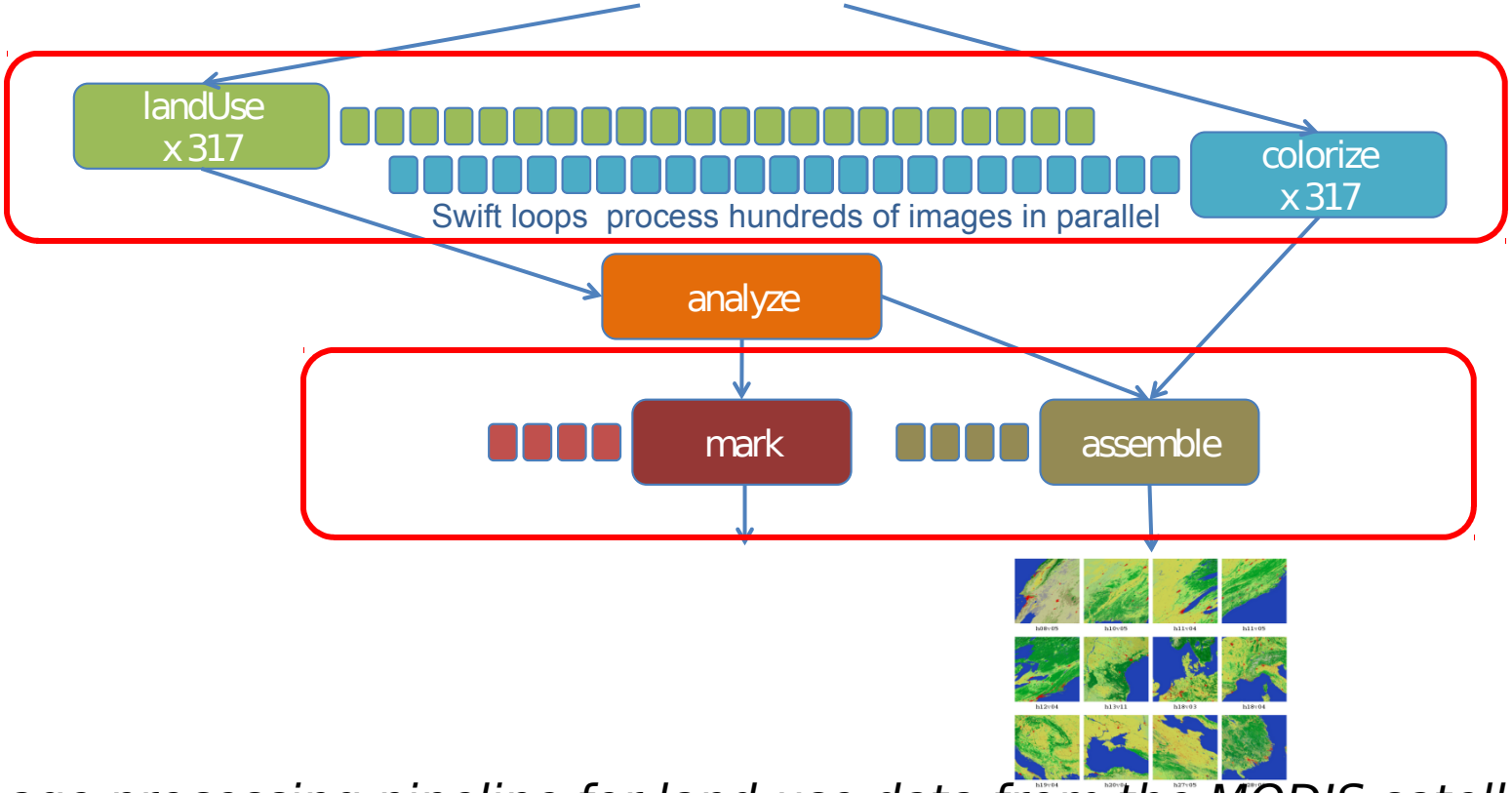
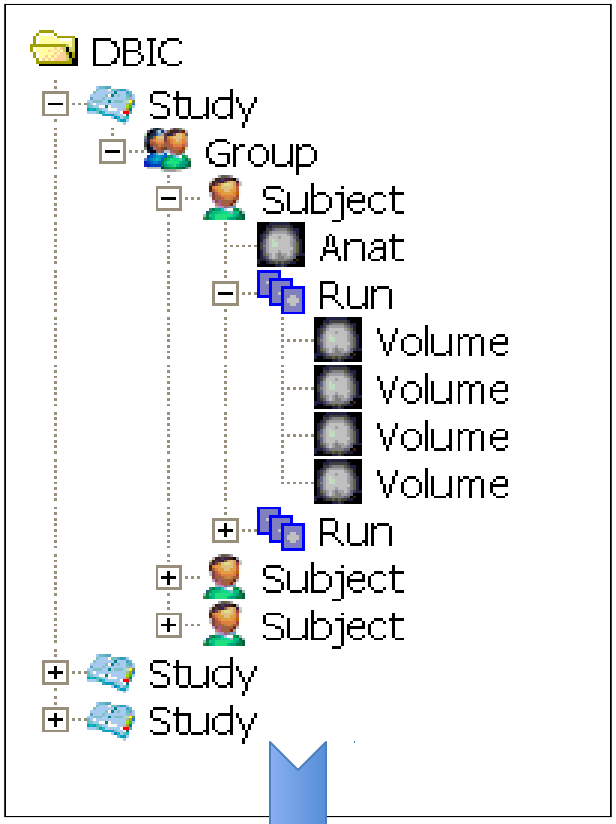


Image processing pipeline for land-use data from the MODIS satellite instrument...

Dataset mapping example: deep fMRI directory tree

On-Disk Data Layout

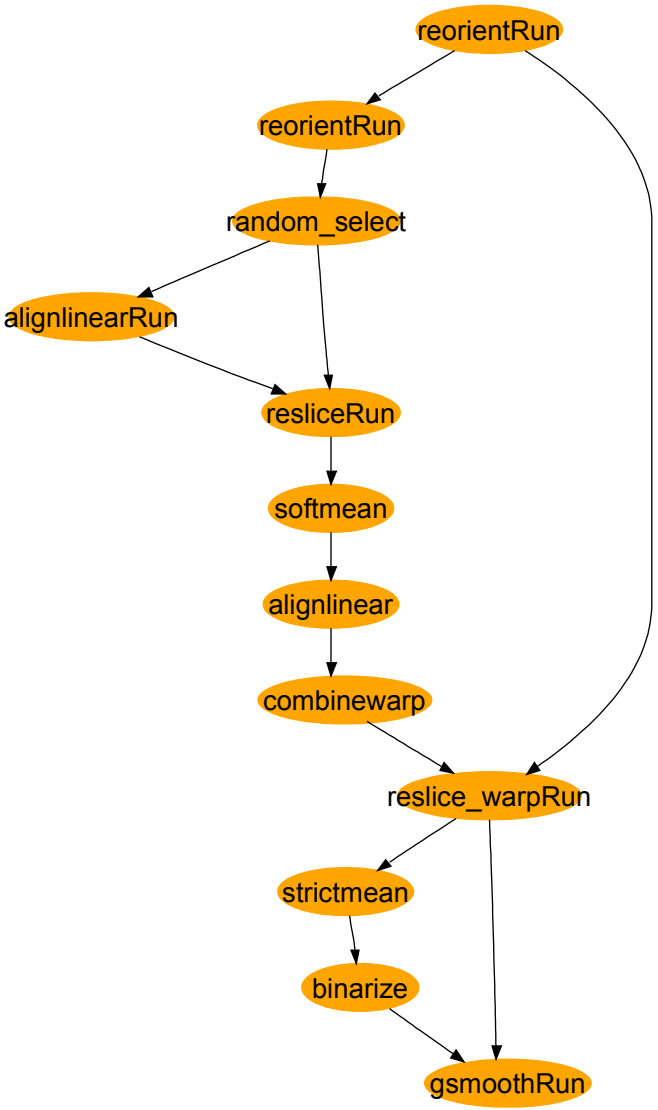


Mapping function or script

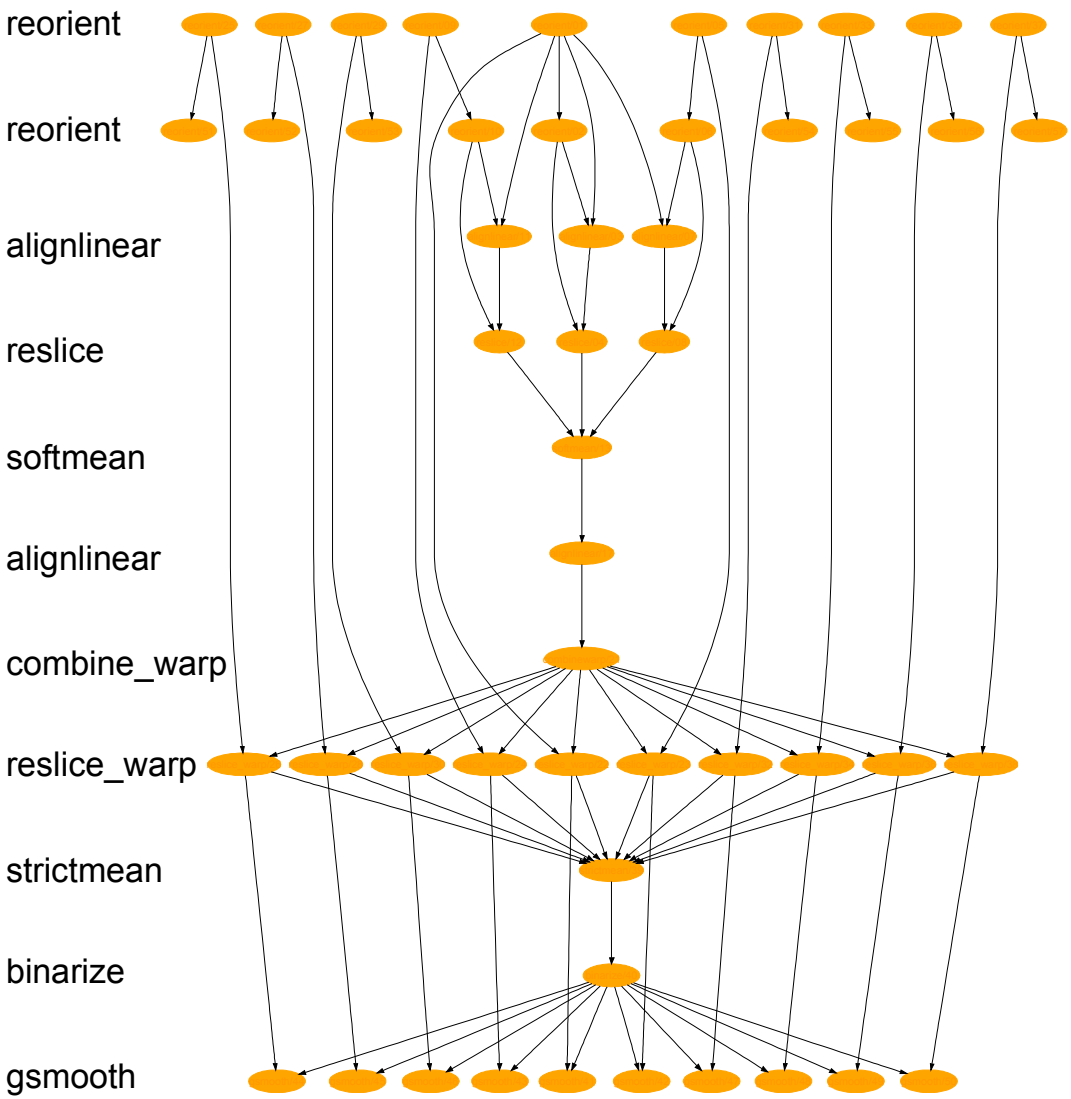
```
type Study {
        Group g[ ];
}
type Group {
        Subject s[ ];
}
type Subject {
        Volume anat;
        Run run[ ];
}
type Run {
        Volume v[ ];
}
type Volume {
        Image img;
        Header hdr;
}
```

Swift's in-memory data model

Spatial normalization of functional MRI runs



Dataset-level workflow



Expanded (10 volume) workflow

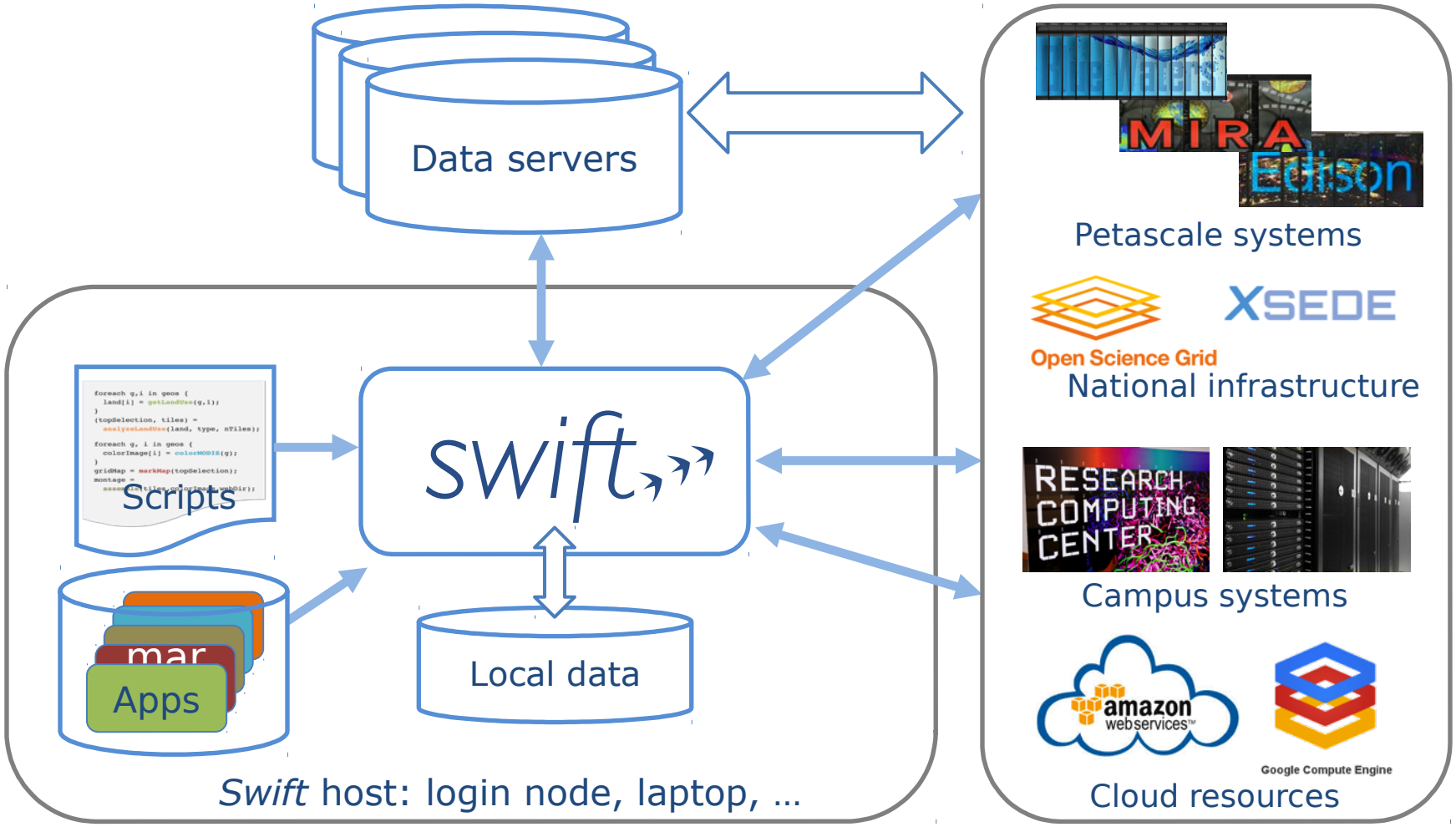
Complex scripts can be well-structured

programming in the large: fMRI spatial normalization script example

```
(Run snr) functional ( Run r, NormAnat a,
                       Air shrink )
{    Run yroRun = reorientRun( r , "y" );
     Run roRun = reorientRun( yroRun , "x" );
     Volume std = roRun[0];
     Run rndr = random_select( roRun, 0.1 );
     AirVector rndAirVec = align_linearRun( rndr, std, 12, 1000, 1000, "81 3 3" );
     Run reslicedRndr = resliceRun( rndr, rndAirVec, "o", "k" );
     Volume meanRand = softmean( reslicedRndr, "y", "null" );
     Air mnQAAir = alignlinear( a.nHires, meanRand, 6, 1000, 4, "81 3 3" );
     Warp boldNormWarp = combinewarp( shrink, a.aWarp, mnQAAir );
     Run nr = reslice_warp_run( boldNormWarp, roRun );
     Volume meanAll = strictmean( nr, "y", "null" )
     Volume boldMask = binarize( meanAll, "y" );
     snr = gsmoothRun( nr, boldMask, "6 6 6" );
}
```

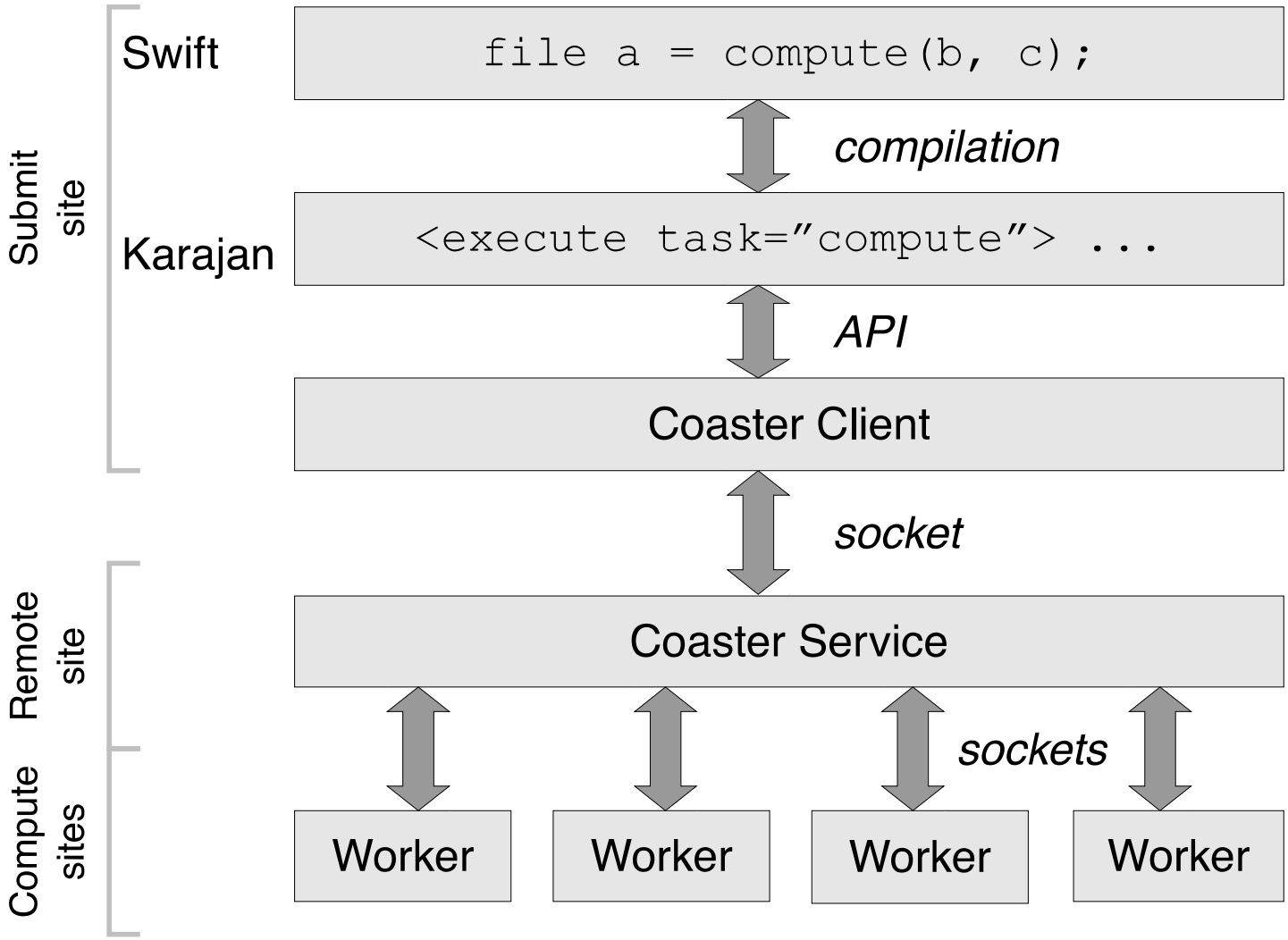
```
(Run or) reorientRun ( Run ir, string direction)
{
        foreach Volume iv, i in ir.v {
                or.v[i] = reorient(iv, direction);
        }
}
```

Swift's distributed architecture is based on a client/worker mechanism (internally named "coasters")



The Swift runtime system has drivers and algorithms to efficiently support and aggregate diverse runtime environments

Worker architecture handles diverse environments



Summary of Swift main benefits

Makes parallelism more transparent

- *Implicitly parallel functional dataflow programming*

- Makes computing location more transparent
- *Runs your script on multiple distributed site and diverse computing resources (desktop to petascale)*

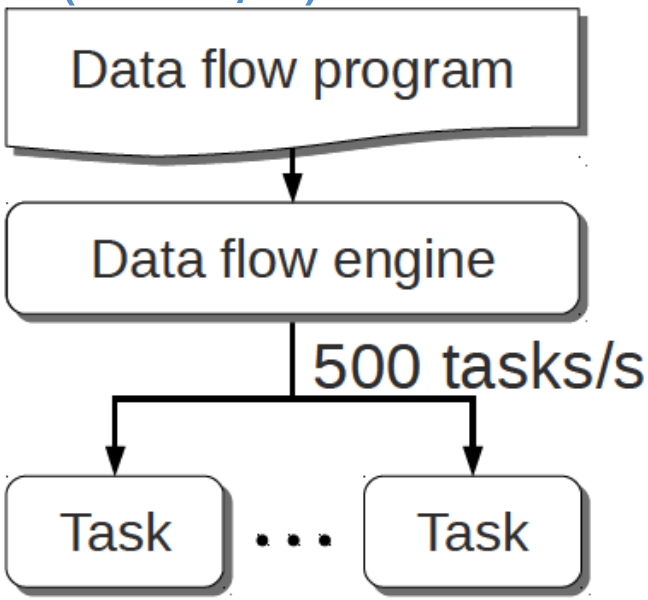
Makes basic failure recovery transparent

- *Retries/relocates failing tasks*
- *Can restart failing runs from point of failur*

Enables provenance capture

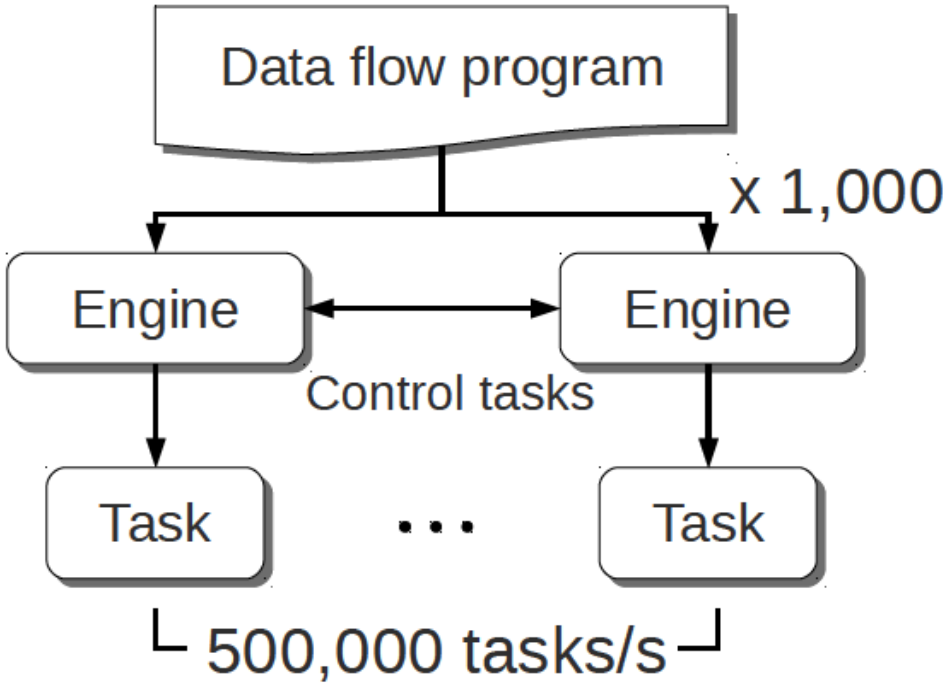
BUT: Centralized evaluation can be a bottleneck at extreme scales

Had this (Swift/K):



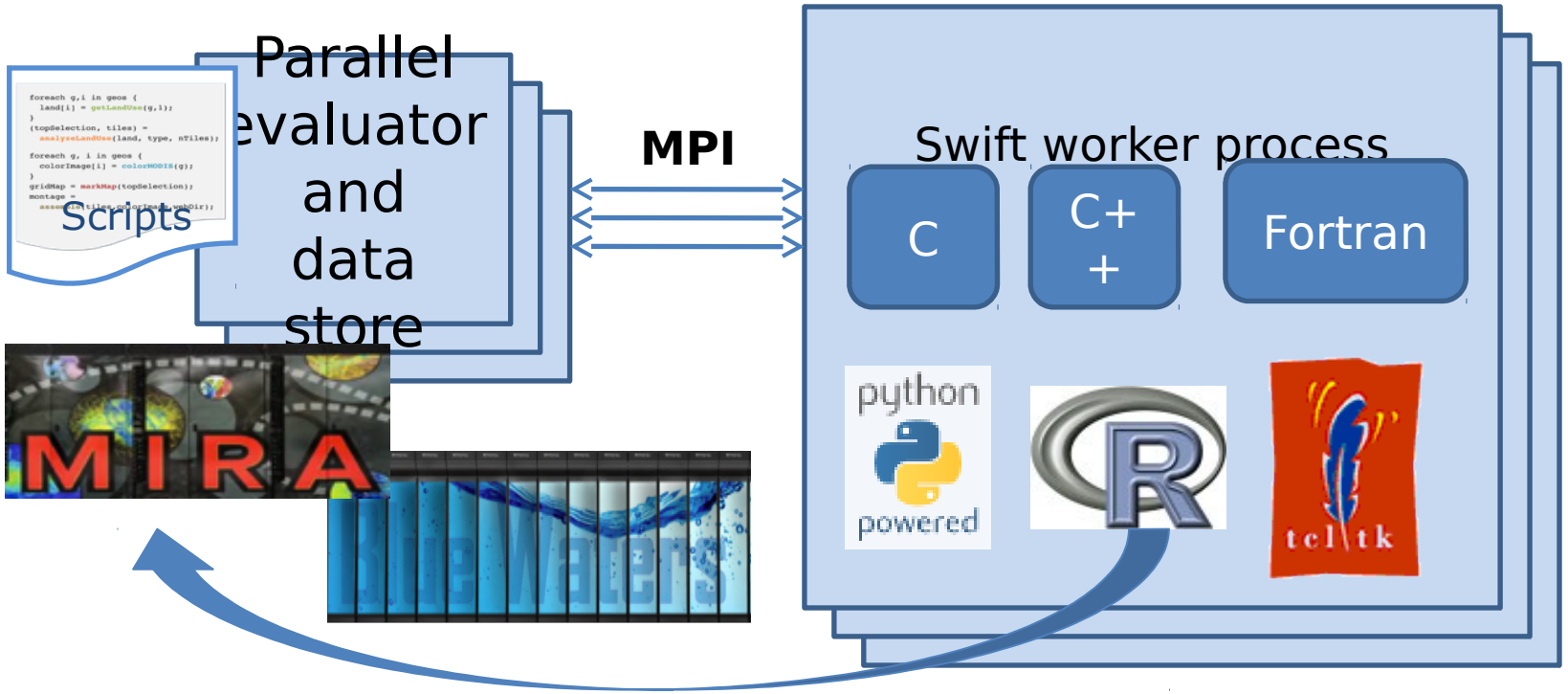
Centralized evaluation

For extreme scale, we need this (Swift/T):



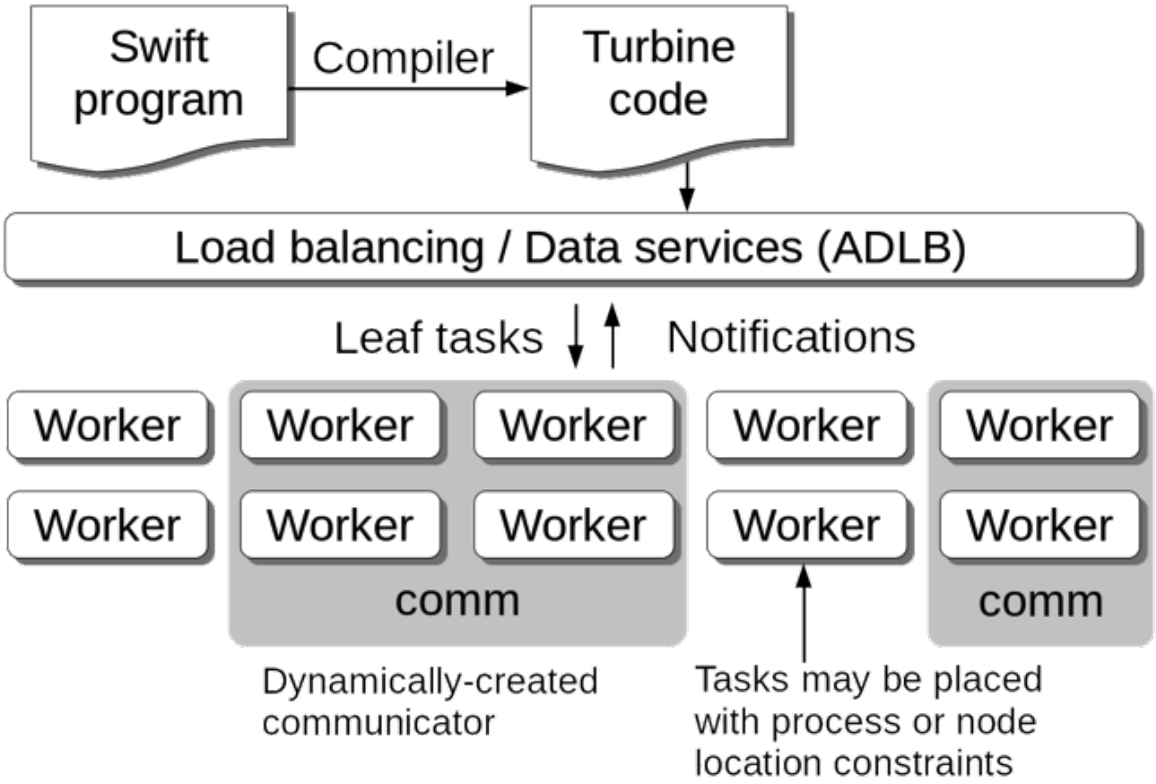
Distributed evaluation

Swift/T: productive extreme-scale scripting



- Script-like programming with “leaf” tasks
  - In-memory function calls in C++, Fortran, Python, R, … passing in-memory objects
  - More expressive than master-worker for “programming in the large”
  - 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

Parallel tasks in Swift/T

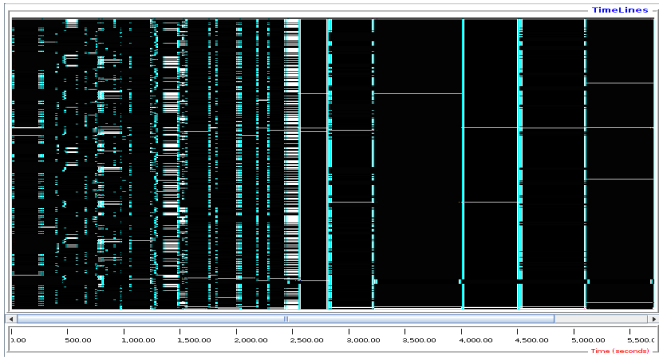


- Swift expression: `z = @par=32 f(x,y);`
- ADLB server finds 8 available workers
  - Workers receive ranks from ADLB server
  - Performs `comm = MPI_Comm_create_group()`
- Workers perform `f(x,y)` communicating on `comm`

LAMMPS parallel tasks

```
foreach i in [0:20] {
    t = 300+i;
sed_command = sprintf("s/_TEMPERATURE_/%i/g", t);
  lammps_file_name = sprintf("input-%i.inp", t);
      lammps_args = "-i " + lammps_file_name;
    file lammps_input<lammps_file_name> =
        sed(filter, sed_command) =>
      @par=8 lammps(lammps_args);
}
```

- LAMMPS provides a convenient C++ API
- Easily used by Swift/T parallel tasks



Tasks with varying sizes packed into big MPI ru

Black: Compute **Blue:** Message **White:** Idl

Swift/T-specific features

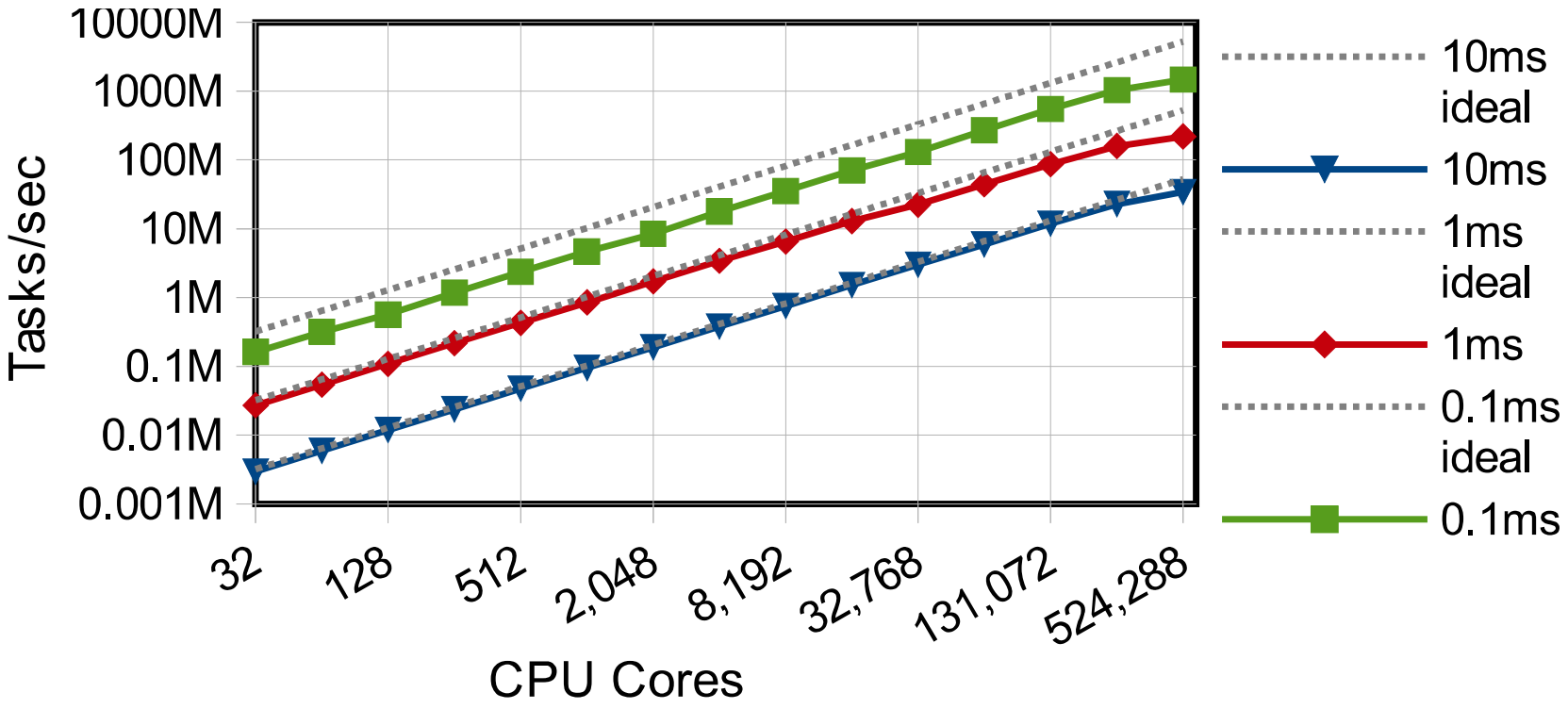
- Task locality: Ability to send a task to a process
  - Allows for big data –type applications
  - Allows for stateful objects to remain resident in the workflow
  - ```
    location L = find_data(D);
    int y = @location=L f(D, x);
    ```
- Data broadcast
- Task priorities: Ability to set task priority
  - Useful for tweaking load balancing
- Updateable variables
  - Allow data to be modified after its initial write
  - Consumer tasks may receive original or updated values when they emerge from the work queue

Wozniak et al. Language features for scalable distributed-memory dataflow computing. Proc. Dataflow Execution Models at PACT, 2014.


    ```

Swift/T: scaling of trivial foreach { } loop

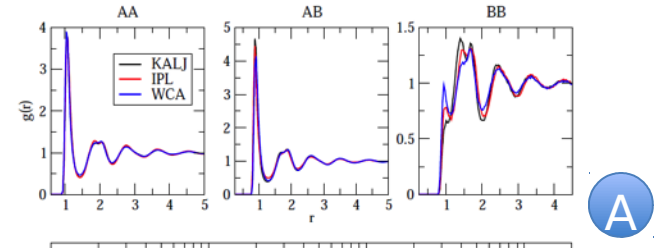
100 microsecond to 10 millisecond tasks on up to 512K integer cores of Blue Waters



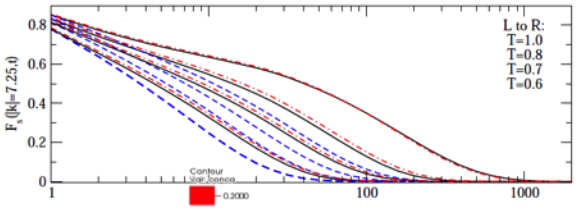
Large-scale applications using Swift

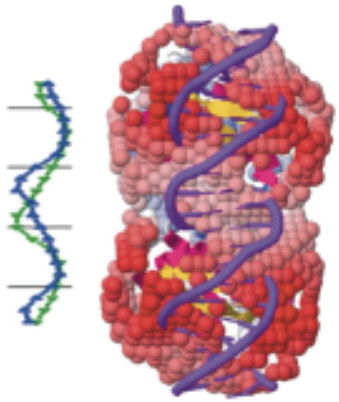
- A: Simulation of super-cooled glass materials
- B: Protein and biomolecule structure and interaction
- C: Climate model analysis and decision making for global food production & supply
- D: Materials science at the Advanced Photon Source
- E: Multiscale subsurface flow modeling
- F: Modeling of power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

All have published science results obtained using Swift



A





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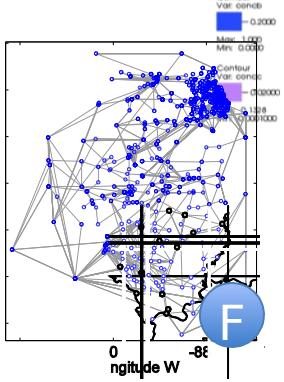

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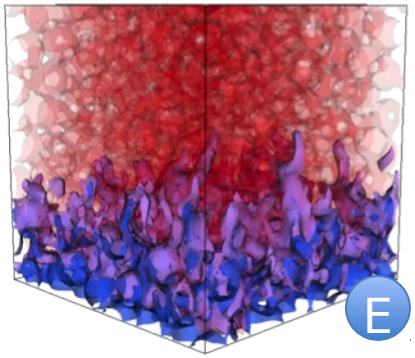

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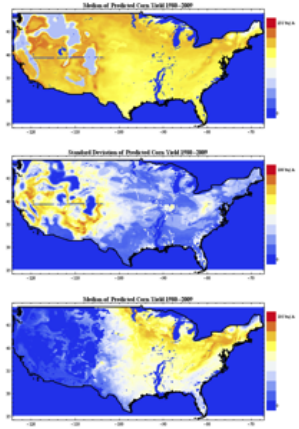
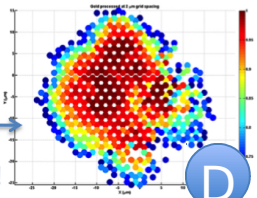
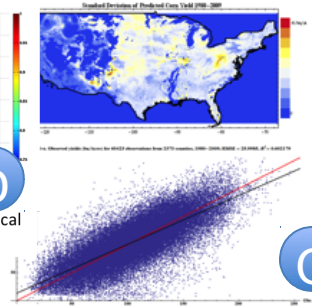




D

Red indicates higher statistical confidence in data



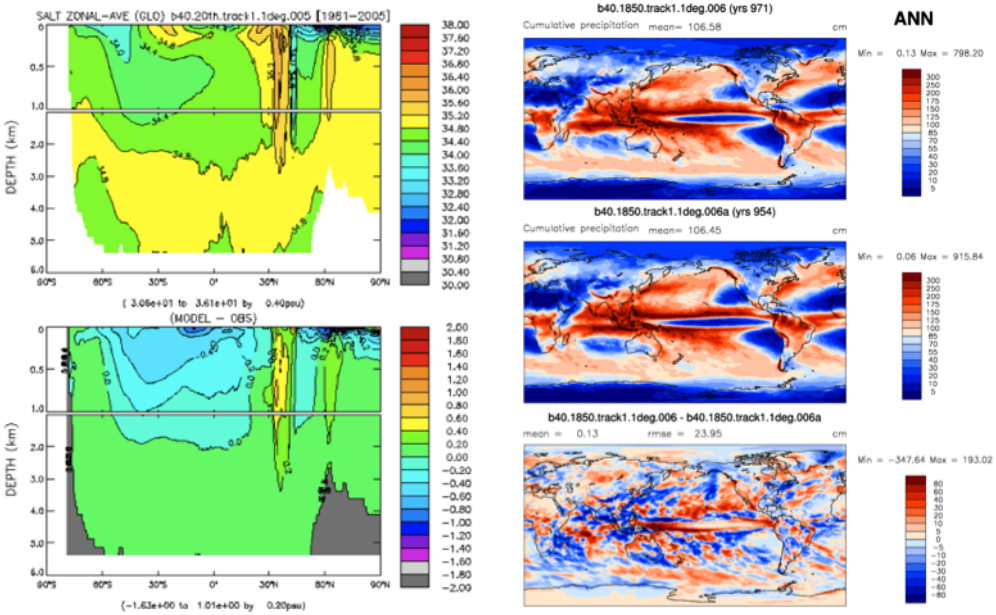
C

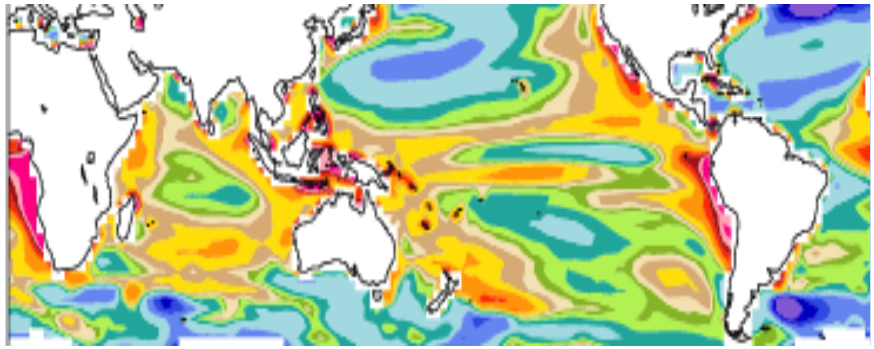
Benefit of implicit pervasive parallelism: Analysis & visualization of high-resolution climate models

powered by *Swift*

parVis

- Diagnostic scripts for each climate model (ocean, atmospehere, land, ice) were expressed in complex shell scripts
- Recoded in Swift, the CESM community has benefited from significant speedups and more modular scripts





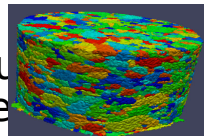
Work of: J Dennis, M Woitasek, S Mickelson, R Jacob, M Vertenstein

Boosting Light Source Productivity with *Swift* ALCF Data Analysis

H Sharma, J Almer (APS); J Wozniak, M Wilde, I Foster (MCS)

Impact and Approach

- HEDM imaging and analysis shows material structu non-destructive



- APS Sector 1 scientists use Mira to process data from live HEDM experiments, providing real-time feedback to correct or improve in-progress experiments
- Scientists working with *Discovery Engines* LDRD developed new *Swift* analysis workflows to process APS data from Sectors 1, 6, and 11

Accomplishments

- Mira analyzes experiment in 10 mins vs. 5.2 hours on APS cluster: > 30X improvement
- Scaling up to ~ 128K cores (driven by data features)
- **Cable flaw was found and fixed at start of experiment,** saving an entire multi-day experiment and valuable user time and APS beam time.
- **In press:** *High-Energy Synchrotron X-ray Techniques for Studying Irradiated Materials* J-S

ALCF Contributions

- Design, develop, support, and trial user engagement to make *Swift* workflow solution on ALCF systems a reliable, secure and supported production service
- Creation and support of the Petrel data server
- Reserved resources on Mira for APS HEDM experiment at Sector 1-ID beamline (8/10/2014 and future sessions in APS 2015 Run 1)

Red indicates higher statistical confidence in

Conclusion: parallel workflow scripting is practical, productive, *and necessary*, at a broad range of scales

- Swift programming model demonstrated feasible and scalable on XSEDE, Blue Waters, OSG, DOE systems
- Applied to numerous MTC and HPC application domains
  - attractive for data-intensive applications
  - and several hybrid programming models
- Proven productivity enhancement in materials, genomics, biochem, earth systems science, …
- Deep integration of workflow in progress at XSEDE, ALCF

Workflow through implicitly parallel dataflow is productive for applications and systems at many scales, including on highest-end system

What's next?

- Programmability
  - New patterns ala Van Der Aalst et al (workflowpatterns.org)
- Fine grained dataflow – programming in the smaller?
  - Run leaf tasks on accelerators (CUDA GPUs, Intel Phi)
  - How low/fast can we drive this model?
- PowerFlow
  - Applies dataflow semantics to manage and reduce energy usage
- Extreme-scale reliability
- Embed Swift semantics in Python, R, Java, shell, make
  - Can we make Swift "invisible"? Should we?
- Swift-Reduce
  - Learning from map-reduce
  - Integration with map-reduce

GeMTC: GPU-enabled Many-Task Computing

Motivation: Support for MTC on all accelerators!

Goals:

1) MTC support 2) Programmability

3) Efficiency 4) MPMD on SIMD

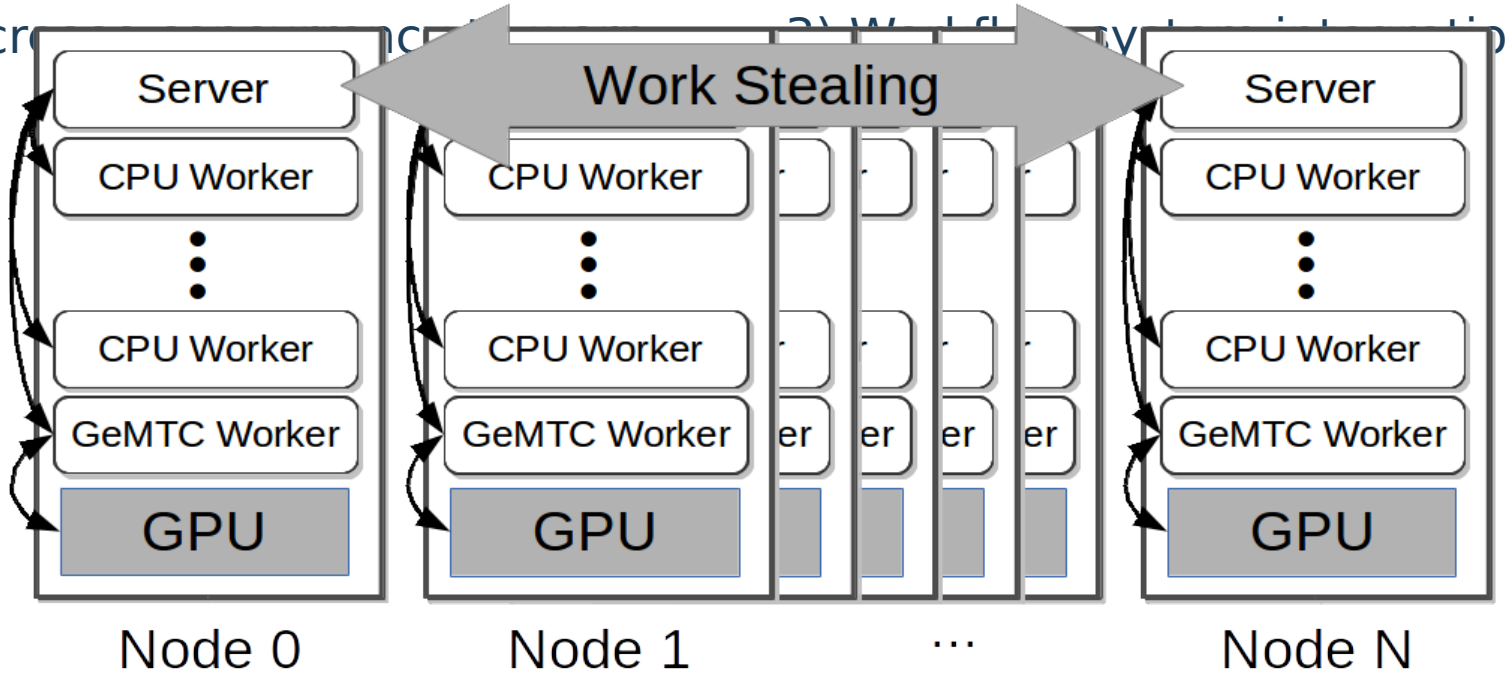
5) Incr… level

Approach:

Design & implement GeMTC middleware:

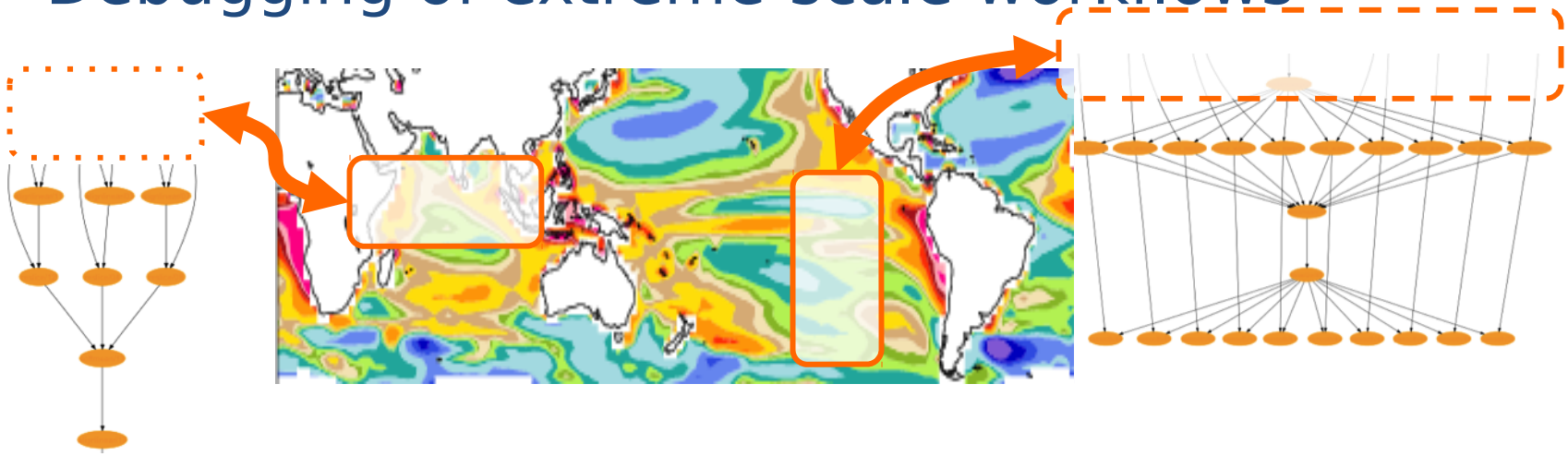
1) Manages GPU 2) Spread host/device

…



Further research directions

- Deeply in-situ processing for extreme-scale analytics
- Shell-like Read-Evaluate-Print Loop ala iPython
- Debugging of extreme-scale workflows



Deeply in-situ analytics of a climate simulation

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Swift: A language for distributed parallel scripting

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ABSTRACT

Scientists, engineers, and statisticians must execute domain-specific application programs many times on large collections of file-based data. This activity requires complex orchestration and data management as data is passed to, from, and among application invocations. Distributed and parallel computing resources can accelerate such processing, but their use further increases programming complexity. The Swift parallel scripting language reduces these complexities by making file system structures accessible via language constructs and by allowing ordinary application programs to be composed into powerful parallel scripts that can efficiently utilize parallel and distributed resources. We present Swift's implicitly parallel and deterministic programming model, which applies external applications to file collections using a functional style that abstracts and simplifies distributed parallel execution.