Many-Task Computing Tools for Multiscale Modeling

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Computation Institute

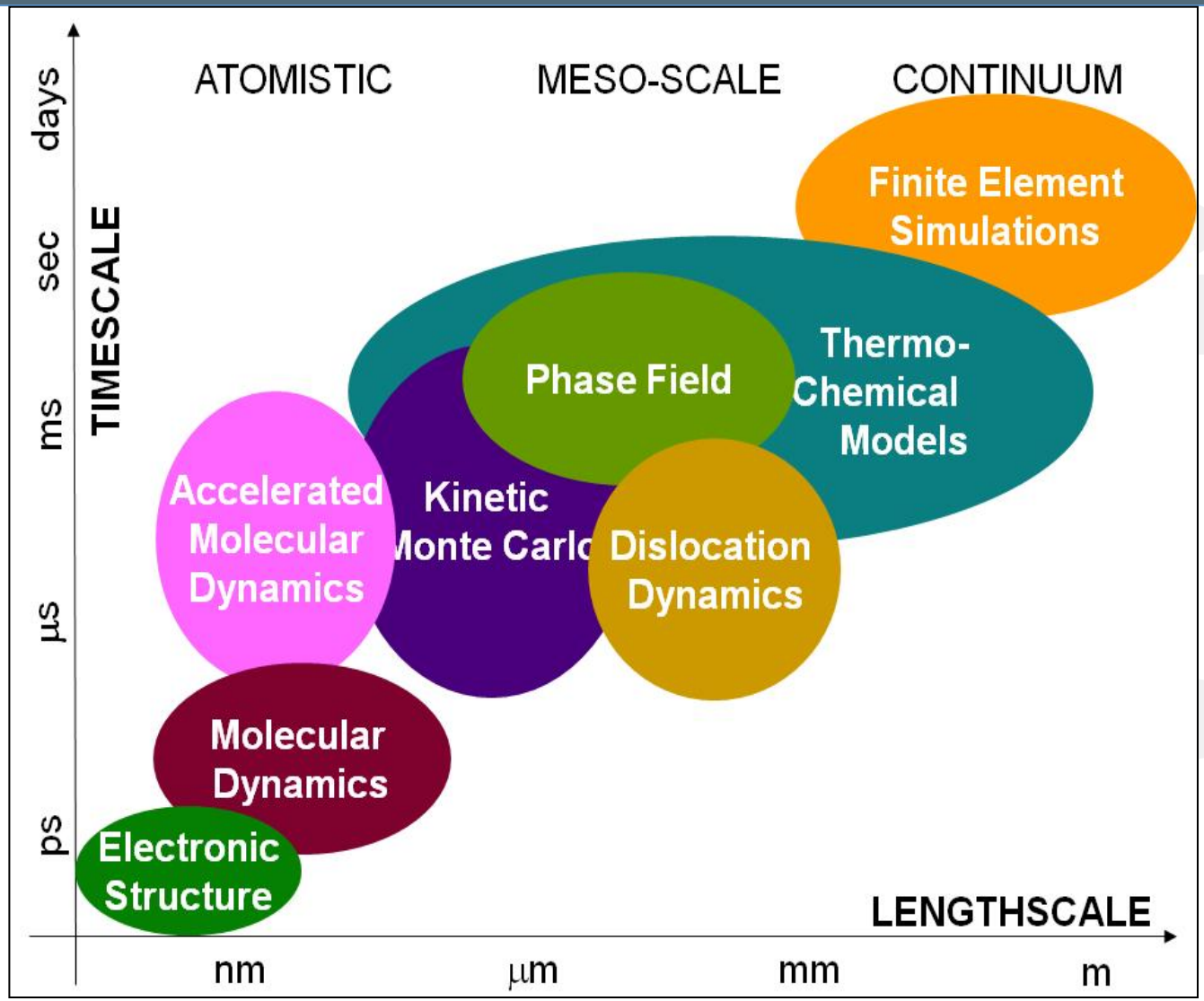
- Mission: address the most challenging problems arising in the use of strategic computation and communications
- Joint Argonne/UChicago institute, ~100 Fellows (~50 UChicago faculty) & ~60 staff
- Primary goals:
  - Pursue new discoveries using multi-disciplinary collaborations and computational methods
  - Develop new computational methods and paradigms required to tackle these problems, and create the computational tools required for the effective application of advanced methods at the largest scales
  - Educate the next generation of investigators in the advanced methods and platforms required for discovery

Multiscale Modeling

Multiscale

- The world is multiscale
- In modeling, a common challenge is determining the correct scale to capture a phenomenon of interest
  - In computer science, a parallel problem is describing a problem with the right level of abstraction
    - Capture the details you care about and ignore those you don't
- But multiple phenomena interact, often at different scales

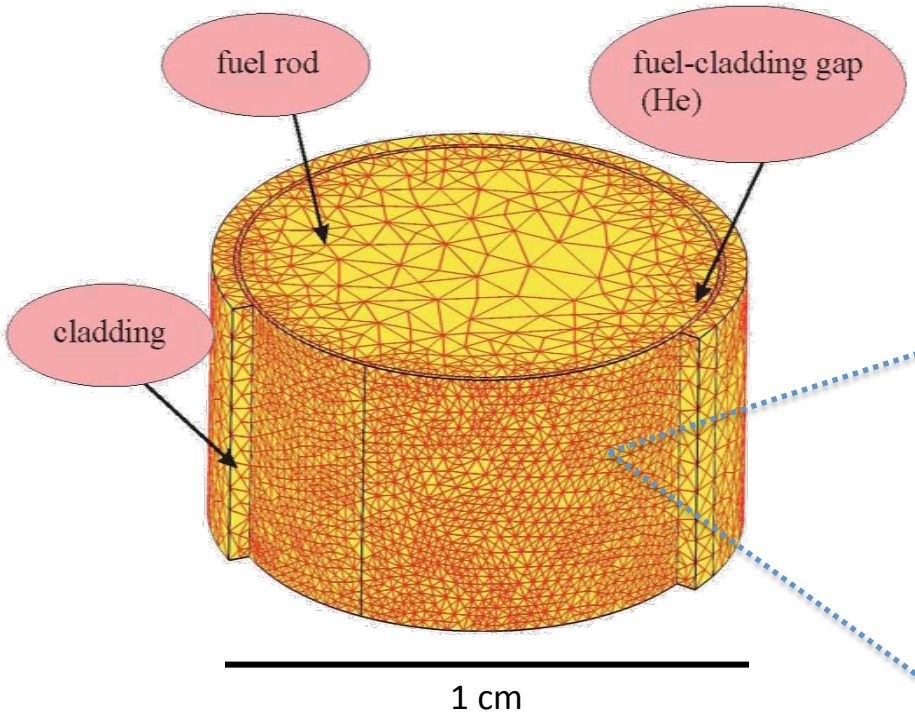
Material Science, Methods and Scales



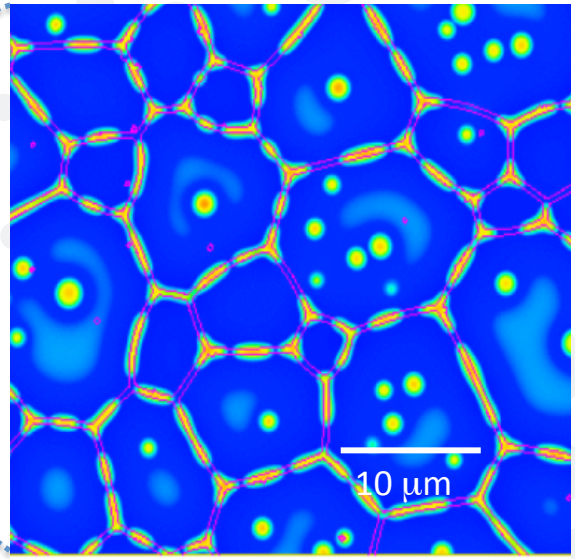
Credit: M. Stan, Materials Today, 12 (2009) 20-28

Modeling nuclear fuel rods

Fuel Element Model (FEM)



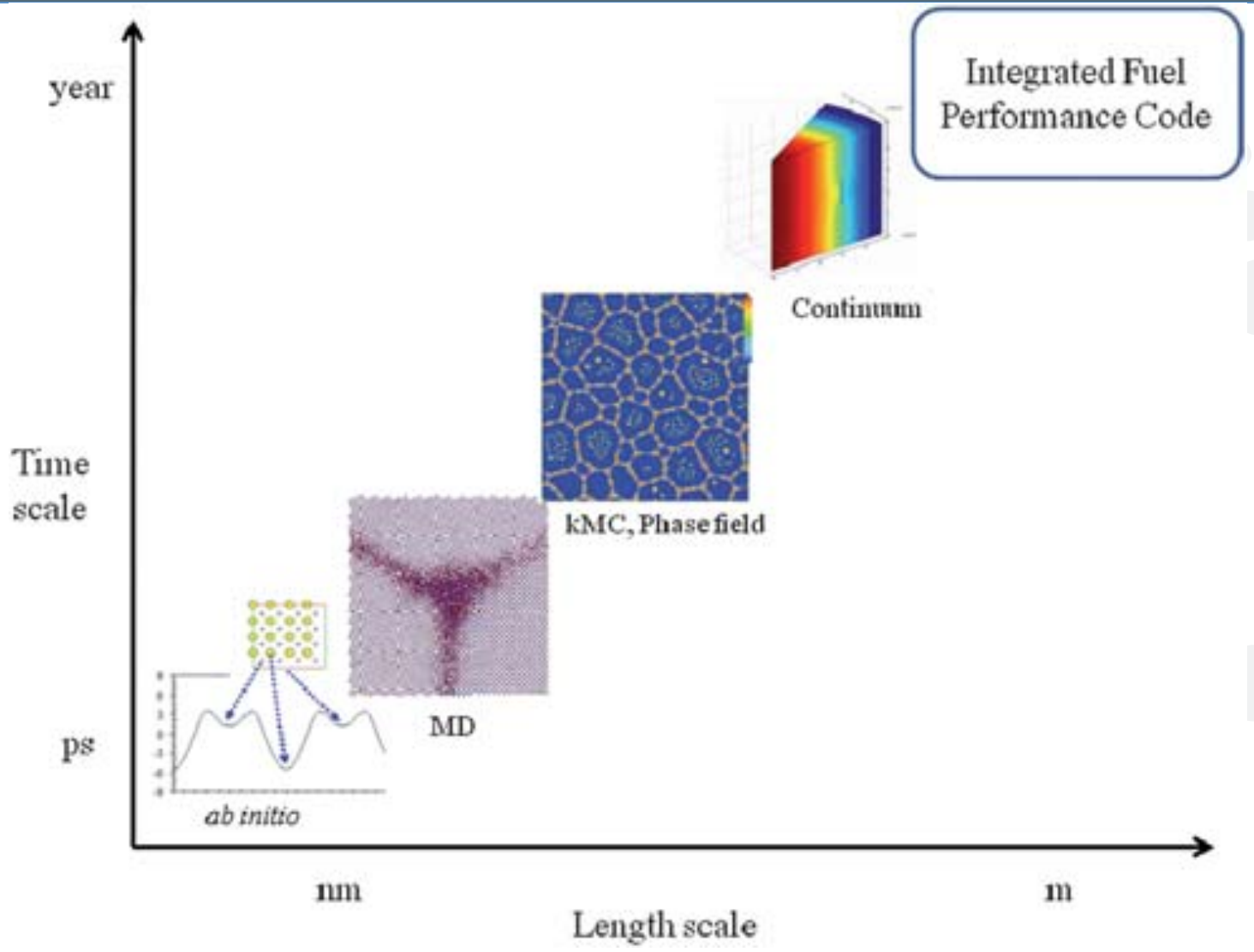
Microstructure Model (PF)



B. Mihaila, et al., J. Nucl. Mater., **394** (2009) 182-189

S.Y. Hu et al., J. Nucl. Mater. **392** (2009) 292–300

Sequential (information passing, hand-shaking, bridging)



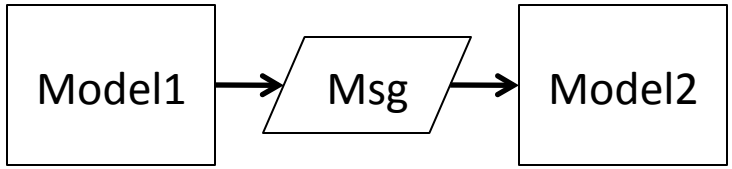
R. Devanathan, et al., Energy Env. Sc., **3** (2010) 1406-1426

Coupling methods

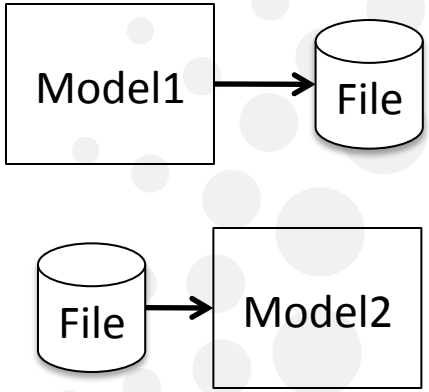
- We often know how to solve a part of the problem with sufficient accuracy, but when we combine multiple parts of the problem at various scales, we need to couple the solution methods too
- Must first determine the models to be run and how they iterate/interact
- Coupling options
  - "Manual" coupling (sequential, manual)
    - Inputs to a code at one scale are influenced by study of the outputs of a previously run code at another scale
    - Coupling timescale: hours to weeks
  - "Loose" coupling (sequential, automated) between codes
    - Typically performed using workflow tools
    - Often in different memory spaces
    - Coupling timescale: minutes
  - "Tight" coupling (concurrent, automated) between codes
    - e.g., ocean-atmosphere-ice-bio
    - Typically performed using coupling methods (e.g., CCA), maybe in same memory space
    - Hard to develop, changes in one code may break the system
    - Coupling timescale: seconds
- Boundary between options can be fuzzy
- Choice often depends on how frequently the interactions are required, and how much work the codes do independently

More on coupling

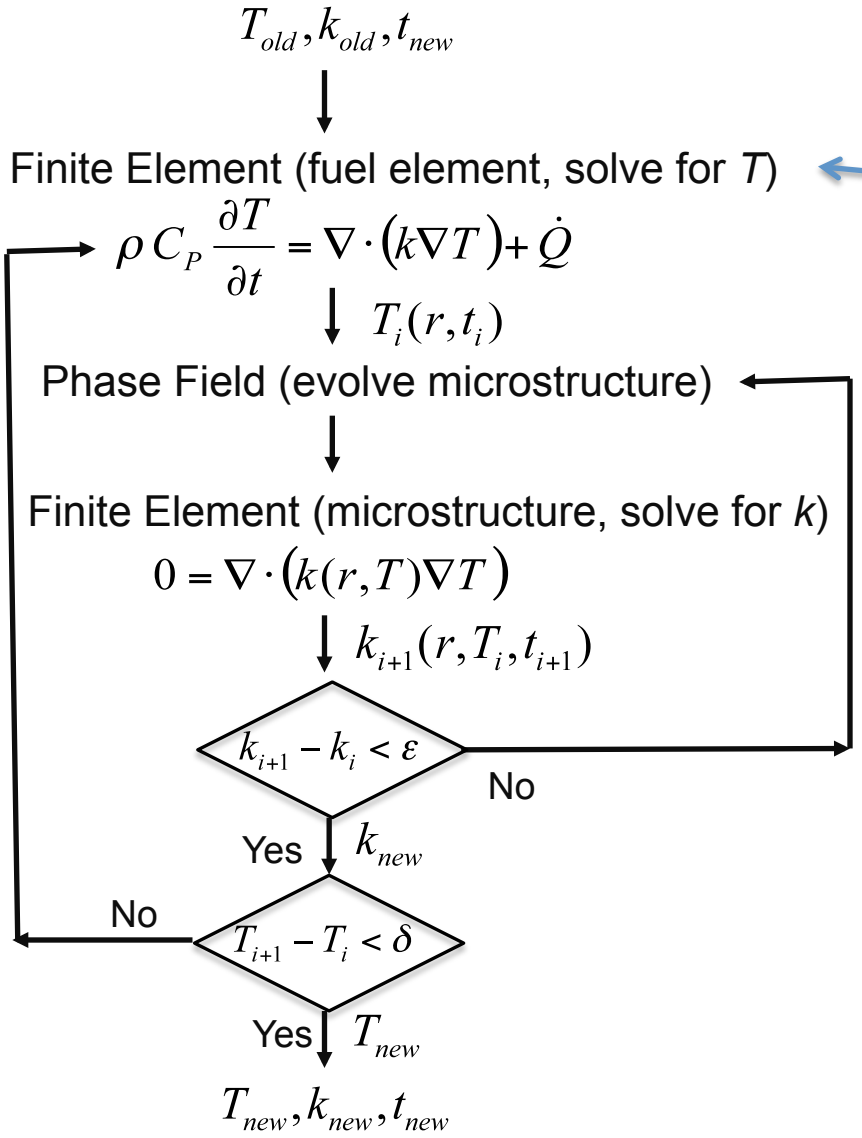
Tight

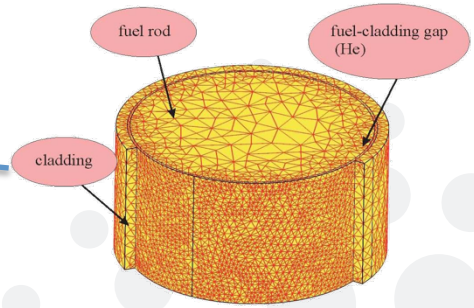


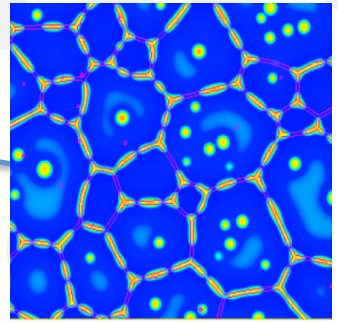
Loose



Coupling Models



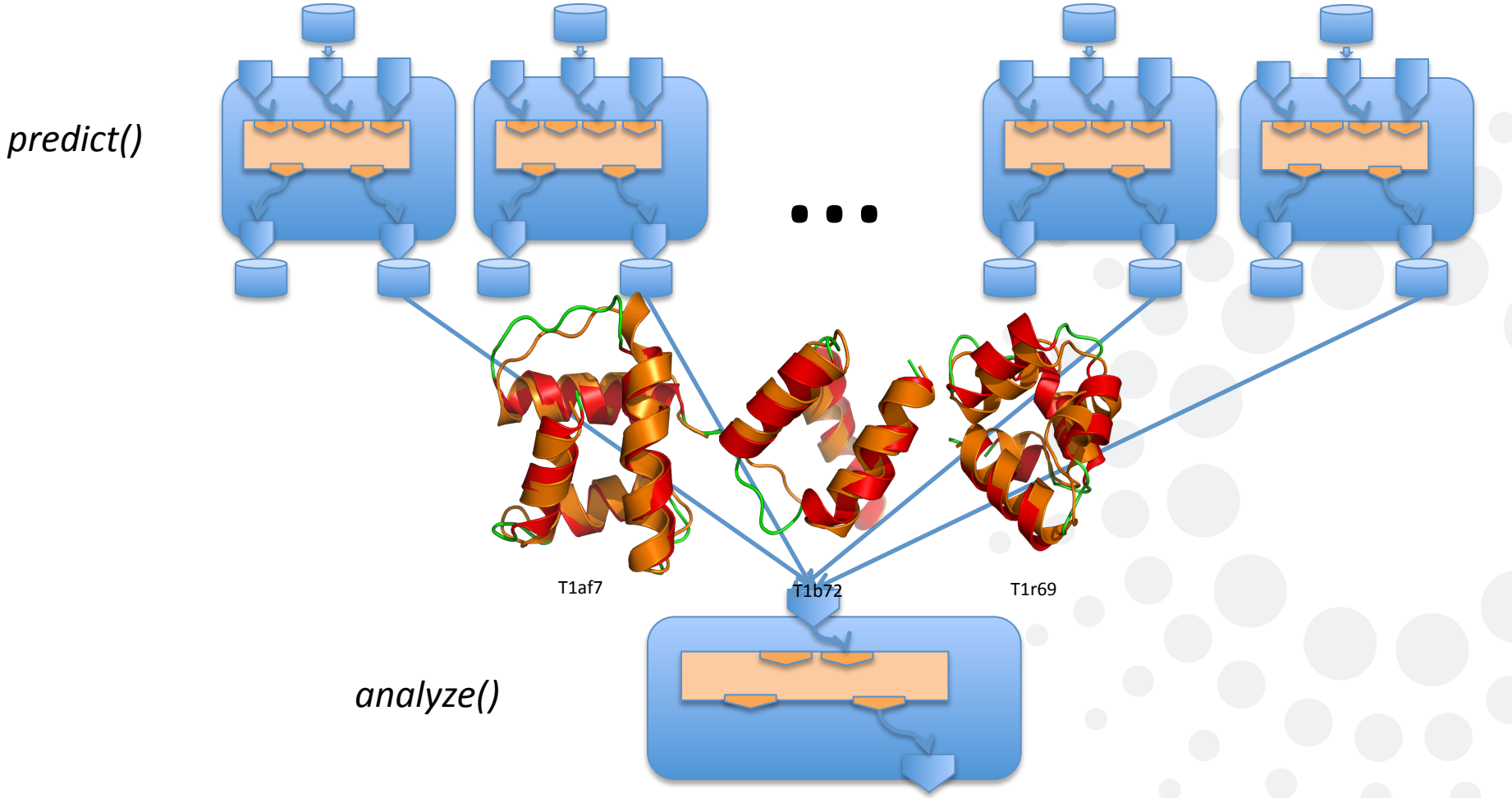




Credit: Marius Stan, Argonne

Swift (for Loose Coupling)

Workflow Example: Protein Structure Prediction



Want to run: 10 proteins x 1000 simulations x
3 MC rounds x 2 temps x 5 deltas = 300K tasks

Swift

- Portable workflows – deployable on many resources
- Fundamental script elements are external processes and data files
- Provides natural concurrency at runtime through automatic data flow analysis and task scheduling
- Data structures and script operations to support scientific computing
- Provenance gathered automatically

Portability: dynamic development and execution

- Separate workflow description from resource and component implementations

<sites.xml>
…

```
rawdata = sim(settings);
stats = analysis(rawdata);
…
```

select resources

write script

allocate resources

Execute
(Swift)

<tc.data>
…

define
components

Swift scripts

- C-like syntax, also Python prototype
- Supports file/task model directly in the language

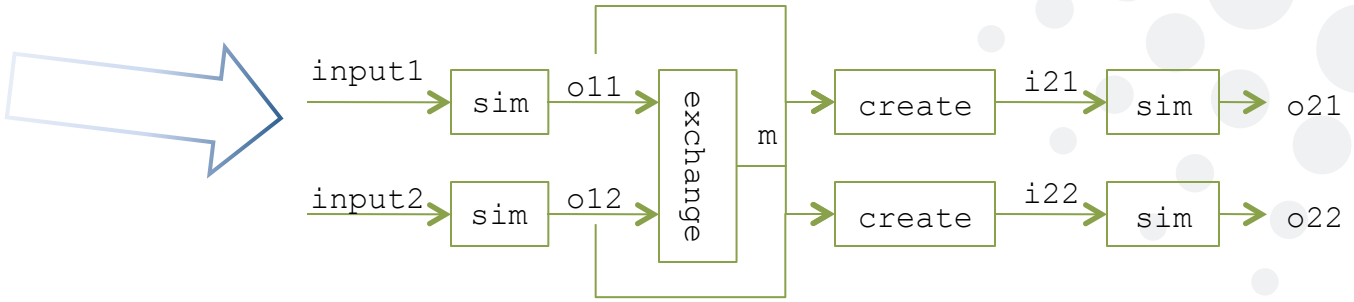
```
type file;

app (file output) sim(file input) {
  namd2 @input @output
}
```

- Historically, most tasks have been sequential applications

Data flow and natural concurrency

- Provide natural concurrency through automatic data flow analysis and task scheduling

```
file o11 = sim(input1);
file o12 = sim(input2);
file m   = exchange(o11, o12);
file i21 = create(o11, m);
file o21 = sim(i21);
...
```

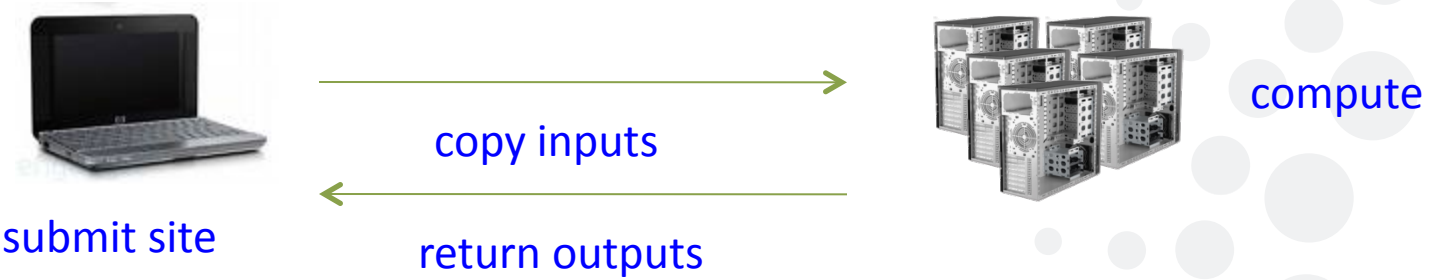


Variables, Tasks, Files, Concurrency

- Variables are single assignment futures
  - Unassigned variables are open
- Variables can represent files
  - When a file doesn't exist, the variable is open
  - When a file exists, the variable is closed
- All tasks found at runtime
- Tasks with satisfied dependencies (closed variables) are run on whatever resources are available
- These runs create files/variables that allow more tasks to run

Execution model

- In a standard Swift workflow, each task must enumerate its input and output files
- These files are shipped to and from the compute site

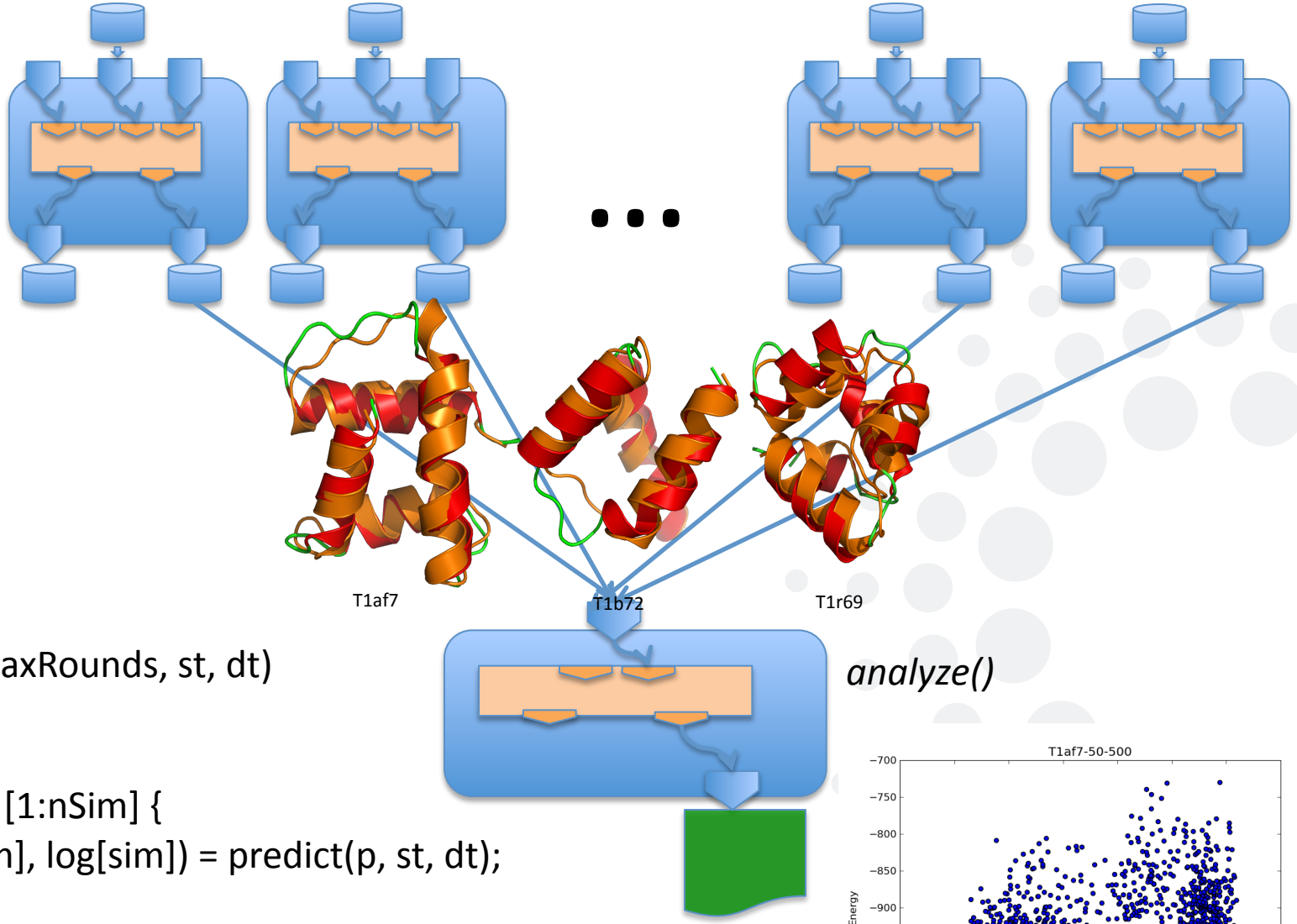


- RPC-like technique, can use multiple queuing systems, data services, and execution environments
  - Uses abstractions for file transfer, job execution, etc.
  - Allows use of local systems (laptop, desktop), parallel systems (HPC), distributed systems (HTC, clouds)
  - Supports grid authentication mechanisms
- Can use multi-level scheduling (Coasters) – alleviates need for reservations?

Performance and Usage

- Swift is fast
  - Uses Karajan (in Java CoG) as powerful, efficient, scalable, and flexible execution engine
  - Scaling close to 1M tasks; .5M in live science work, and growing
- Swift usage is growing (~300 users in last year):
  - Applications in neuroscience, proteomics, molecular dynamics, biochemistry, climate, economics, statistics, astronomy, etc.
  - And earthquake modeling (to be discussed in seasonal school Wed.)

nSim (1000) predict()s




```
ItFix(p, nSim, maxRounds, st, dt)
{
  ...
  foreach sim in [1:nSim] {
    (structure[sim], log[sim]) = predict(p, st, dt);
  }
  result = analyze(structure)
  ...
}
```

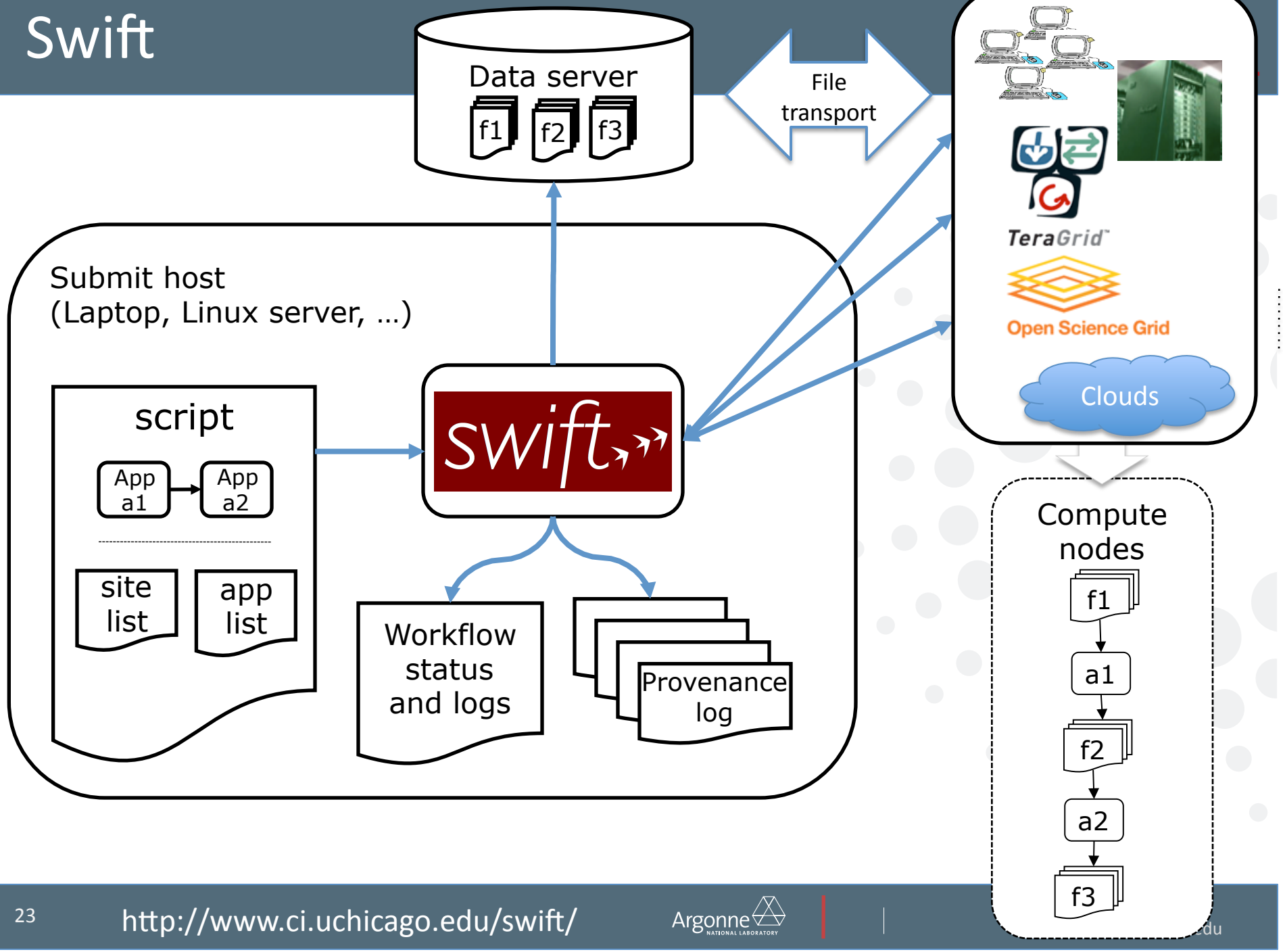
analyze()

Powerful parallel prediction loops in *Swift*

```
1.  Sweep( )
2.  {
3.    int nSim = 1000;
4.    int maxRounds = 3;
5.    Protein pSet[ ] <ext; exec="Protein.map">;
6.    float startTemp[ ] = [ 100.0, 200.0 ];
7.    float delT[ ] = [ 1.0, 1.5, 2.0, 5.0, 10.0 ];
8.    foreach p, pn in pSet {
9.      foreach t in startTemp {
10.       foreach d in delT {
11.         ItFix(p, nSim, maxRounds, t, d);
12.       }
13.     }
14.   }
15. }
```

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

Swift



http://www.ci.uchicago.edu/swift/

Swift summary

- Structures and arrays of data
- Typed script variables intermixed with references to file data
- Natural concurrency
- Integration with schedulers such as PBS, Cobalt, SGE, GT2, …
- Advanced scheduling settings
- A variety of useful workflows can be considered

Using Swift for Loose Coupling

Multiscale Molecular Dynamics

- Problem: many systems are too large to solve using all-atom molecular dynamics (MD) models
- Potential solution: coarse-grained (CG) models where each site represents multiple atoms
- In order to do this, have to decide how to coarsen the model
  - How many sites are needed?
  - Which atoms are mapped to which sites?
  - What is the potential energy as a function of coordinates of those CG sites?

Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Building a CG model – initial data processing

- Stage 0 – run multiple short-duration trajectories of all-atom MD simulation, e.g., using NAMD, capture dcd files
  - Can require large run time and memory, so run on TeraGrid system
  - Download (binary) dcd files to local resources for archiving
  - Remove light atoms (e.g., water, H)
  - Performed manually
- Stage 1 – remove non α-Carbon atoms on a subset of the dcd files from each trajectory
  - Need to know how many steps were in each trajectory – not always what was planned, and final file may be corrupt, so some manual checking needed
  - Performed by fast Tcl script

Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Building CG model – covariance matrix

- Stage 2 – join trajectory files together into ascii file
  - Requires trajectory length from previous stage
  - Performed by fast Tcl script
- Stage 3 – generate covariance matrix for each trajectory
  - Find deviation of each atom from its average position across all time steps
  - Covariance matrix determines which atoms can be grouped into rigid bodies (roughly)
  - Performed by shell script that runs a compiled C code
    - Takes several hours per trajectory

Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Building a CG model – CG mapping

- Stage 4 – for a given number of sites (#sites), find best mapping for each trajectory
  - Pick 3 to 5 values for #sites that should cover the likely best value
  - For each #sites, can find χ^2 value for each mapping
  - Overall, want lowest χ^2 and corresponding mapping
  - Uses a group of random initial values and simulated annealing from each
  - Performed by shell script to launch compiled C code, O(50k) trials, takes several days on 100-1000 processors
- Stage 5 – check χ^2 values for each trajectory
  - χ^2 vs. #sites on a log-log plot should be linear
  - Performed by script
  - If a point is not close to the line, it's probably not a real minimum χ^2 for that #sites
    - Go back to Stage 4 – run more initial case to get a lower χ^2

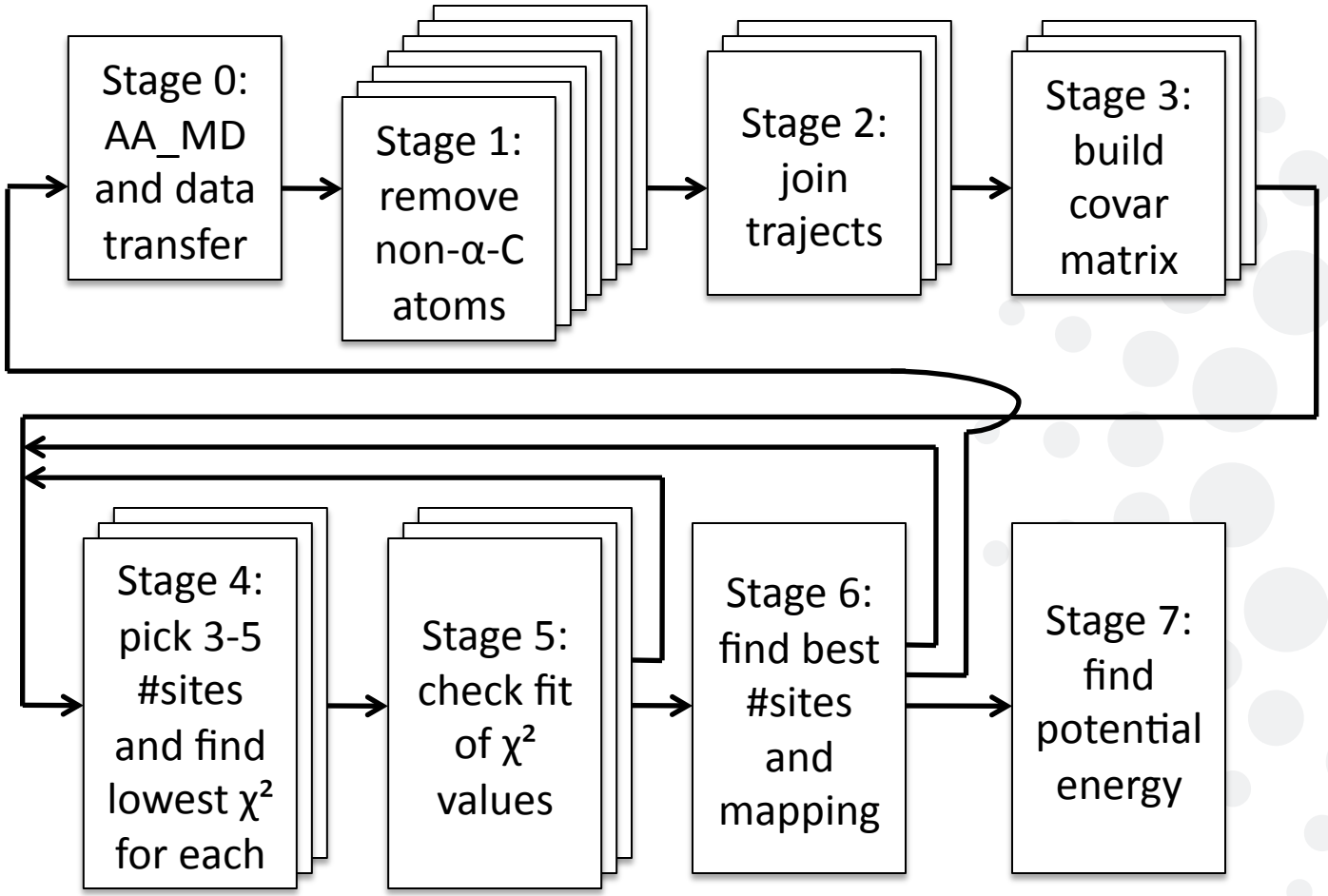
Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Building a CG model – finding #sites

- Stage 6 – determine #sites
  - Estimate best #sites (b#sites) from slope/intercept of line in stage 5, and compare results of all trajectories
  - Performed by script
  - If results for each trajectory are different, trajectories didn't sample enough of the phase space – go back to Stage 0 and run more/longer trajectories
  - If b#sites is outside the range of #sites that have been calculated, add to initial range and go back to Stage 4
  - If b#site is inside the range, create a smaller range around b#sites and go back to Stage 4
    - b#sites is an integer, so don't have to do this too much
  - Outputs final b#sites and corresponding mapping
- Stage 7 – building potential energy as function of site coordinates
  - Can be done by different methods, e.g., Elastic Network Models (ENM)
    - Currently under construction

Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Bio workflow: AA->CG MD



Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

Multiscale?

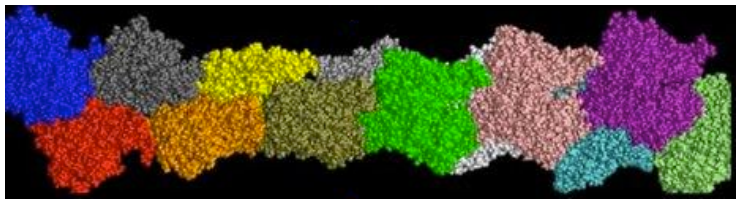
- So far, this isn't really multiscale
- It has just used fine grain information to build the best coarse grained model
- But it's a needed part of the process
- Overall, can't run AA_MD as much as desired.
  - Here, limited AA_MD simulations -> structural information for a rough CG model of the internal molecular structure
  - With rough CG model, user can parameterize interactions for CG "atoms" via targeted all-atom simulations -> determine average energies and forces etc. for the CG beads
- Doing this automatically is a long-term goal

Credit: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago

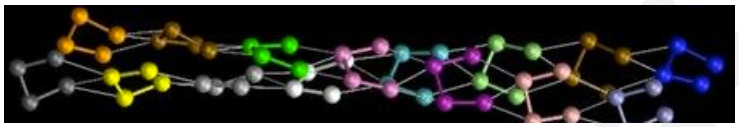
NSF Center for Chemical Innovation Phase I award: "Center for Multiscale Theory and Simulation"

- ... development of a novel, powerful, and integrated theoretical and computational capability for the description of biomolecular processes across multiple and connected scales, starting from the *molecular scale and ending at the cellular scale*
- Components:
  - A theoretical and computer **simulation capability to describe biomolecular systems at multiple scales** will be developed, includes atomistic, coarse-grained, and mesoscopic scales ... all scales will be connected in a multiscale fashion so that key information is passed upward in scale and vice-versa
  - Latest generation scalable computing and **a novel cyberinfrastructure** will be implemented
  - A high profile demonstration projects will be undertaken using the resulting theoretical and modeling advances which involves the **multiscale modeling of the key biomolecular features of the eukaryotic cellular cytoskeleton (i.e., actin-based networks and associated proteins)**
- Core CCI team includes a diverse group of leading researchers at the University of Chicago from the fields of theoretical/computational chemistry, biophysics, mathematics, and computer science:
  - Gregory A. Voth (PI, Chemistry, James Franck Institute, Institute for Biophysical Dynamics, Computation Institute); Benoit Roux (co-PI, Biochemistry and Molecular Biology, Institute for Biophysical Dynamics); Nina Singhal Hinrichs (co-PI, Computer Science and Statistics); Aaron Dinner (co-PI, Chemistry, James Franck Institute, Institute for Biophysical Dynamics); Karl Freed (co-PI, Chemistry, James Franck Institute, Institute for Biophysical Dynamics); Jonathan Weare (co-PI, Mathematics); Daniel S. Katz (Senior Personnel, Computation Institute)

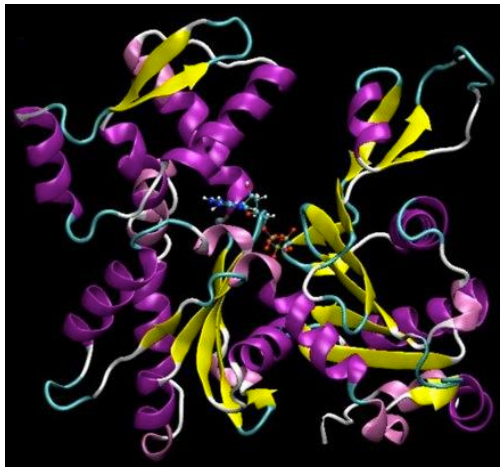
Actin at multiple scales



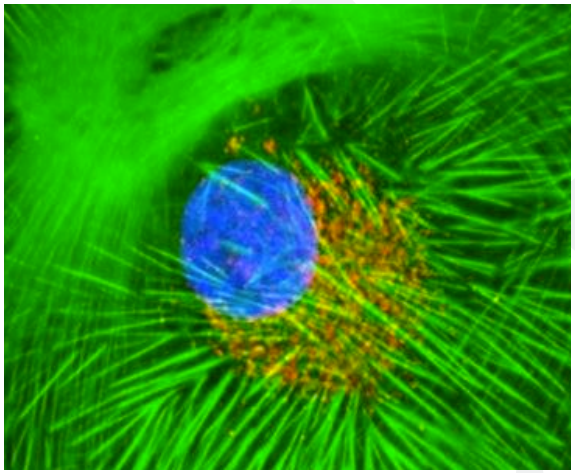
Actin filament (F-Actin) – complex of G-Actins



Actin filament (F-Actin) – CG representation



Single Actin monomer (G-Actin) – all-atom representation



Actin in cytoskeleton – mesoscale representation

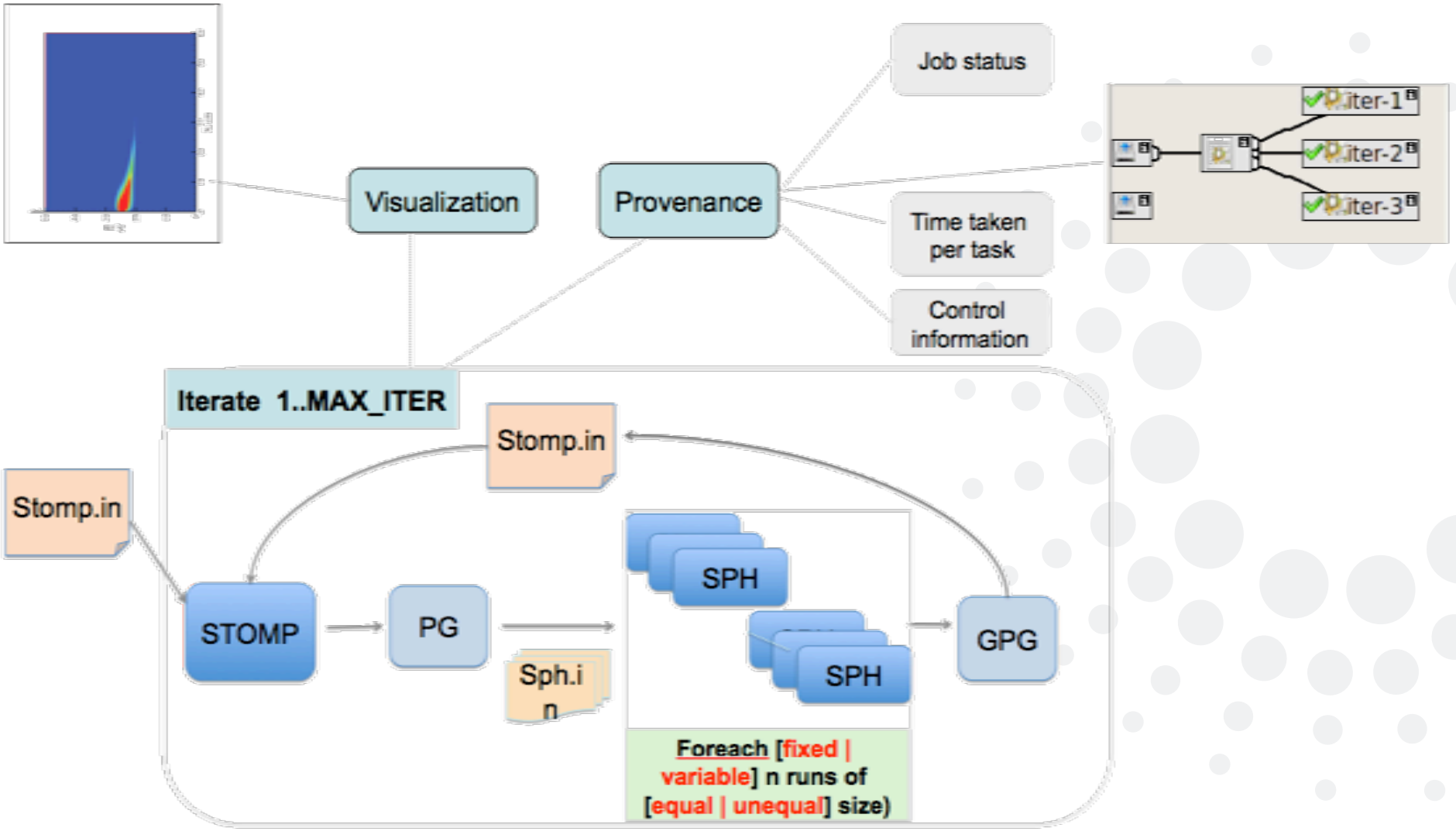
Credit: Greg Voth, U. Chicago

Geophysics Application

- Subsurface flow model
- Couples continuum and pore scale simulations
  - Continuum model: exascale Subsurface Transport Over Multiple Phases (eSTOMP)
    - Scale: meter
    - Models full domain
  - Pore scale model: Smoothed Particle Hydrodynamics (SPH)
    - Scale: grains of soil (mm)
    - Models subset of domain as needed
- Coupler codes developed
  - Pore Generator (PG) – adaptively decides where to run SPH and generates inputs for each run
  - Grid Parameter Generator (GPG) – uses outputs from SPH to build inputs for next eSTOMP iteration

Credit: Karen Schuchardt , Bruce Palmer, Khushbu Agarwal, Tim Scheibe, PNNL

Subsurface Hybrid Model Workflow



Credit: Karen Schuchardt , Bruce Palmer, Khushbu Agarwal, Tim Scheibe, PNNL

Swift code

```
// Driver
file stompIn <"stomp.in">;

iterate iter {
        output = HybridModel(inputs[iter]);
        inputs[iter+1] = output;
        capture_provenance(output);

} until(iter >=  MAX_ITER);
```

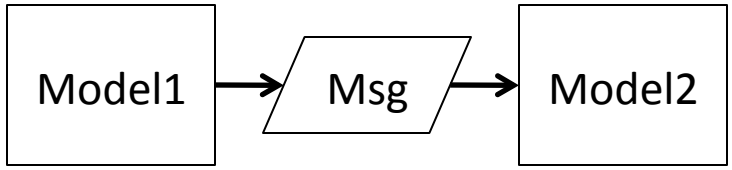
```
//Hybrid Model

(file  simOutput) HybridModel (file input) {
    …
     stompOut = runStomp(input);

    (sphins, numsph) = pg(stompOut, sphinprefix);

     //Find number of pore scale runs
     int n = @toint(readData(numsph));
      foreach i in [1:@toint(n)]  {
         sphout[i]= runSph(sphins[i],  procs_task)
      }

    simOutput = gpg(sphOutArr, n, sphout);
}
```

Credit: Karen Schuchardt , Bruce Palmer, Khushbu Agarwal, Tim Scheibe, PNNL

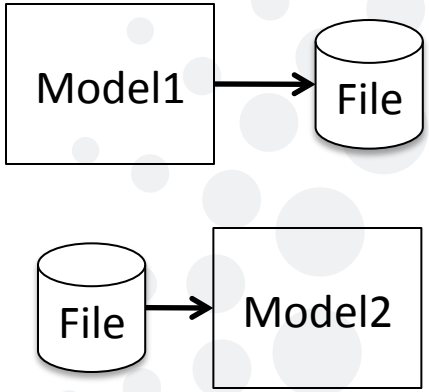
Towards Tighter Coupling

More on coupling

Tight



Loose



More on coupling

- Message vs. file issues:
  - Performance: overhead involved in writing to disk vs. keeping in memory
  - Semantics: messages vs. Posix
  - Fault tolerance: file storage provides an automatic recovery mechanism
  - Synchronicity: messages can be sync/async, files must be async
- Practical issues:
  - What drives the application?
    - Loose case: A driver script calls multiple executables in turns
    - Tight case: No driver, just one executable
  - What's the cost of initialization?
    - Loose case: Executables initialized each time
    - Tight case: All executables exist at all times, only initialized once
  - How much can components be overlapped?
    - Loose case: If all components need the same number of resources, all resources can be kept busy all the time
    - Tight case: Components can be idle waiting for other components

Work in progress towards tighter coupling in Swift: Collective Data Management (CDM)

- Data transfer mechanism is: transfer input, run, transfer output
- Fine for single node systems, could be improved to take advantage of other system features, such as intermediate file system (or shared global file system on distributed sites)
- Define I/O patterns (gather, scatter, broadcast, etc.) and build primitives for them
- Improve support for shared filesystems on HPC resources
- Make use of specialized, site-specific data movement features
- Employ caching through the deployment of distributed storage resources on the computation sites
- Aggregate small file operations into single larger operations

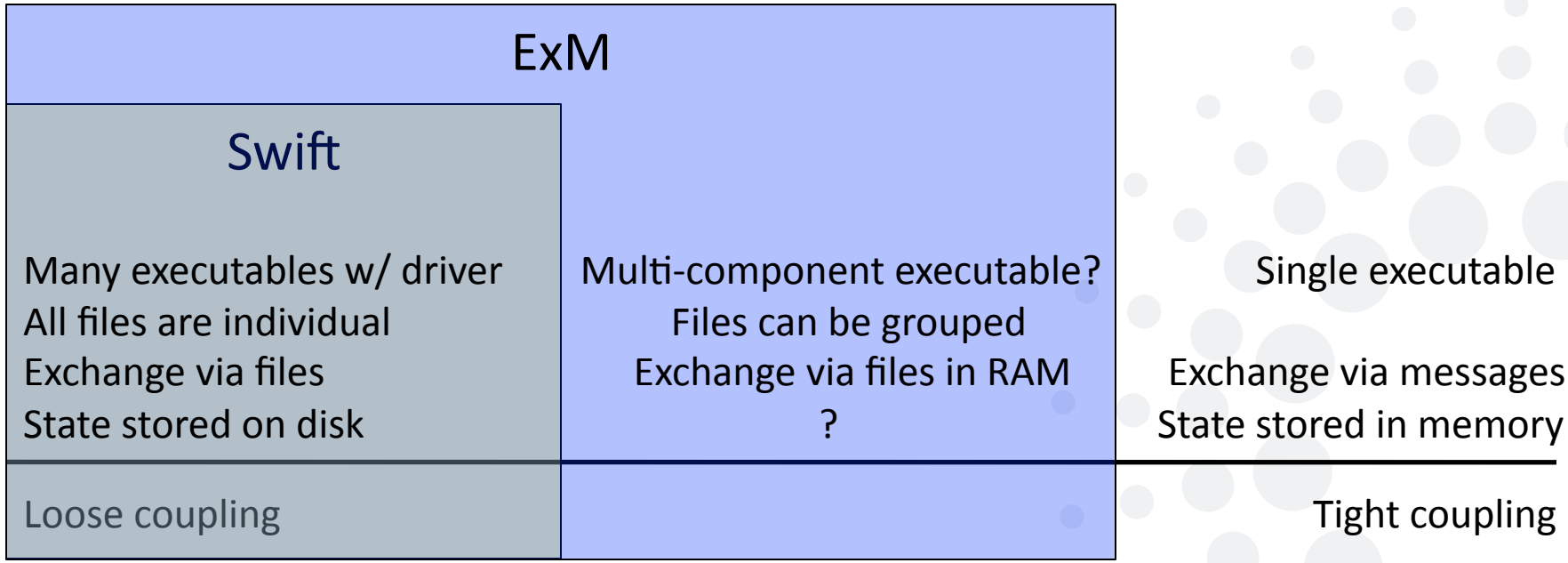
CDM examples

- Broadcast an input data set to workers
  - On Open Science Grid, just send it to the shared file system of each cluster once, the let worker nodes copy it from there
  - On IBM BG/P, use intermediate storage on I/O nodes on each pset similarly
- Gather an output data set
  - Rather than sending each job's output, if multiple jobs are running on a node and sufficient jobs are already runnable, wait and bundle multiple output files, then transfer bundle

Work in progress towards tighter coupling after Swift: ExM (Many-task computing on extreme-scale systems)

- Deploy Swift applications on exascale-generation systems
- Distributed task (and function management)
  - Break the bottleneck of a single execution engine
  - Call functions, not just executables
- JETS: Dynamically run multiple MPI tasks on an HPC resource
  - Allow dynamic mapping of workers to resources – both ways
  - Add resilience – allow mapping of workers to dynamic resources
- MosaStore: intermediate file storage
  - Use files for message passing, but stripe them across RAMdisk on nodes (single distributed filesystem w/ shared namespace), backing store in shared file system, potentially cache in the middle
- AME: intermediate file storage
  - Use files for message passing, but store them in RAMdisk on nodes where written (multiple filesystems w/ multiple namespaces), copy to new nodes when needed for reading

Increased coverage of scripting



- Questions:
  - Will we obtain good-enough performance in ExM?
  - How far can we go towards the tightly-coupled regime without breaking the basic Swift model?

Conclusions

- Multiscale modeling is important now, and use will grow
- Can think of multiscale modeling instances on a spectrum of loose to tight coupling
- Swift works for loose coupling
  - Examples shown for nuclear energy, biomolecular modeling, and subsurface flows
- Improvements in Swift (and ExM) will allow it to be used along more of the spectrum

Acknowledgments

- Swift is supported in part by NSF grants OCI-721939, OCI-0944332, and PHY-636265, NIH DC08638, DOE and UChicago SCI Program

- http://www.ci.uchicago.edu/swift/
- The Swift team:
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- Scientific application collaborators and usage described in this talk:
  - Material Science: Marius Stan, Argonne
  - Biomolecular Modeling: Anton Sinitskiy, John Grime, Greg Voth, U. Chicago
  - Subsurface Flows: Karen Schuchardt , Bruce Palmer, Khushbu Agarwal, Tim Scheibe, PNNL

- Thanks! – questions now or later – d.katz@ieee.org

8-12 October 2012 Chicago, IL, USA

http://www.ci.uchicago.edu/escience2012/

THE UNIVERSITY OF CHICAGO

Argonne NATIONAL LABORATORY

eScience Conference main events Wednesday – Friday
(keynotes, papers, panels, posters)

Paper submissions due 11 July; posters due 24 Aug

Microsoft eScience Workshop Monday – Tuesday

Additional eScience workshops Monday – Tuesday

Open Grid Forum OGF36 Monday – Wednesday

GLIF Annual Meeting Thursday – Friday

General Chair Ian Foster

Program Co-Chairs Daniel S. Katz, Heinz Stockinger

Program Vice Co-Chairs David Abramson, Gabrielle Allen, Rosa M. Badia, Geoffrey Fox

Early Results and Works-in-Progress Posters Chair Roger Barga

Workshops Chair Ruth Pordes

Sponsorship Chair Charlie Catlett

Conference Manager and Finance Chair Julie Wulf-Knoerzer

Publicity Chairs Kento Aida, Ioan Raicu, David Wallom

Conference Tracks:

eScience Algorithms and Applications

- eScience application areas, including:
  - Physical sciences
  - Biomedical sciences
  - Social sciences and humanities
- Data-oriented approaches and applications
- Compute-oriented approaches and applications
- Extreme scale approaches and applications

Cyberinfrastructure to support eScience

- Novel hardware
- Novel uses of production infrastructure
- Software and services
- Tools