Kepler Scientific Workflow System

Introduction to Workflow-Driven Scientific Computing in Kepler

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Slides for Blue Waters Webinar Series, 04/26/2017

Computing Today has Many Shapes and Sizes

hadoop

NVIDIA TESLA

amazon web services

+

COMPUTING AT SCALE

BIG DATA

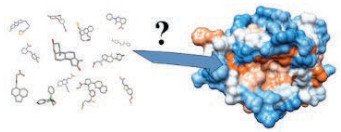
Enables dynamic data-driven applications

Requires software for dynamic coordination and resource optimization

Workflow Systems

Smart Manufacturing

Computer-Aided Drug Discovery



Personalized Precision Medicine

Smart Cities

Smart Grid and Energy Management

Let's make pasta this evening!

Shop → Prepare → Cook → Store

30 minutes

30 minutes

15 minutes

3 minutes

15 minutes

3 minutes

How to Cook Everything Fast

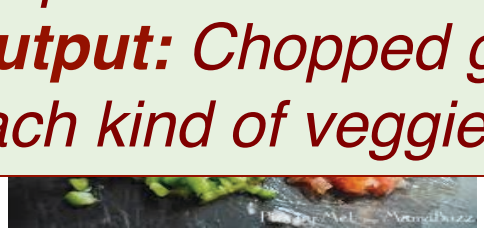
"How to Cook Everything Fast is a book of kitchen innovations. ***Time management****— the essential principle of fast cooking— is woven into revolutionary recipes that do the thinking for you. You'll learn how* ***to take advantage of downtime to prepare vegetables while a soup simmers or toast croutons while whisking a dressing****. Just cook as you read—and let the recipes guide you quickly and easily toward a delicious result."*

Image and quote source: amazon.com

What if you have more than one cooks?

MAP

- ***Input:*** *veggies*
- ***User defined function(UDF):*** *chop*
- ***Output:*** *Chopped groups of each kind of veggie*



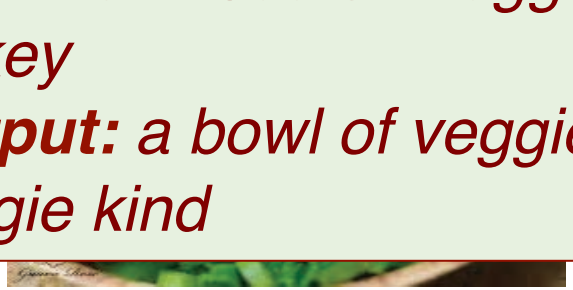
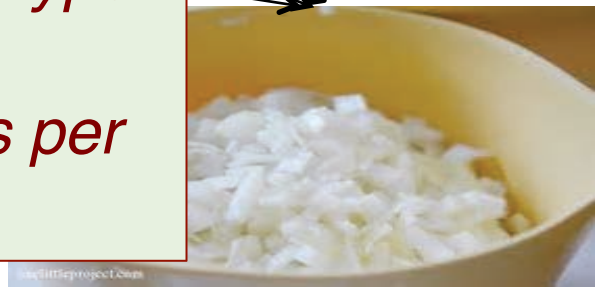
...



REDUCE

- ***Input:*** *chopped batches for each veggie type*
- ***User defined function(UDF):*** *combine based on veggie type as key*
- ***Output:*** *a bowl of veggies per veggie kind*



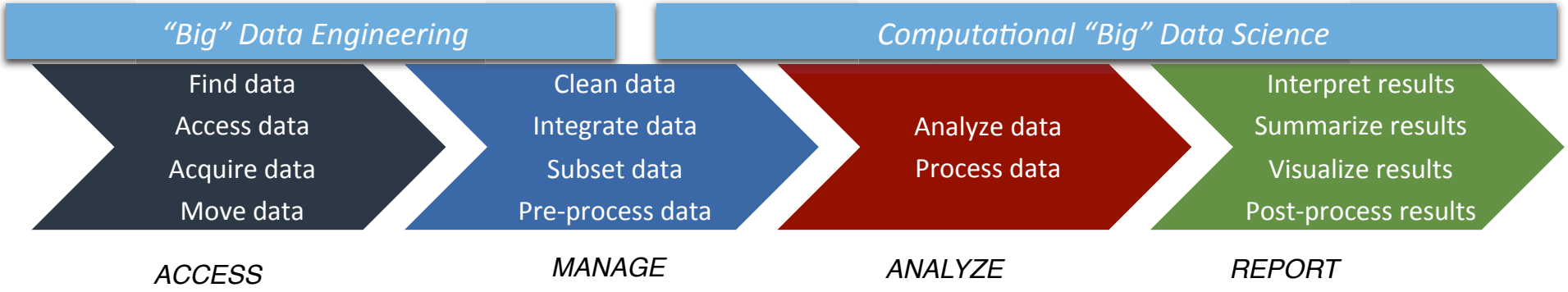
Thanksgiving dinner preparation: more planning and tasks?

PHOTOS COURTESY OF LOL FOODIE, KING ARTHUR FLOUR, SAVORY SWEET LIFE, MY RECIPES, FOOD NETWORK, WHAT WE'RE EATING AND FOODIE TOTS

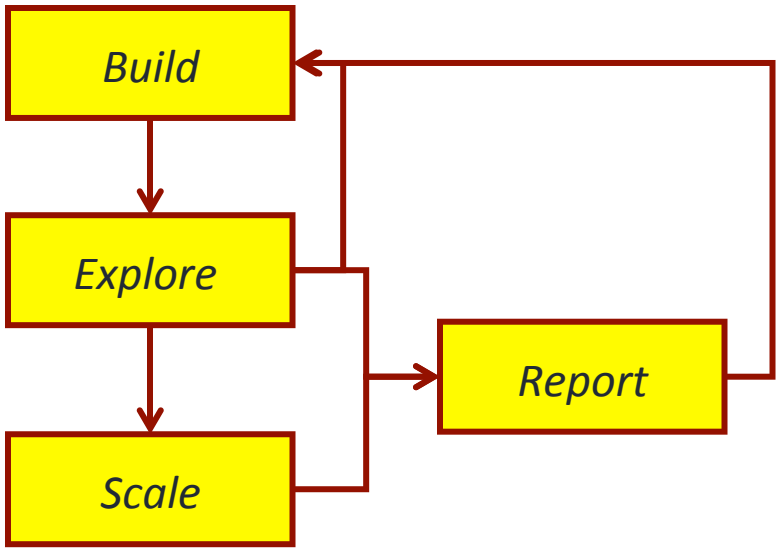
Vintage Family Cooking Thanksg... by YesterdayCafe Zazzle

Menu Item	Preparation Time	Cooking Time	Cooling Time
Turkey	30 minutes	4 hours	15 minutes
Veggies	30 minutes	45 minutes	None
Cranberry Sauce	5 minutes	30 minutes	2 hours
Soup	20 minutes	30 minutes	None
Pie	30 minutes	5 minutes	1 day

- *When do you start cooking?*
- *What order do you cook?*
- *Can you cook some menu items in parallel?*
- *Who cooks what?*
- *…*



Many ways to look at the process for HPC and Big Data… not every step is automatable!



Facilitating and Accelerating XXX-Data Science or Comp-XXX Research using Scientific Workflows

Important Attributes

Assemble complex processing easily

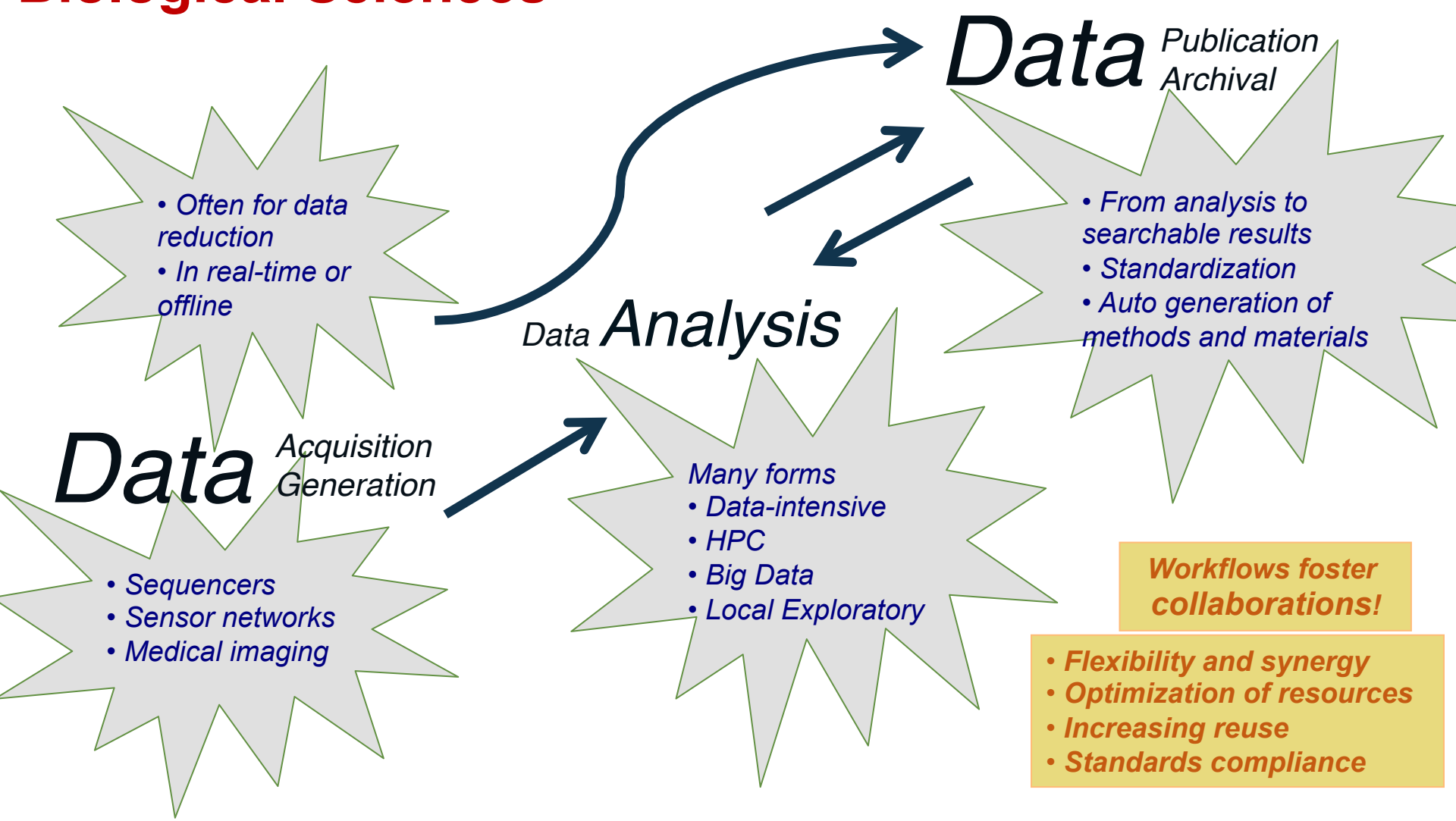
Access transparently to diverse resources

Incorporate multiple software tools

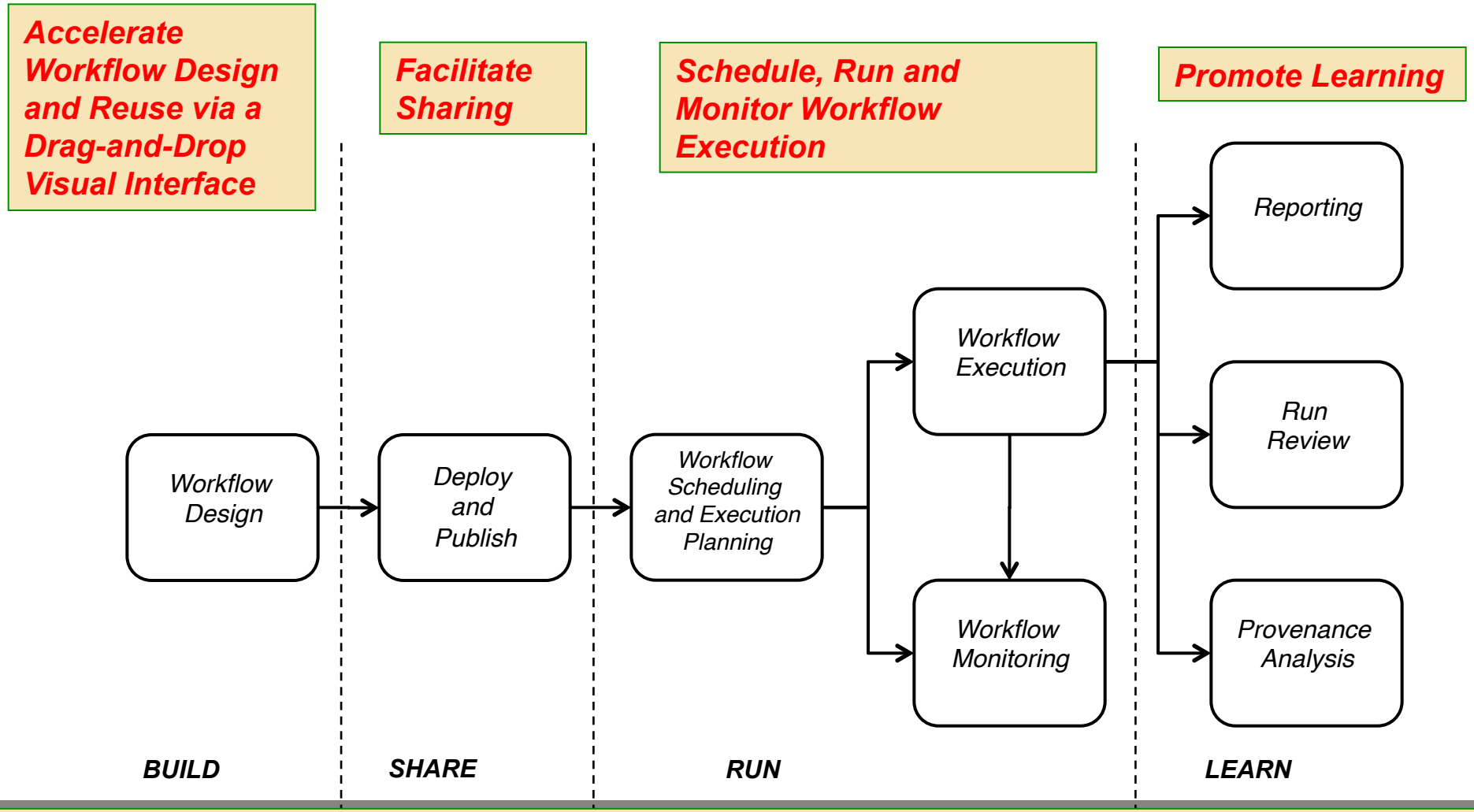
Assure reproducibility and robustness

Build around community development model

Workflows are Used in These Diverse Scenarios in Biological Sciences



Workflows are a Part of Cyberinfrastructure



Support for end-to-end computational scientific process

Graphical Workflow Systems

-Toolboxes with Many Tools-

- *Data*
  - *Search, database access, IO operations, streaming data in real-time…*
- *Compute*
  - *Data-parallel patterns, external execution, …*
- *Network operations*
- *Provenance and fault tolerance*

Need expertise to identify which tool to use when and how!
Require computation models to schedule and optimize execution!

Kepler is a Scientific Workflow System

www.kepler-project.org

- A cross-project collaboration
  … initiated August 2003
- 2.4 released in 2015
- Frequent module release updates

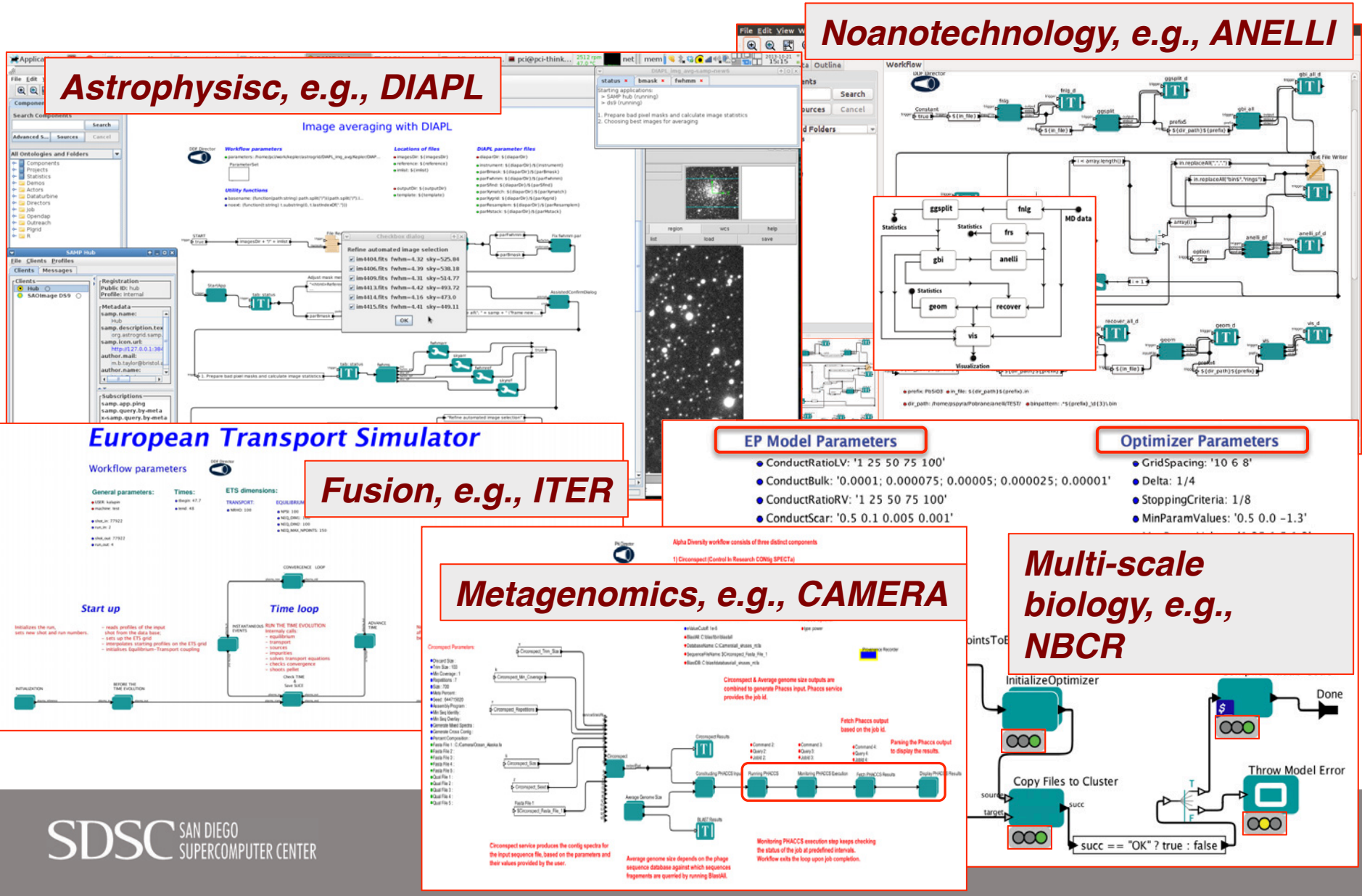
- *Builds upon the open-source Ptolemy II framework*

Ptolemy II: A laboratory for investigating design

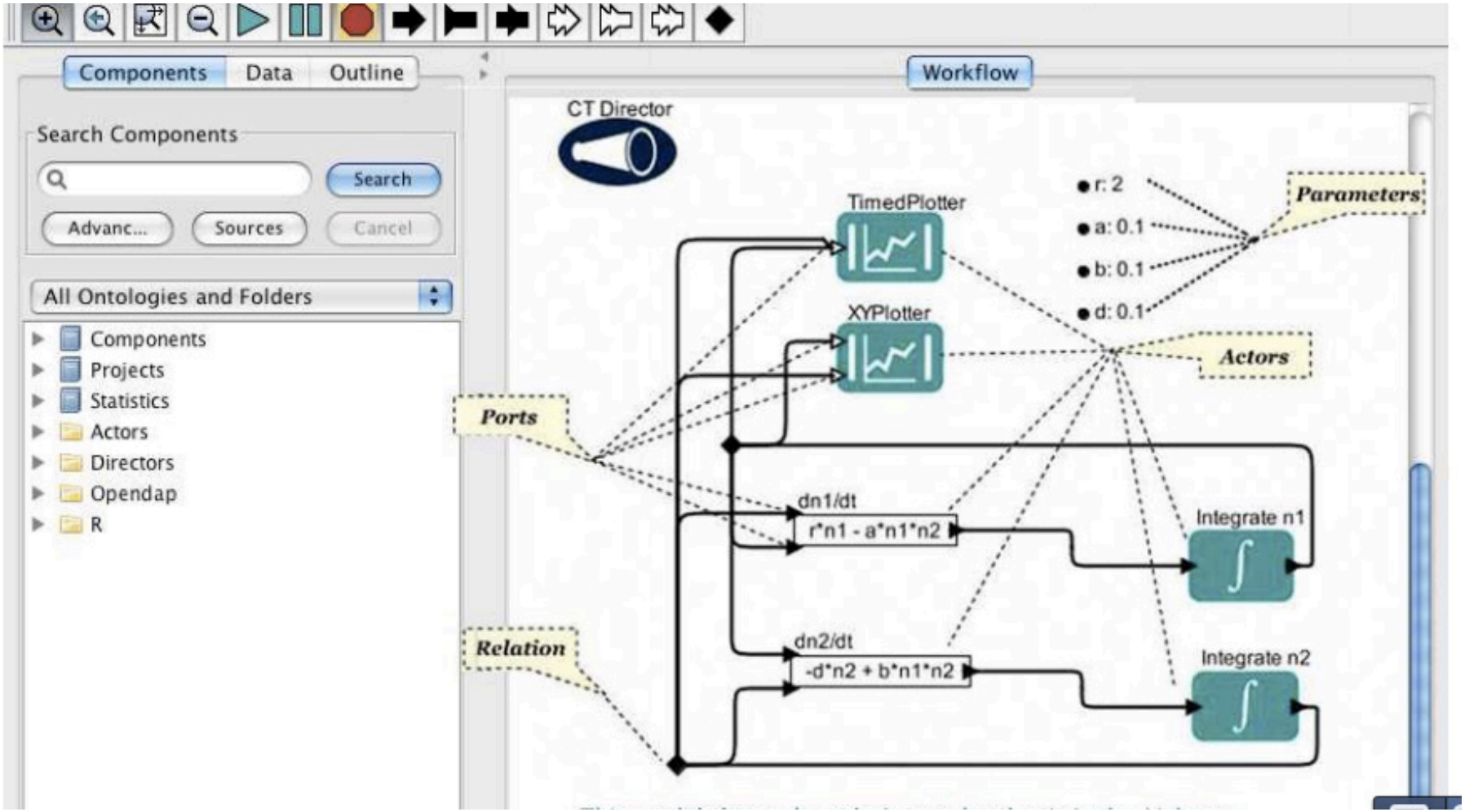
KEPLER: A problem-solving environment for Scientific Workflow

KEPLER = "Ptolemy II + X" for Scientific Workflows

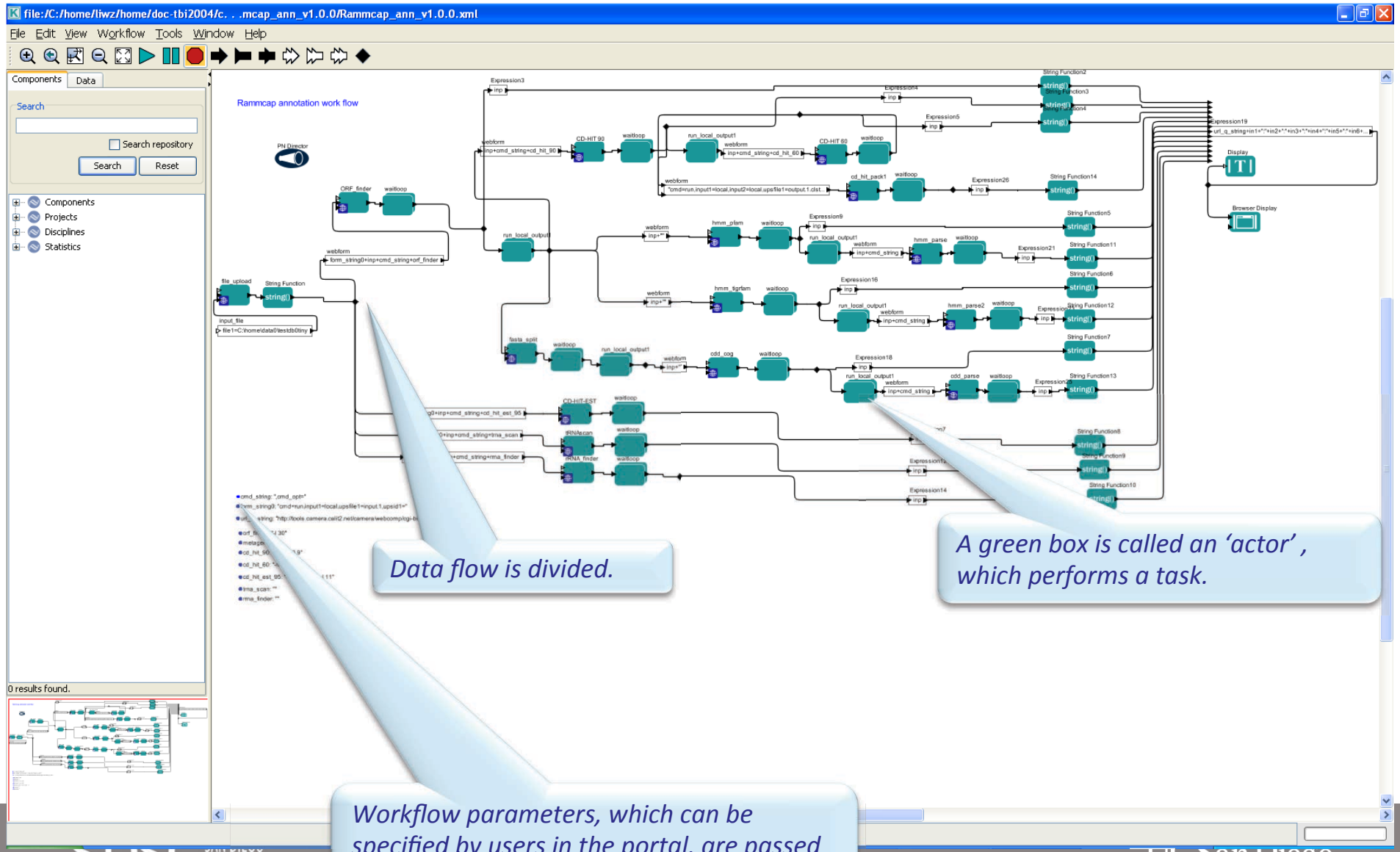
Kepler can be applied to problems in different scientific disciplines: some here and many more…



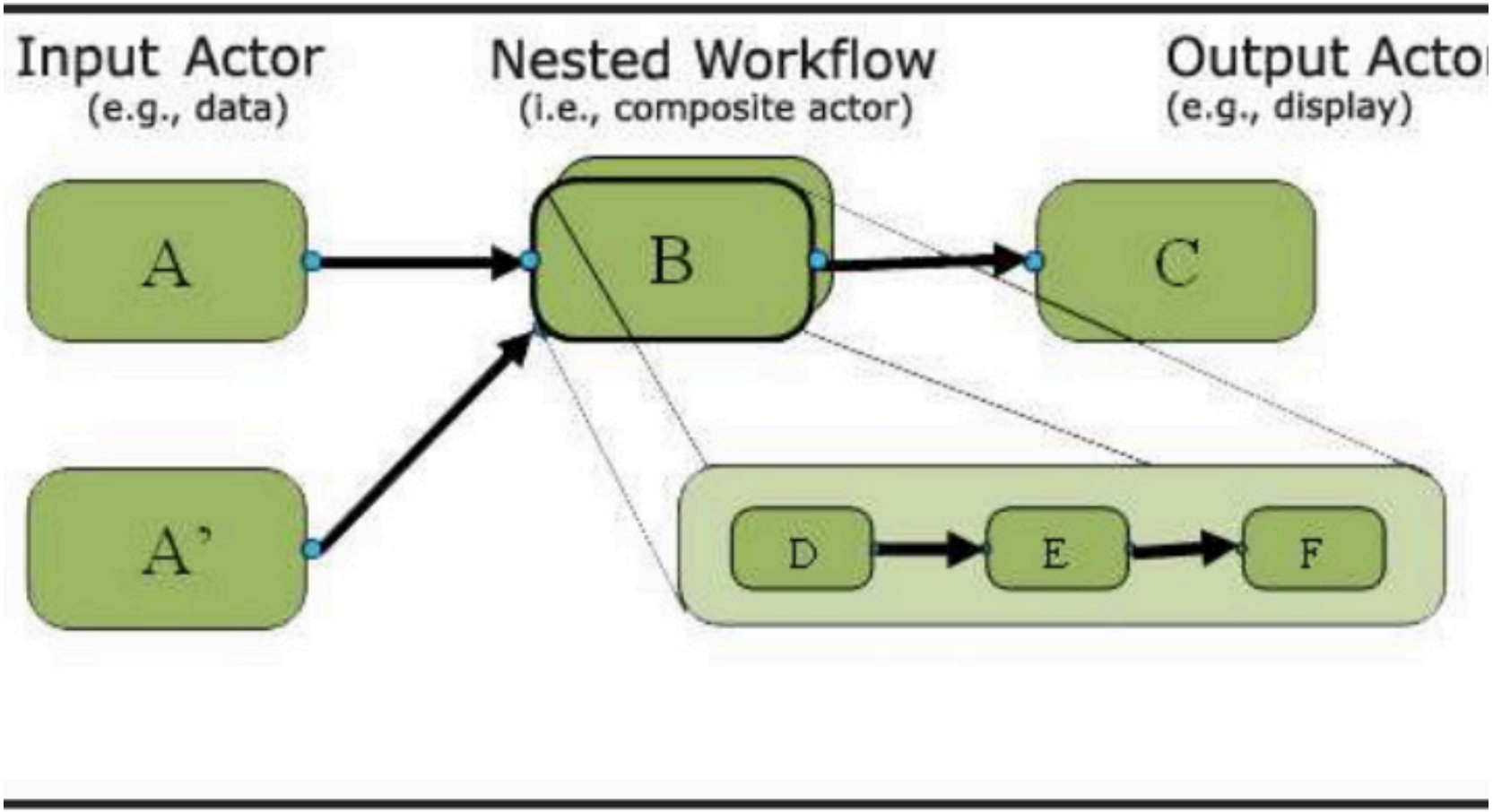
Basic components and terminologies in Kepler



A Typical Kepler Workflow



Kepler Actor Types



Some actors in place for…

- *Command Line wrapper tools (**local execution**, **ssh**, **scp**, ftp, etc.)*
- *Generic Web Service Clients for SOAP and **REST***
- *A suite of **cloud computing** actors for VM instantiation and management*
- *Job management actors for **HPC, GPU, SGE** and other commodity clusters*
- *Customizable **RDBMS** query and update*
- *Distributed data parallel patterns, e.g., Map, Reduce, Cross*
- ***Hadoop**, Stratosphere, and **Spark** integration*
- *iRODS support*
- *Native **R** and **Matlab** support*
- *Open **GIS** tools*
- *Communication with external workflow engines, e.g., **KNIME***
- *Communication with sensor data loggers through actors and services*
- *Imaging, Gridding, Vis Support*
- *Textual and Graphical Output*
- *Integration with **Jython, JavaScript, Java, JRuby***
- *…more generic and domain-oriented actors…*

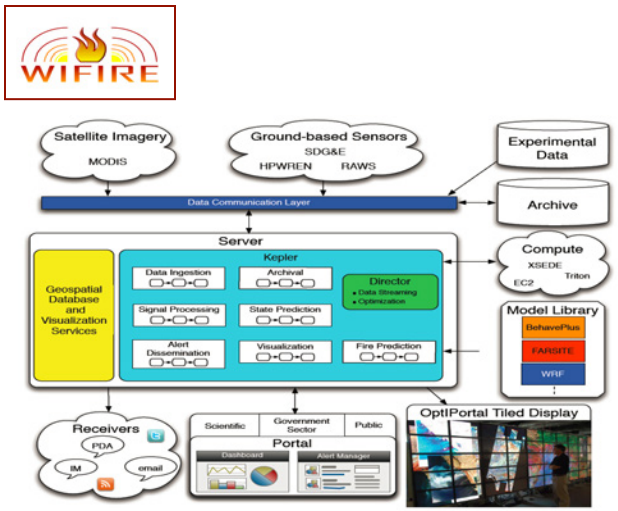
Workflow Execution across Multiple Environments

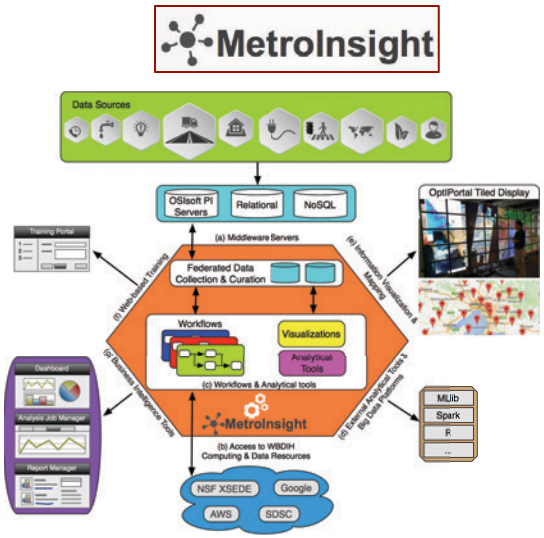
- Execution Choice Actor: Multiple types of executions within one workflow
  - **Local** execution
  - **Hadoop** execution
  - **EC2** execution
  - **Remote job** execution

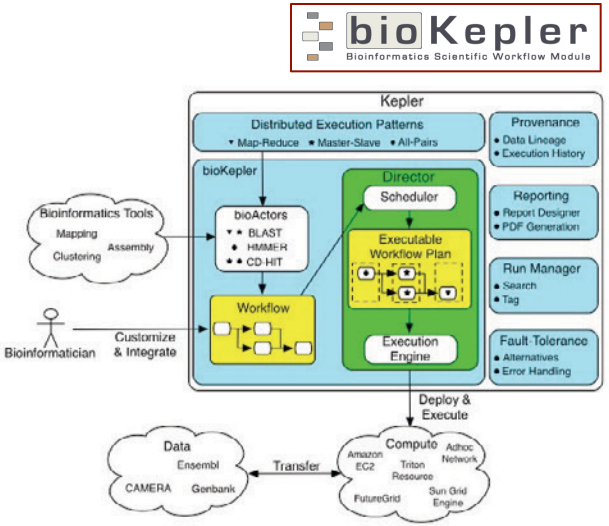
- Useful for heterogeneous execution requirements

Some Recent Kepler Workflow Examples

Examples: Use of Workflows as an Application Integration Tool for "Big" Data and Computational Science







Using Workflows and Cyberinfrastructure for Wildfire Resilience

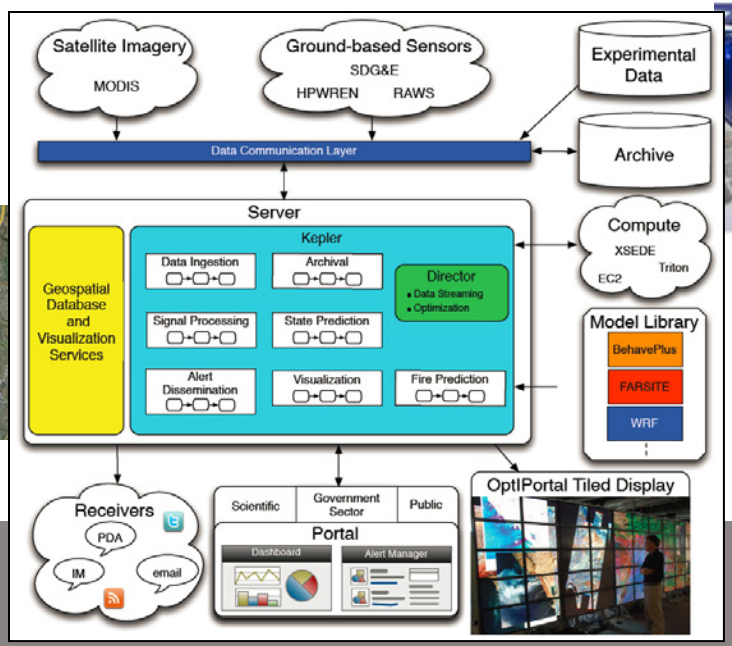
- A Scalable Data-Driven Monitoring and Dynamic Prediction Approach -

wifire.ucsd.edu

Big Data

WIFIRE

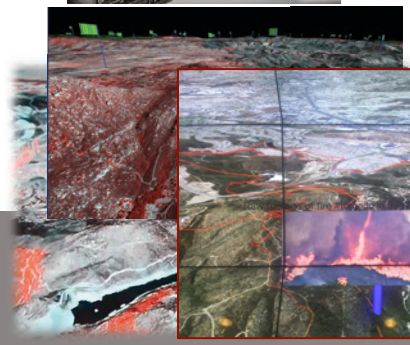
Monitoring
Visualization
Fire Modeling



hadoop

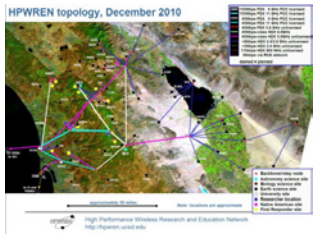
NVIDIA TESLA

amazon web services

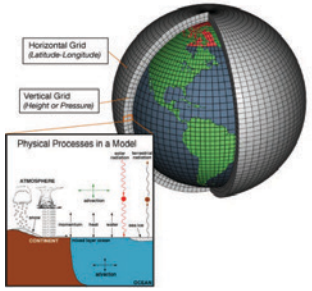


SDSC SAN DIEGO SUPERCOMPUTER CENTER

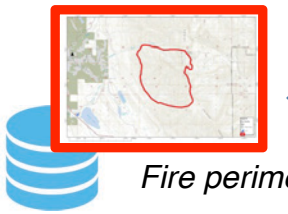
Fire Modeling Workflows in WIFIRE



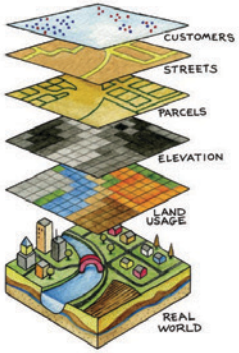
Real-time sensors



Weather forecast

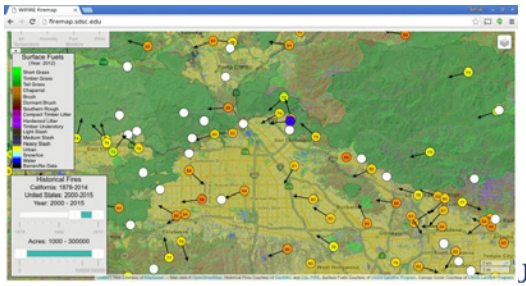


Fire perimeter



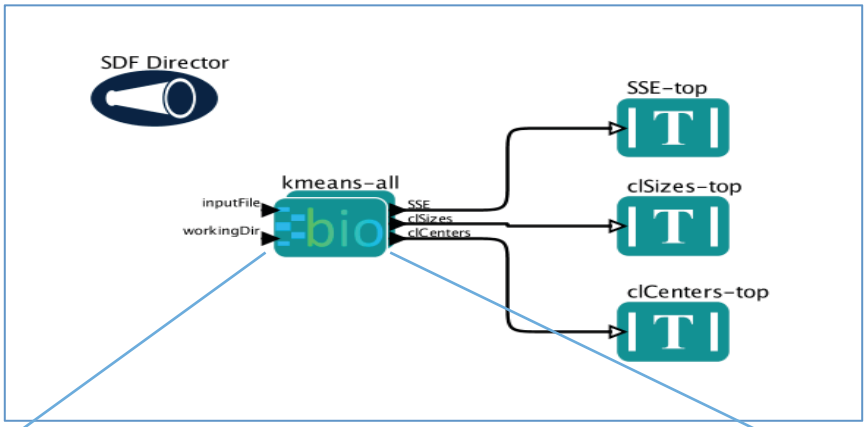
Landscape data

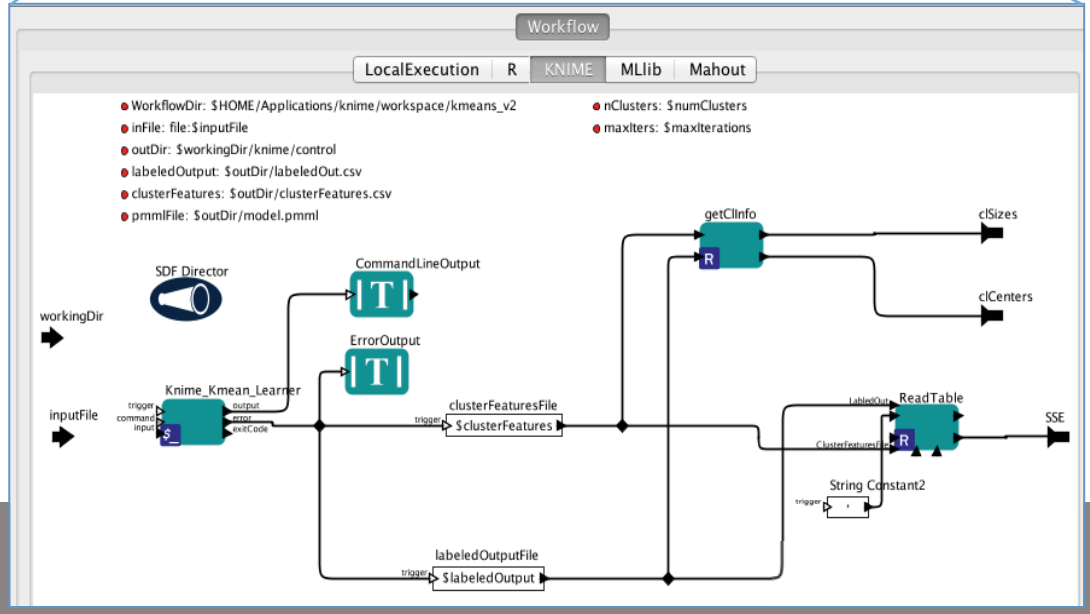
Monitoring & fire mapping



Flexible programming of K-means

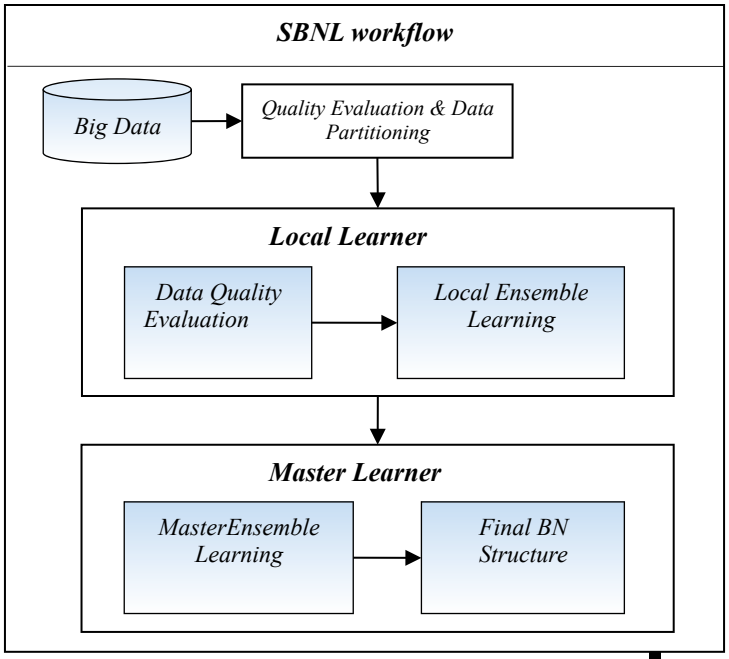
- **R:** Programming language and software environment for statistical computing and graphics.
- **KNIME:** Platform for data analytics.
- **MlLib:** Scalable machine learning library running on Spark cluster computing framework
- **Mahout:** Scalable machine learning library based on MapReduce.





Scalable Bayesian Network Learning

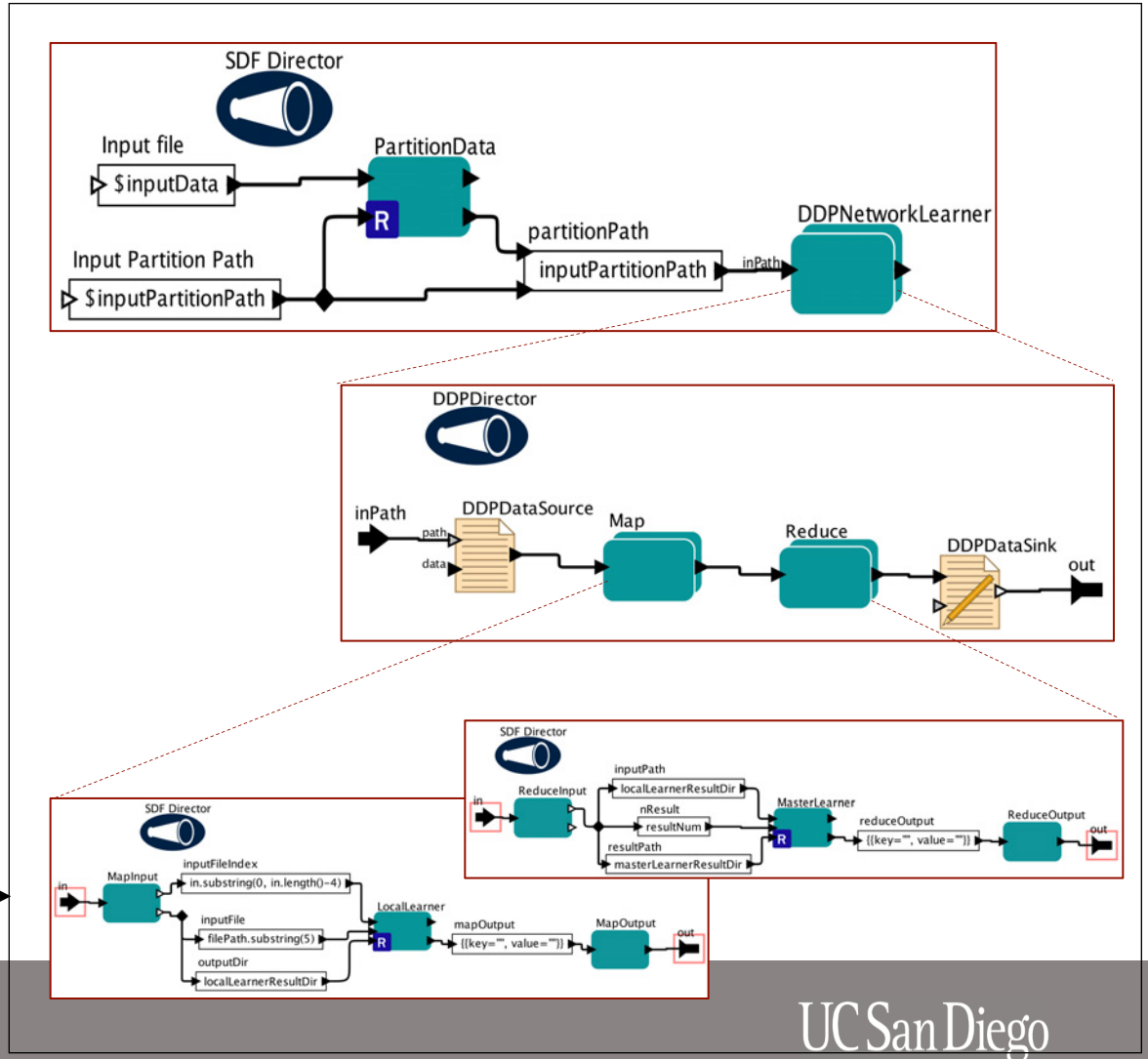
From "Napkin Drawings" to Executable Workflows…



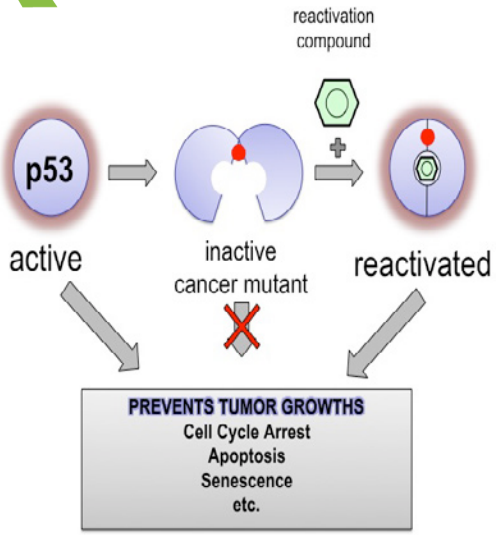
Conceptual SWF

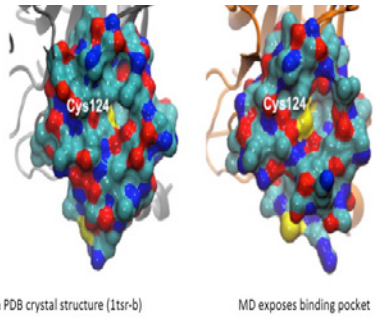
Insurance and Traffic Data Analytics using Big Data Bayesian Network Learning

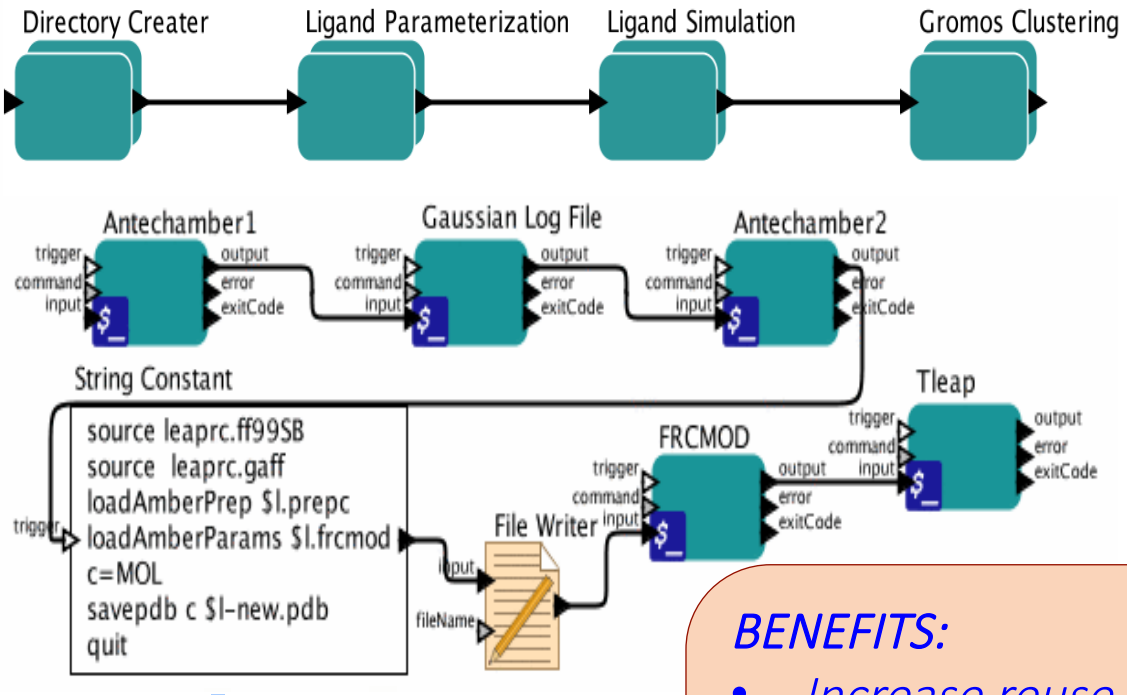
Executable SWF

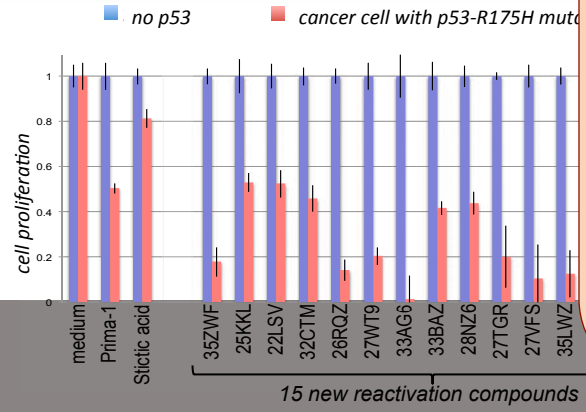


Scalable Drug Discovery









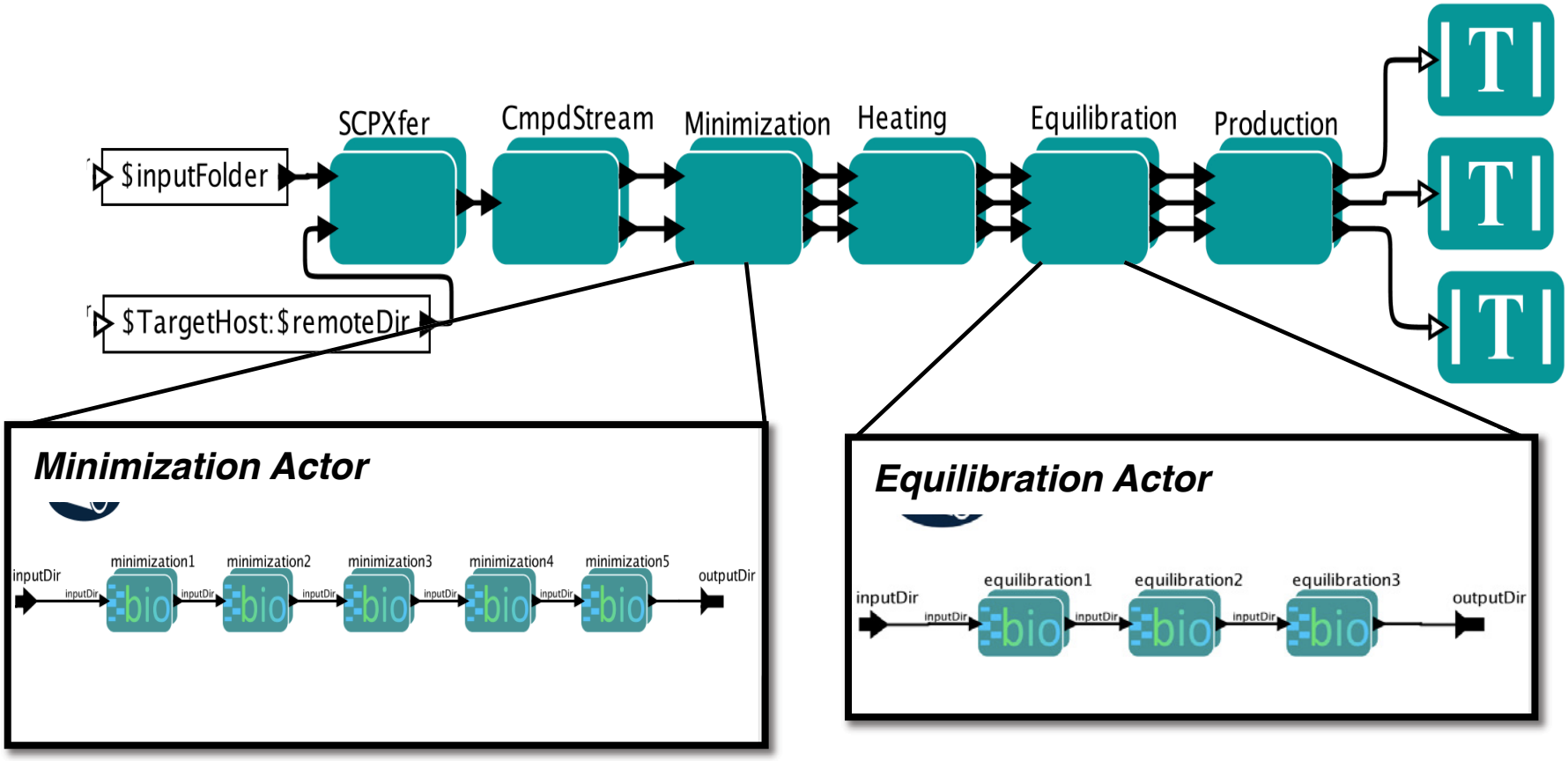
BENEFITS:

- *Increase reuse*
- *Reproducibility*
- *Scale execution, problem & solution*
- *Compare methods*
- *Training*

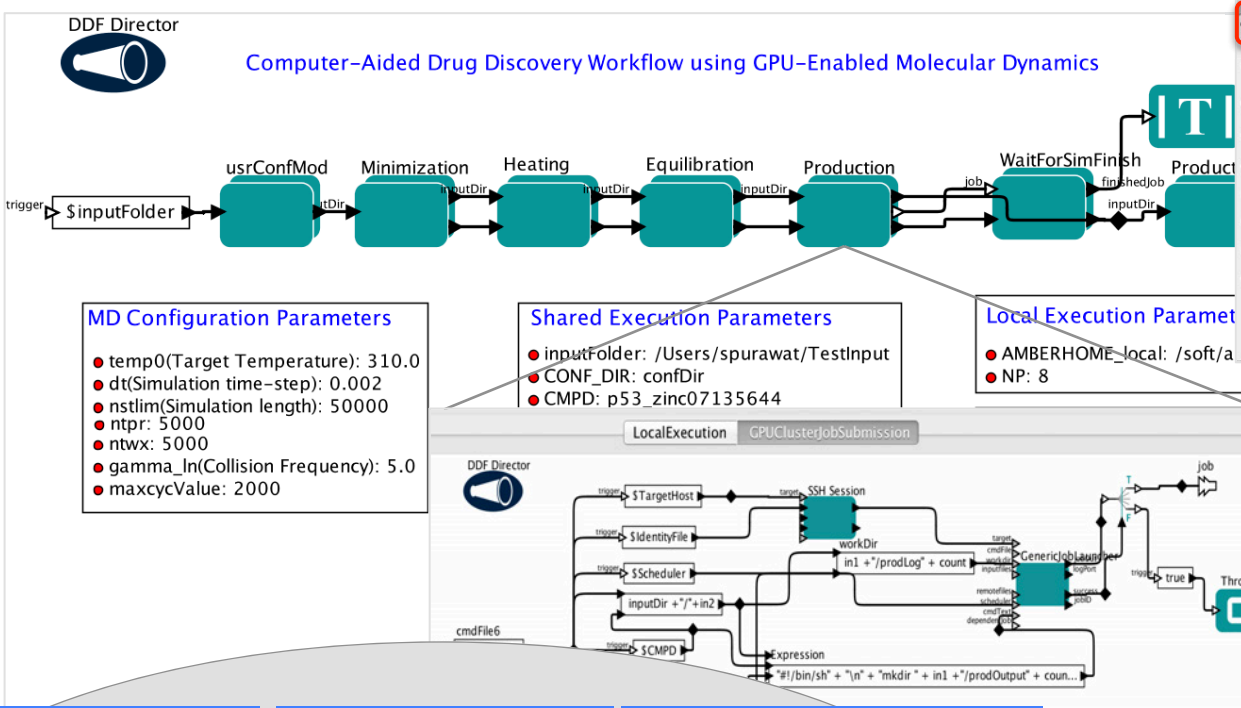
Ieong et al., 2014

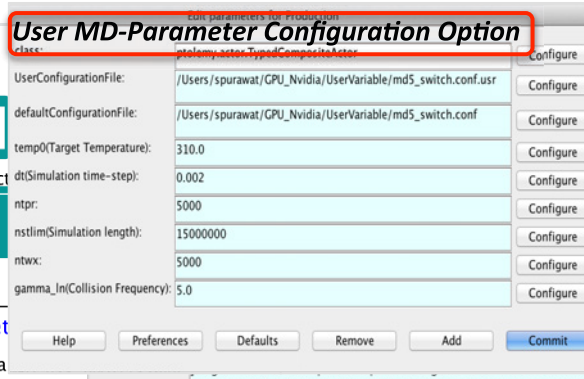
COMPUTE THE CURE

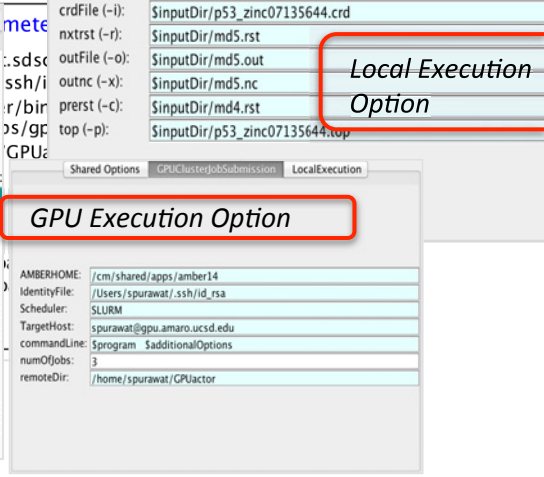
AMBER GPU Molecular Dynamics Workbench



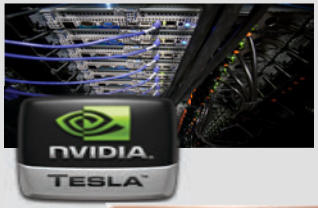
Parametric execution of each step







Local: *NBCR Cluster Resources*



NSF/DOE: *TeraScale Resources (XSEDE)*

SDSC *(Comet)*

TACC *(Stampede)*

Private Cluster: *User Owned Resources*

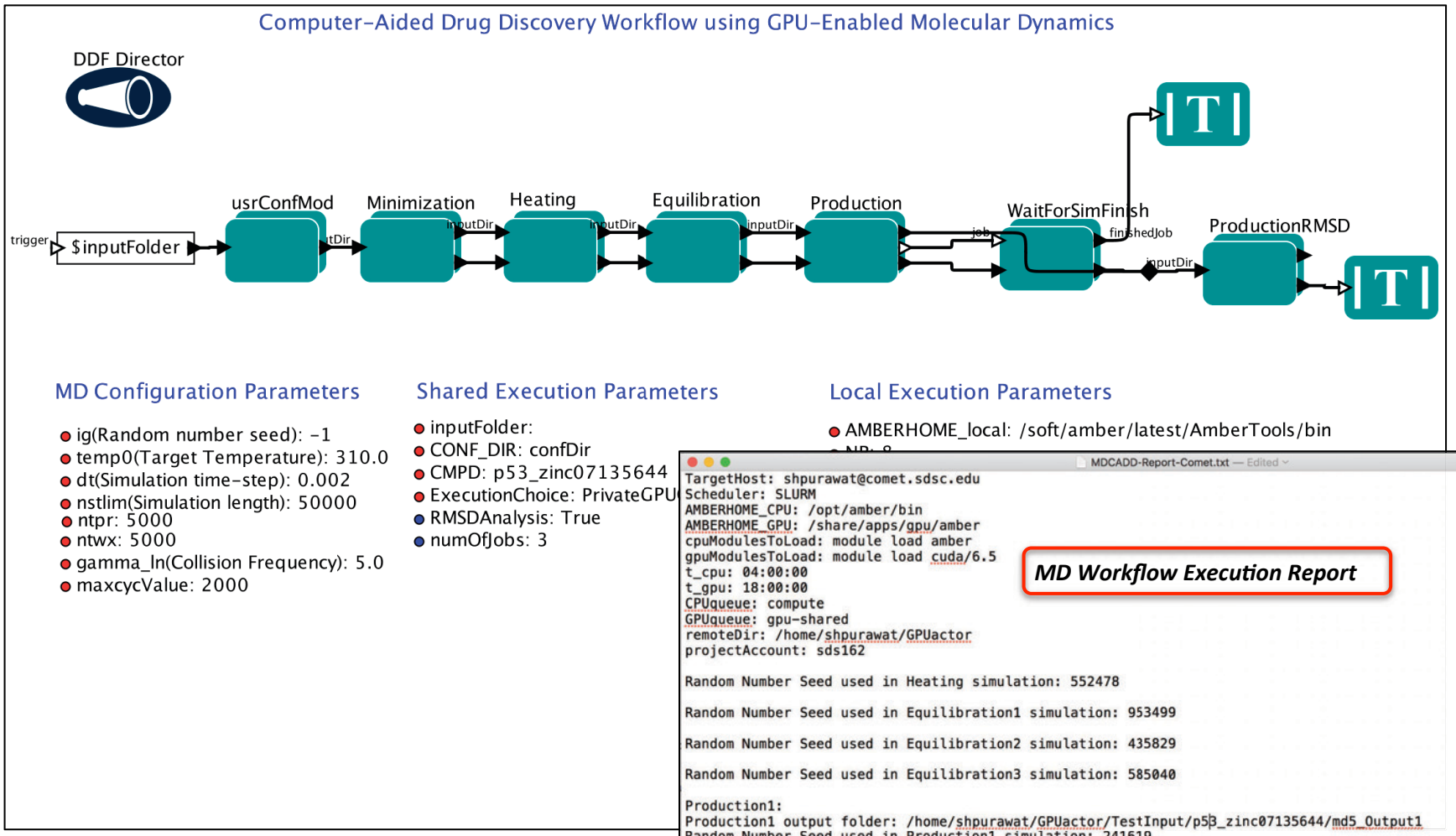
amazon web services

Amber Molecular Dynamics Package

BENEFITS:

- *Flexible configuration of MD job parameters*
- *Scalability at compound level*
- *Computing platform portability*
- *Increased reuse*
- *Provenance*

MDCADD WF – Workflow Execution Report

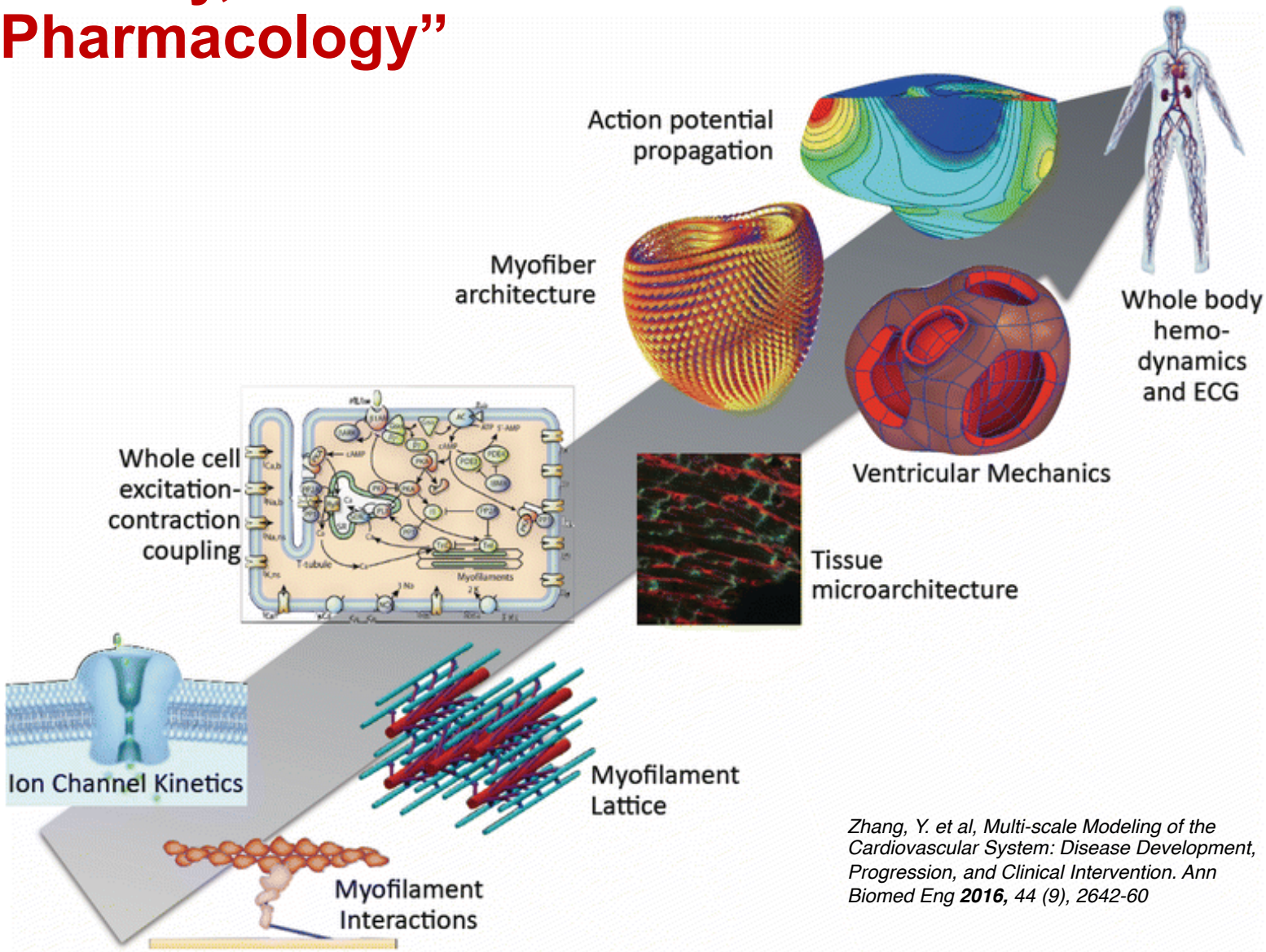


MDCADD-Report-Comet.txt — Edited

MD Workflow Execution Report

```
TargetHost: shpurawat@comet.sdsc.edu
Scheduler: SLURM
AMBERHOME_CPU: /opt/amber/bin
AMBERHOME_GPU: /share/apps/gpu/amber
cpuModulesToLoad: module load amber
gpuModulesToLoad: module load cuda/6.5
t_cpu: 04:00:00
t_gpu: 18:00:00
CPUqueue: compute
GPUqueue: gpu-shared
remoteDir: /home/shpurawat/GPUactor
projectAccount: sds162

Random Number Seed used in Heating simulation: 552478

Random Number Seed used in Equilibration1 simulation: 953499

Random Number Seed used in Equilibration2 simulation: 435829

Random Number Seed used in Equilibration3 simulation: 585040

Production1:
Production1 output folder: /home/shpurawat/GPUactor/TestInput/p53_zinc07135644/md5_Output1
Random Number Seed used in Production1 simulation: 241619


Production3:
Production3 output folder: /home/shpurawat/GPUactor/TestInput/p53_zinc07135644/md5_Output3
Random Number Seed used in Production3 simulation: 740887

Amber Version:
pmemd.cuda: Version 14.0

nvcc: NVIDIA (R) Cuda compiler driver
Copyright (c) 2005-2014 NVIDIA Corporation
Built on Thu_Jul_17_21:41:27_CDT_2014
```

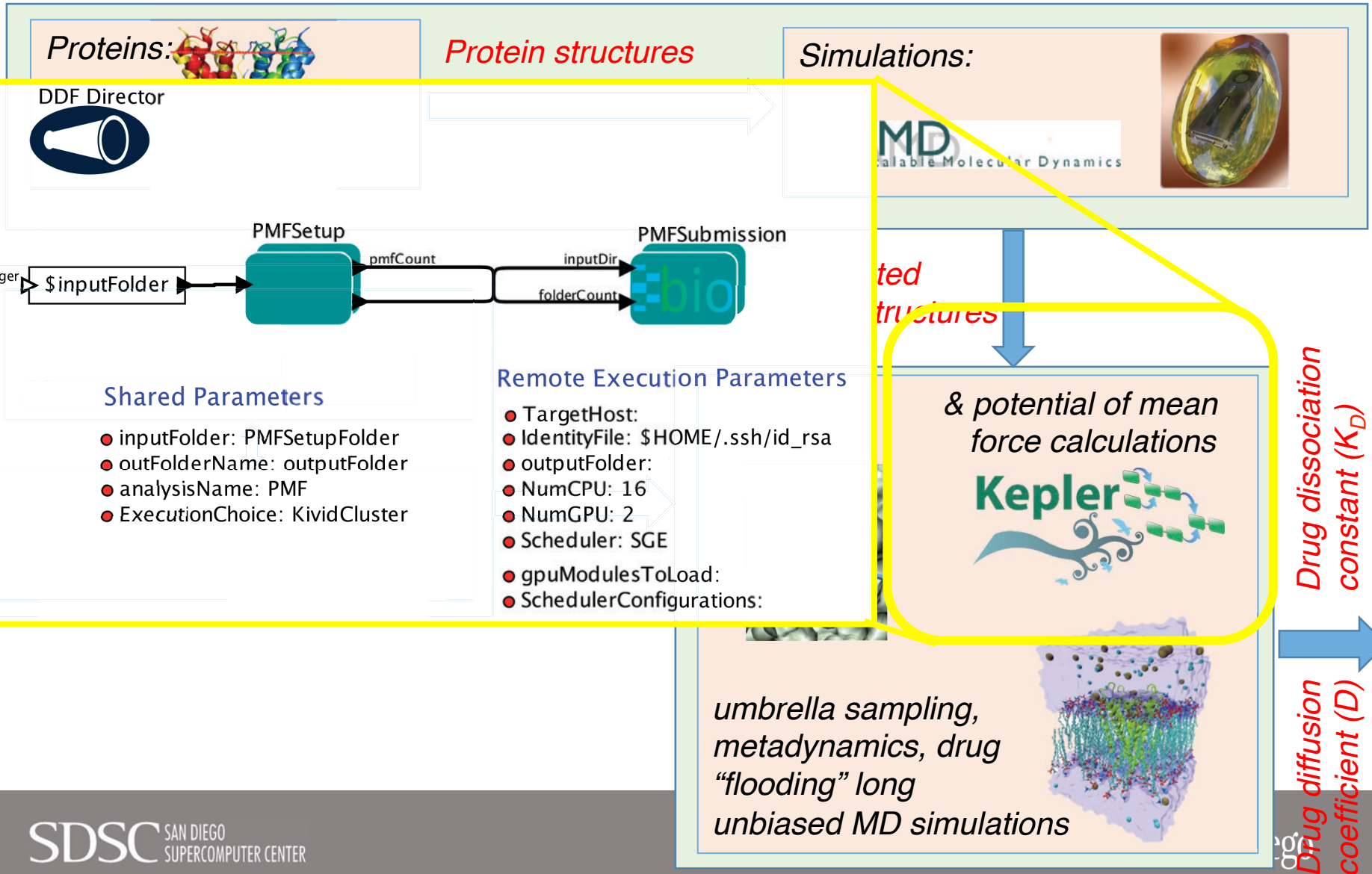
Colleen Clancy, "Predictive Multiscale in silico Cardio-Pharmacology"



Zhang, Y. et al, Multi-scale Modeling of the Cardiovascular System: Disease Development, Progression, and Clinical Intervention. Ann Biomed Eng ***2016,*** *44 (9), 2642-60*

A flow-chart of proposed multi-scale simulations.

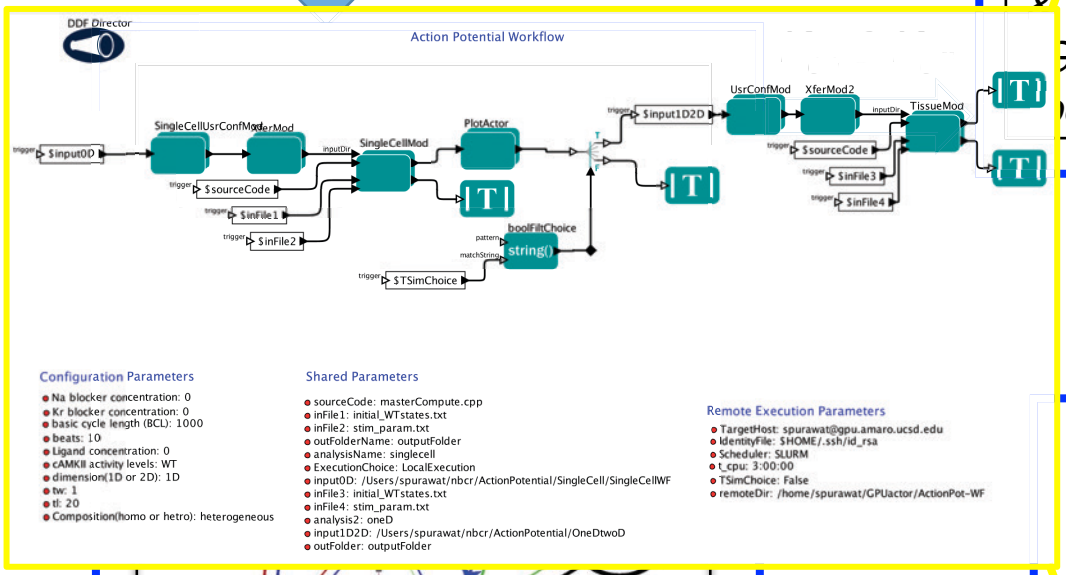
Part 1: Atomistic level simulations.

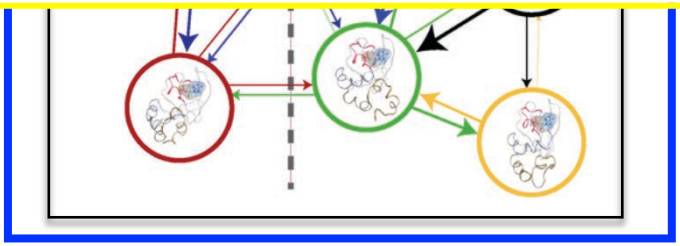


Part 2: Functional level simulations

Atomistic level simulations

K_D





Cell simulations

Markov model into cell
& validations
Generates
"populations" cells)

Kepler

Tissue simulations

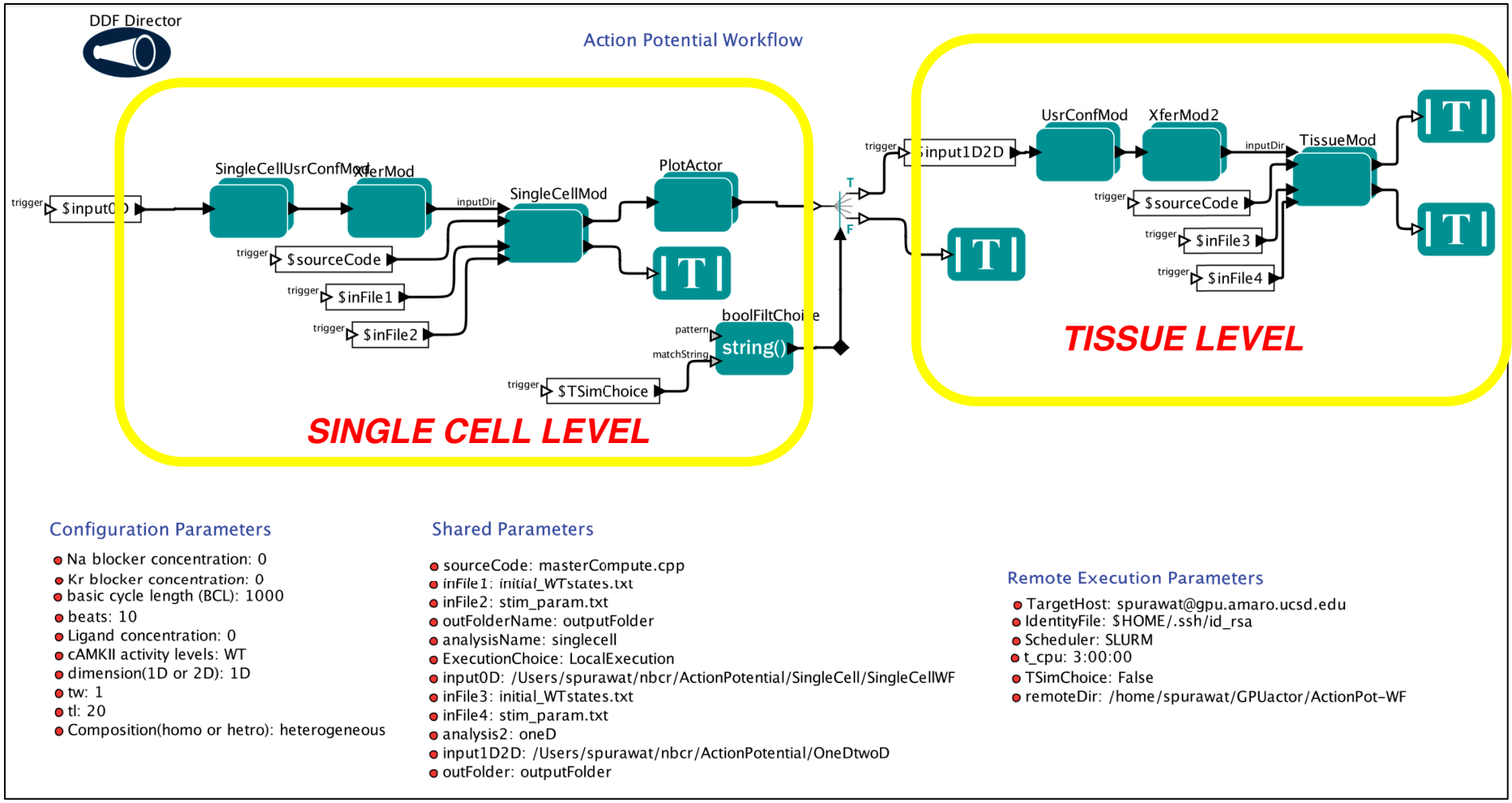
Kepler

Cable/tissue maps
Compare to experiments

Pseudo ECG

Compare to clinical ECG

Cell and Tissue Simulation Workflow



Configuration Parameters

- Na blocker concentration: 0
- Kr blocker concentration: 0
- basic cycle length (BCL): 1000
- beats: 10
- Ligand concentration: 0
- cAMKII activity levels: WT
- dimension(1D or 2D): 1D
- tw: 1
- tl: 20
- Composition(homo or hetro): heterogeneous

Shared Parameters

- sourceCode: masterCompute.cpp
- inFile1: initial_WTstates.txt
- inFile2: stim_param.txt
- outFolderName: outputFolder
- analysisName: singlecell
- ExecutionChoice: LocalExecution
- input0D: /Users/spurawat/nbcr/ActionPotential/SingleCell/SingleCellWF
- inFile3: initial_WTstates.txt
- inFile4: stim_param.txt
- analysis2: oneD
- input1D2D: /Users/spurawat/nbcr/ActionPotential/OneDtwoD
- outFolder: outputFolder

Remote Execution Parameters

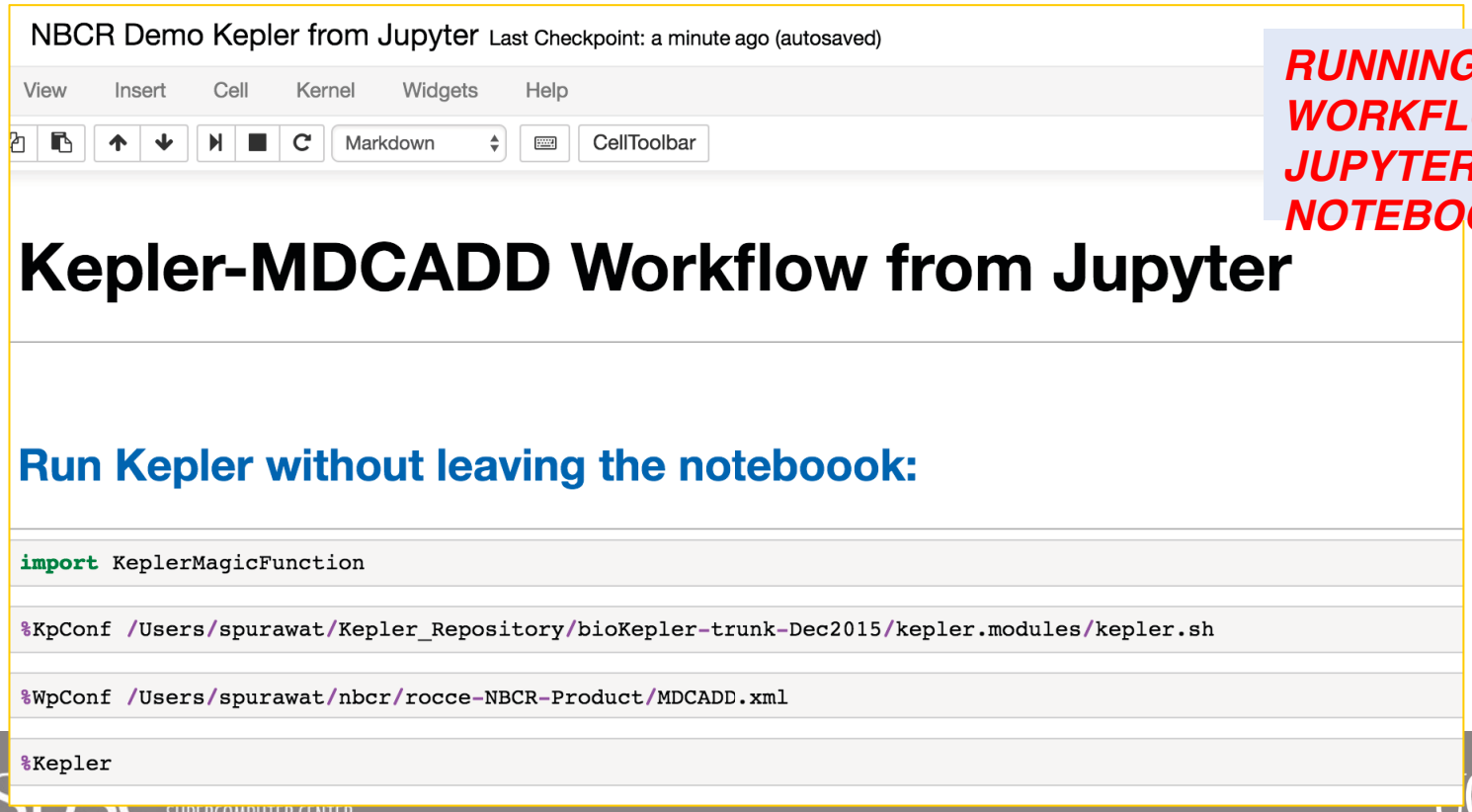
- TargetHost: spurawat@gpu.amaro.ucsd.edu
- IdentityFile: $HOME/.ssh/id_rsa
- Scheduler: SLURM
- t_cpu: 3:00:00
- TSimChoice: False
- remoteDir: /home/spurawat/GPUactor/ActionPot-WF

Integration with Scientific Process and Communication

Aim: Integrate the workflow-driven, scalable and reproducible science with notebooks and exploratory nature of the scientific process.

jupyter Notebooks as Workflow Execution and Reporting Interfaces

- ✓ Jupyter Kepler Magics: https://github.com/words-sdsc/Jupyter_Kepler_Integration/blob/master/README.md



RUNNING MDCADD WORKFLOW IN JUPYTER NOTEBOOKS

jupyter Notebooks as Workflow Execution and Reporting Interfaces

jupyter NBCR Demo Kepler from Jupyter Last Checkpoint: 3 minutes ago (autosaved) Logout

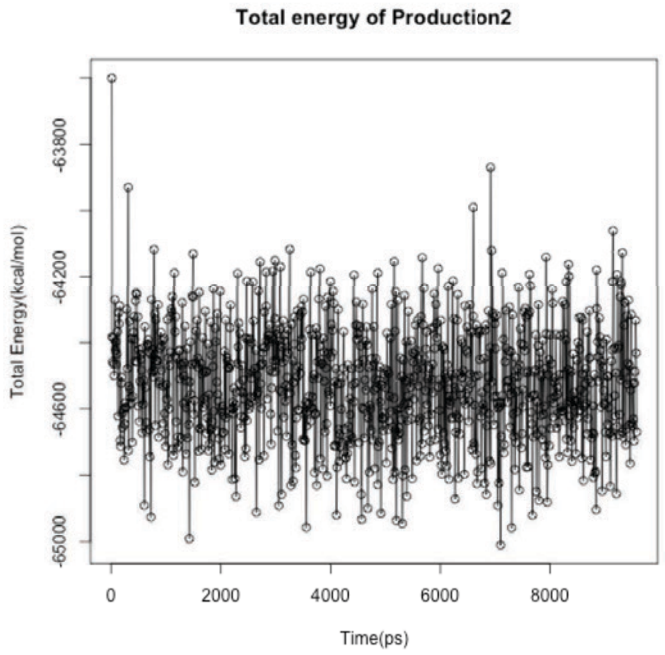
File Edit View Insert Cell Kernel Widgets Help Kernel

Markdown CellToolbar

Plot out graphs from Kepler execution:

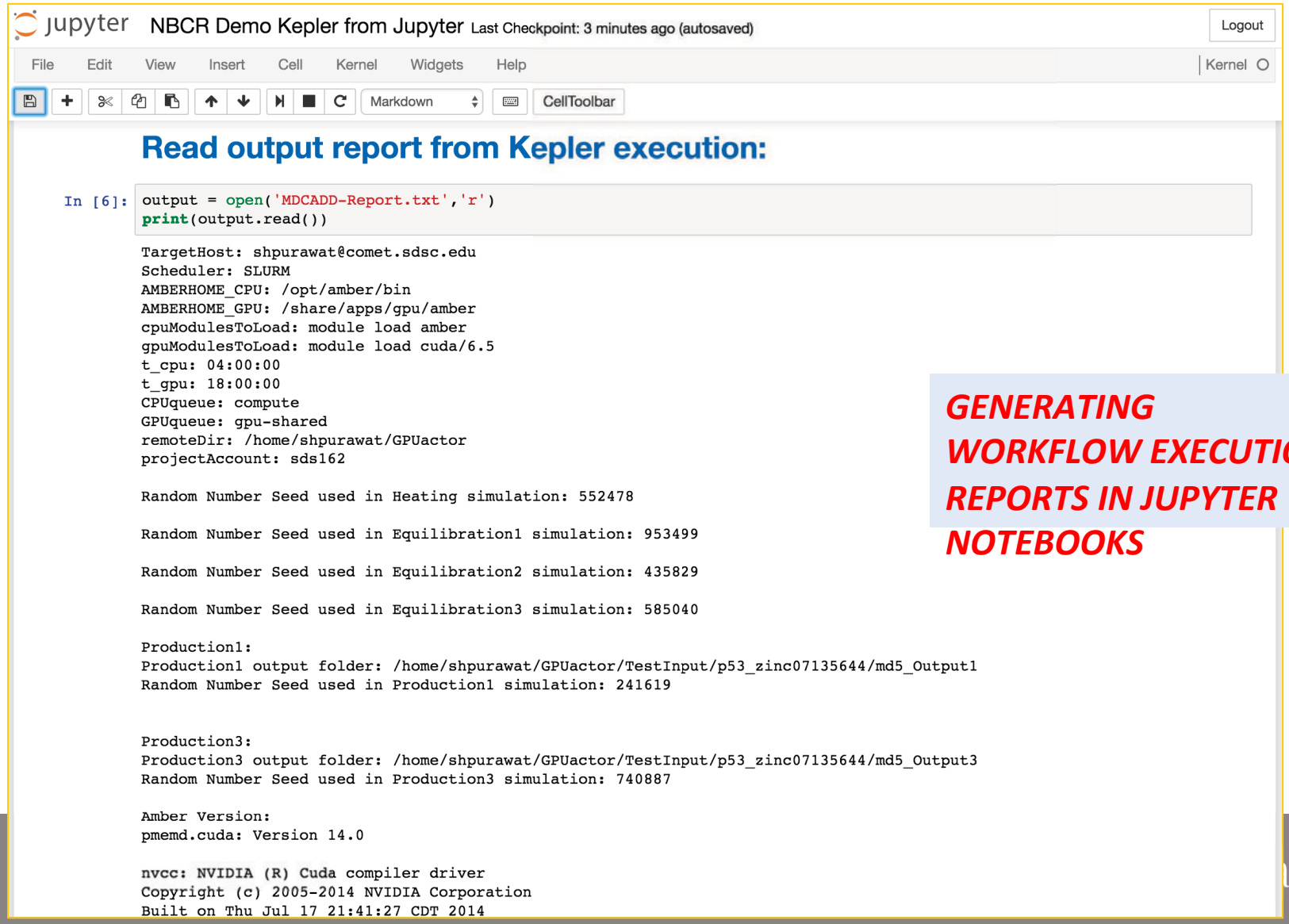
```
In [12]: graph = '/Users/spurawat/NBCR_Demo_Feb17/IPython-Kepler-Magic-Function/p53_zinc07135644/prod2_total_energy.png'
         from IPython.display import Image
         Image(filename=graph)
```

Out[12]:



VIEWING WORKFLOW RESULTS IN JUPYTER NOTEBOOKS

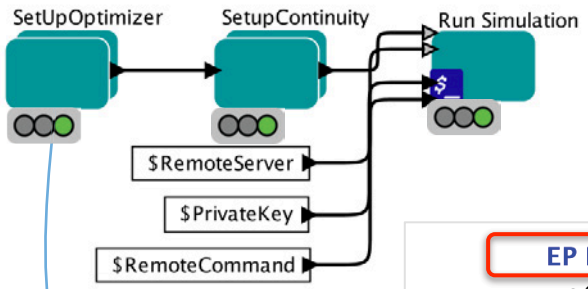
Notebooks as Workflow Execution and Reporting Interfaces



GENERATING WORKFLOW EXECUTION REPORTS IN JUPYTER NOTEBOOKS

Run Parameters

- RunId: "Cond-1"
- LocalWorkingDirectory: "/Users/jeffvandorn/work/myStuff/psm_workflow/"
- StimulusLocationsFile: "stimLocations-RVendo-38"
- RemoteServer: "rocce.ucsd.edu"
- RemoteWorkingDir: "/home/jvandorn/psm_workflow/"
- RemoteCommand: "python runEPbatch.py"
- PrivateKey: "/Users/jeffvandorn/.ssh/id_rsa"



Details of SetUpOptimizer

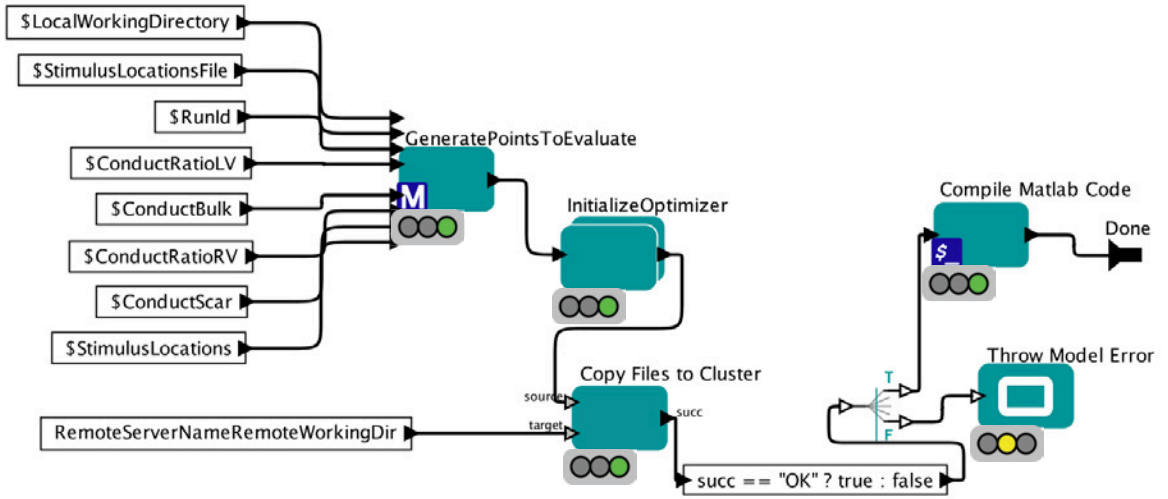
CONTINUITY 6
A Problem Solving Environment for Multi-Scale Biology

EP Model Parameters

- ConductRatioLV: '1 25 50 75 100'
- ConductBulk: '0.0001; 0.000075; 0.00005; 0.000025; 0.00001'
- ConductRatioRV: '1 25 50 75 100'
- ConductScar: '0.5 0.1 0.005 0.001'
- StimulusLocations: 50

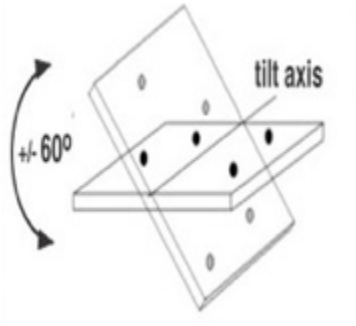
Optimizer Parameters

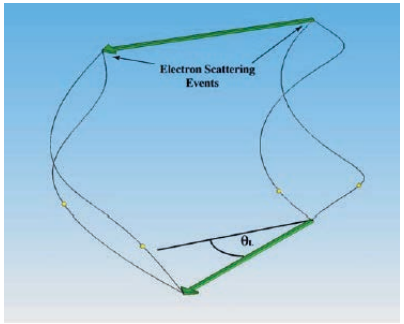
- GridSpacing: '10 6 8'
- Delta: 1/4
- StoppingCriteria: 1/8
- MinParamValues: '0.5 0.0 -1.3'
- MaxParamValues: '1.25 1.5 1.3'



Example: *Integration of Software Tools for Iterative Reconstruction*

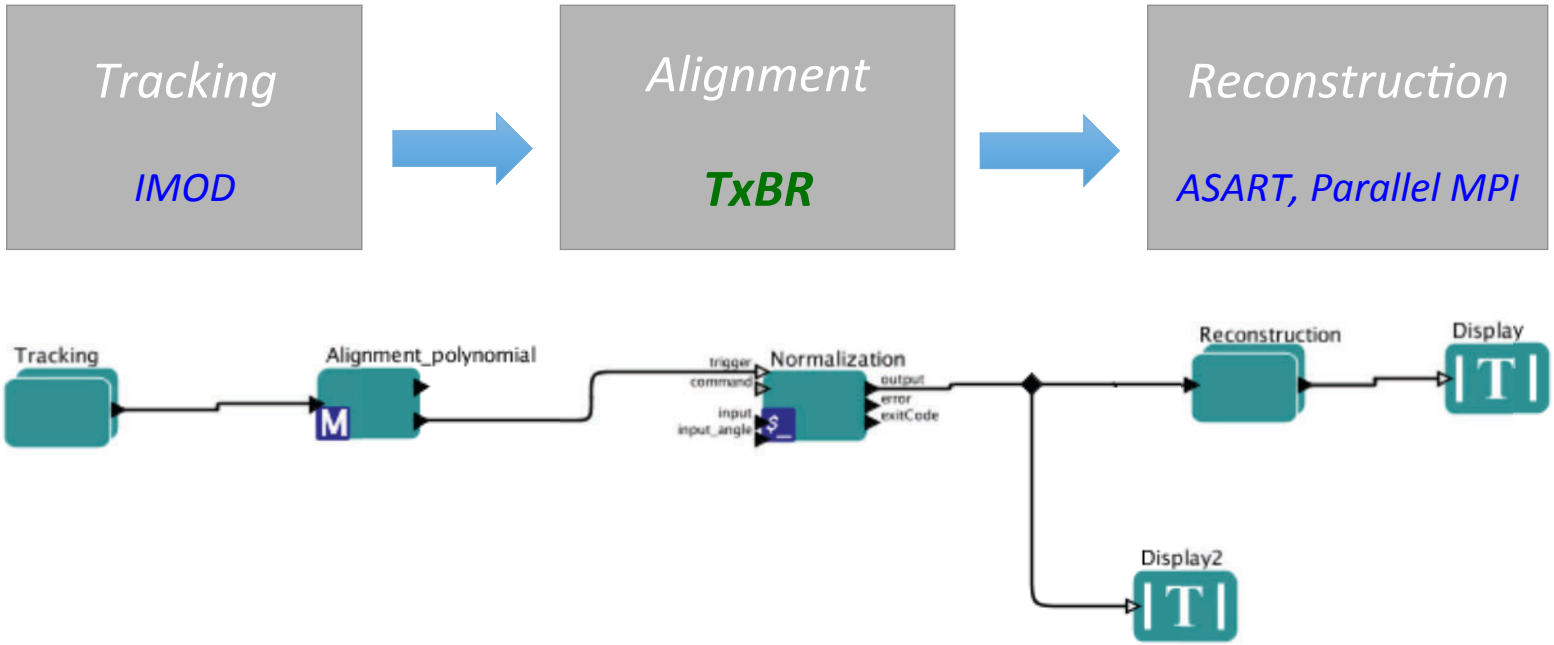
Tracking	Alignment	Reconstruction
IMOD	***TxBR***	*ASART, Parallel MPI*





From "Conceptual Steps"
To Integrated, Executable and Portable Workflows

Electron Microscope Processing in Kepler (EPiK) Workflow for TxBR Streamlines Iterative Reconstruction



In Partnership with
Sun Yat Sen Foundation

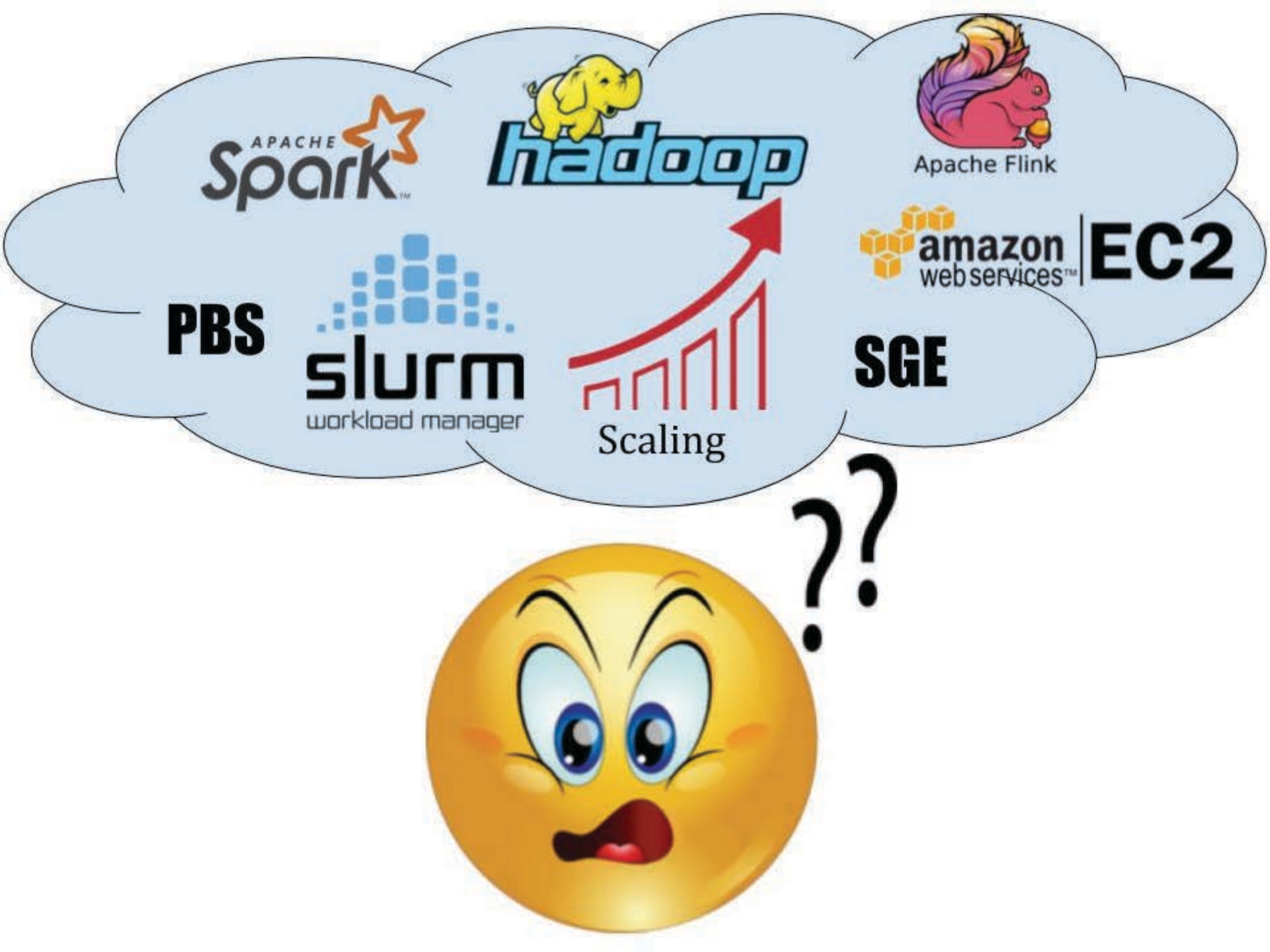
BENEFITS:

- *Improved programmability*
- *Ability to use and compare multiple methods in one integrated workflow*
- *Reduction of complexity*

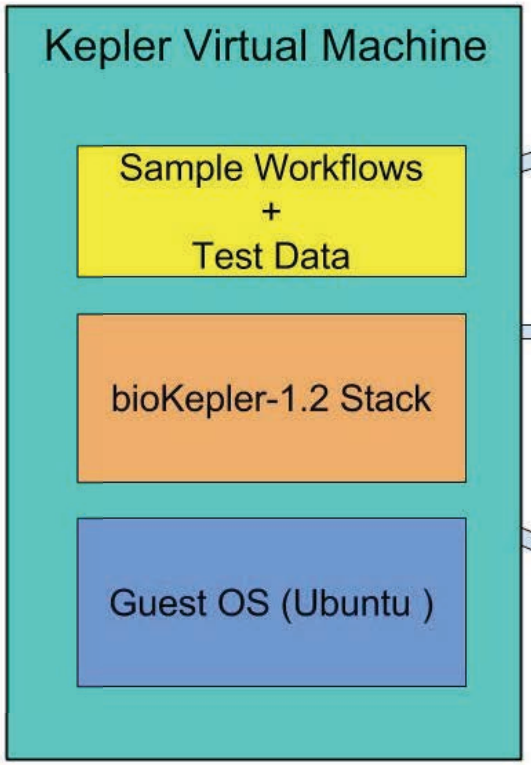
Kepler workflows are used for:

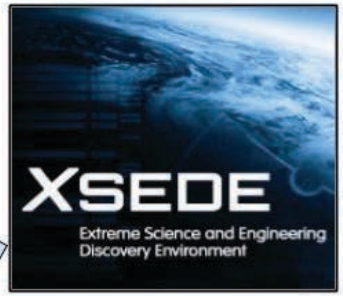
- **documentation** of the analysis
- **visual representation** of analytical steps
- ability to work **across multiple software and platforms**
- **distributed data-parallel** scheduling and execution
- **reproducibility** of a given project with little effort
- **reuse** of part or all of a workflow in a different project

Kepler Demo!


APACHE
Spark
hadoop
Apache Flink
amazon
web services
EC2
PBS
slurm
workload manager
Scaling
SGE
??

Kepler – XSEDE Architecture





https://biobigdata.ucsd.edu/

Downloading and Installing Kepler

- Java 1.8 or later is a prerequisite to run Kepler 2.5

- Download Kepler installer for Windows, Mac, or Linux-based platforms.

  https://kepler-project.org/users/downloads

- Add-on Modules can be added to Kepler to enhance its functionality. Example: bioKepler, Provenance, Reporting.

Useful Links

- https://kepler-project.org/users/downloads
- https://kepler-project.org/users/documentation
- http://www.biokepler.org/userguide
- https://biobigdata.ucsd.edu/
- http://words.sdsc.edu
- https://github.com/words-sdsc/Jupyter_Kepler_Integration
- https://words.sdsc.edu/publications

Please use the following reference:

- To cite Kepler:

  Kepler: an extensible system for design and execution of scientific workflows. Altintas, I. and Berkley, C. and Jaeger, E. and Jones, M. and Ludascher, B. and Mock, S. (2004) Scientific and Statistical Database Management, 2004. Proceedings. 16th International Conference on. Pages: 423--424.

- To cite bioKepler:

  Altintas, J. Wang, D. Crawl, W. Li, "Challenges and approaches for distributed workflow-driven analysis of large-scale biological data", in: Proceedings of the Workshop on Data analytics in the Cloud at EDBT/ICDT 2012 Conference, DanaC2012, 2012, pp 73-78.

- To cite Biomedical Big Data Training Collaborative (BBDTC):

  S. Purawat, C. Cowart, R. E. Amaro, and I. Altintas, "Biomedical Big Data Training Collaborative (BBDTC): An effort to bridge the talent gap in biomedical science and research", Journal of Computational Science, March 2017. http://dx.doi.org/10.1016/j.jocs.2017.03.010

Please use the following reference:

- To cite Molecular Dynamics Computer Aided Drug-Discovery Workflow:

  S. Purawat, P. Ieong, R. Malmstrom, G. Chan, R. Walker, I. Altintas, and R. Amaro, “A Kepler Workflow Tool for Reproducible Molecular Dynamics”, Biophysical Journal, 2017

- To cite WIFIRE:

  Altintas I., Block J., de Callafon R., Crawl D., Cowart C., Gupta A., Nguyen M., Braun H.W., Schulze J., Gollner M., Trouve A., Smarr L., Towards an Integrated Cyberinfrastructure for Scalable Data-Driven Monitoring, Dynamic Prediction and Resilience of Wildfires. In Proceeedings of the Workshop on Dynamic Data-Driven Application Systems (DDDAS) at the 15th International Conference on Computational Science (ICCS 2015). doi:10.1016/j.procs.2015.05.296

  Crawl, D., Block, J., Lin, K., Altintas, I., Firemap: A Dynamic Data-Driven Predictive Wildfire Modeling and Visualization Environment, In Proceedings of the Workshop on Urgent Computing (UC) at the 17th International Conference on Computational Sciences (ICCS 2017), 2017.

Please use the following reference:

- To cite Machine Learning Integration in the Kepler

  Nguyen, M., Crawl, D., Masoumi, T., Altintas, T., Integrated Machine Learning in the Kepler Scientific Workflow System, In proceedings of the Third International Workshop on Advances in the Kepler Scientific Workflow System and Its Applications at the International Conference on Computational Science (ICCS 2016). doi:10.1016/j.procs.2016.05.545

- To cite Scalable Bayesian Network Learning

  Wang J., Tang Y., Nguyen M., Altintas I., A Scalable Data Science Workflow Approach for Big Data Bayesian Network Learning. Accepted by the International Symposium on Big Data Computing (BDC 2014)

- To cite EPiK - Electron Tomography Kepler Workflow:

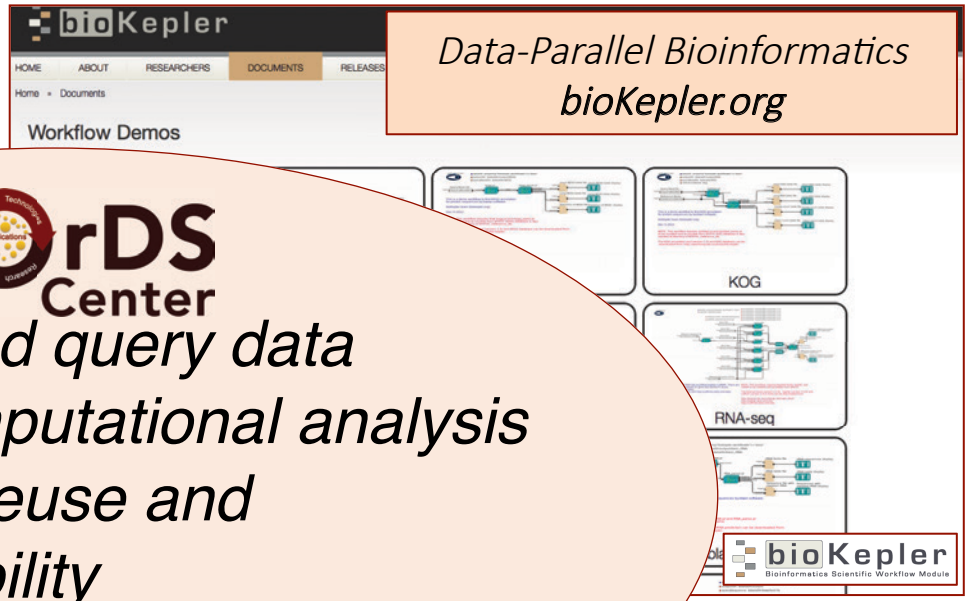
  Chen R., Wan X., Lawrence A., Wang J., Crawl D., Phan S., Altintas. I, Ellisman M., EPiK - a Workflow for Electron Tomography in Kepler. In Proceedings of the Second International Workshop on Advances in the Kepler Scientific Workflow System and Its Applications at the 14th International Conference on Computational Science (ICCS 2014).

Workflows for Data Science Center of Excellence

- Exploring Programmable, Reusable and Reproducible Scalability using Workflows-

Real-Time Hazards Management
wifire.ucsd.edu

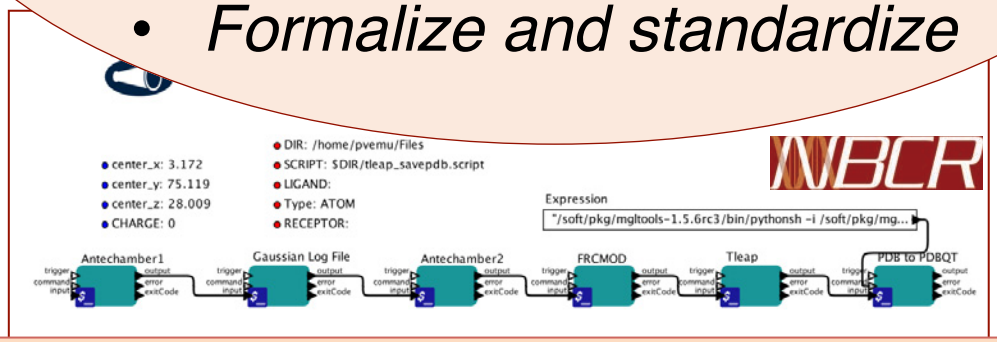
Data-Parallel Bioinformatics
bioKepler.org



WorDS Center

- *Access and query data*
- *Scale computational analysis*
- *Increase reuse and reproducibility*
- *Save time, energy and money*
- *Formalize and standardize*

kepler-project.org



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