

Workflow-Driven Scalable Data Analysis

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Discussion I:

How do you define local
execution?

Discussion II:

How do you define distributed execution?

Distributed Computing

Computing using **more than one computers** connected through a **network**.

- Types of distributed computing:
 - Computers in local area network
 - Cluster or High-Performance Computing
 - Grid
 - Cloud

Cluster or High-Performance Computing

- Built from *multiple computers*
- May have
 - *parallel file system*
 - *high-speed network*
- Provides a **scheduler** to manage the machines and submitted jobs
 - SGE/OGE, PBS, Condor, LSF, SLURM



SGE Clusters

- Each compute node has multiple CPUs
- Resource and Job Management

– SGE/OGE

- Job Submission

```
qsub -pe pvm 6- -l h_rt=30:00 your_script.sh
```

- Job Status Checking

```
qstat -u your_account
```

- Job Killing

```
qdel job_id
```

HPC on NSF XSEDE Gordon (at SDSC)

- Each compute node has *multiple CPUs*
- Each I/O node has 4.8 TB SSD *Flash Memory*
- Resource and Job Management
 - TORQUE, similar with PBS
- Job Submission

```
qsub -l nodes=2:ppn=8,walltime=30:00 your_script.sh
```
- Job Status Checking

```
qstat -u your_account
```
- Job Killing

```
qdel job_id
```



Discussion III:

What is scalability?

Why is it important to know multiple modes of scalability?

How can different modes be applied in bioinformatics?

Workflows Enable Distribution of Execution to Heterogeneous Computing Resources.

- Execution of models on where they run most efficiently -

Different models have different computing architecture needs!

e.g., memory-intensive, compute-intensive, I/O-intensive

Local: NBCR Cluster Resources



NSF/DOE: TeraScale Resources (XSEDE)



(Gordon)



(Lonestar)



(Trestles)



(Stampede)

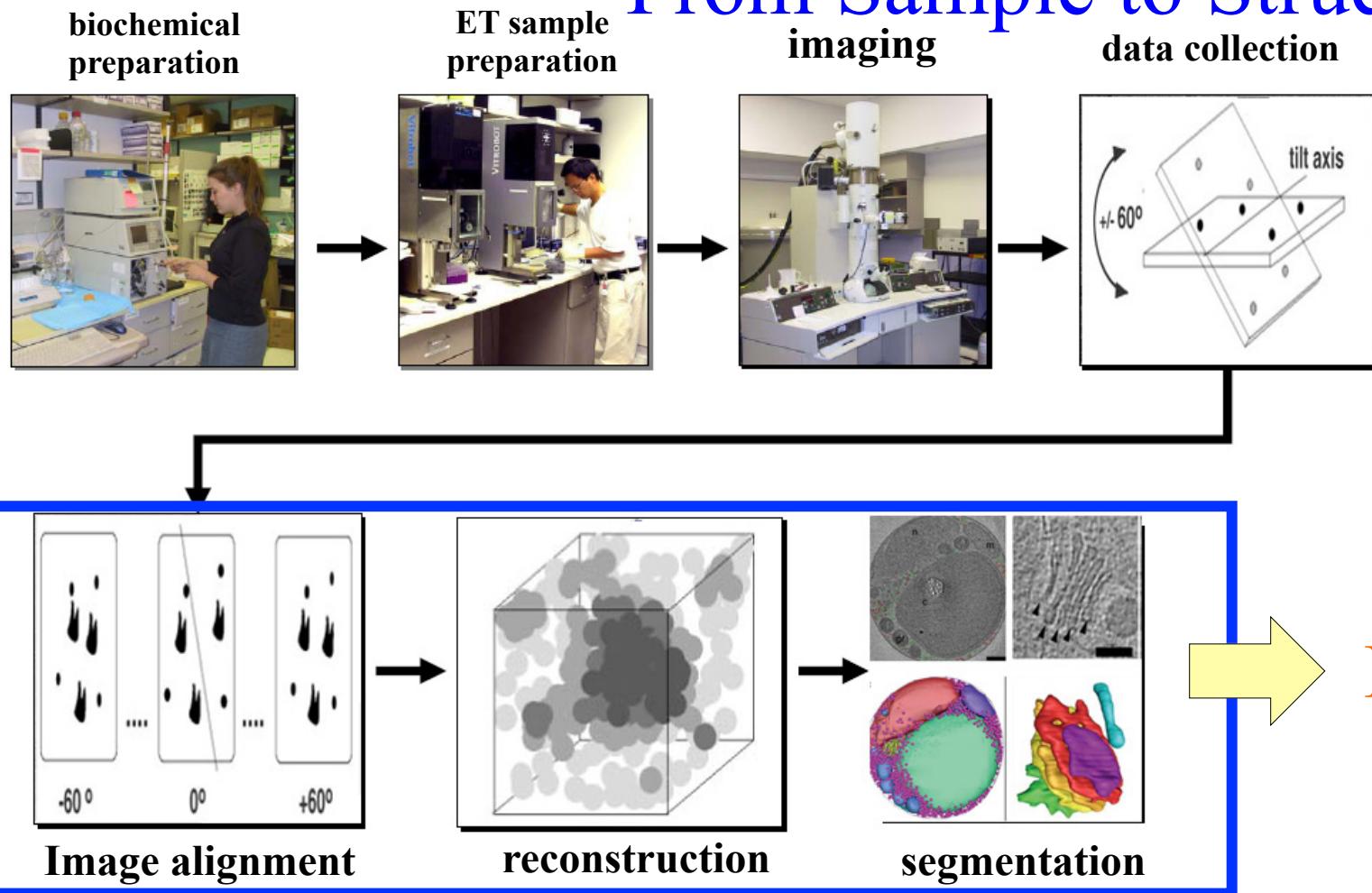
Private Cluster:
User Owned Resources



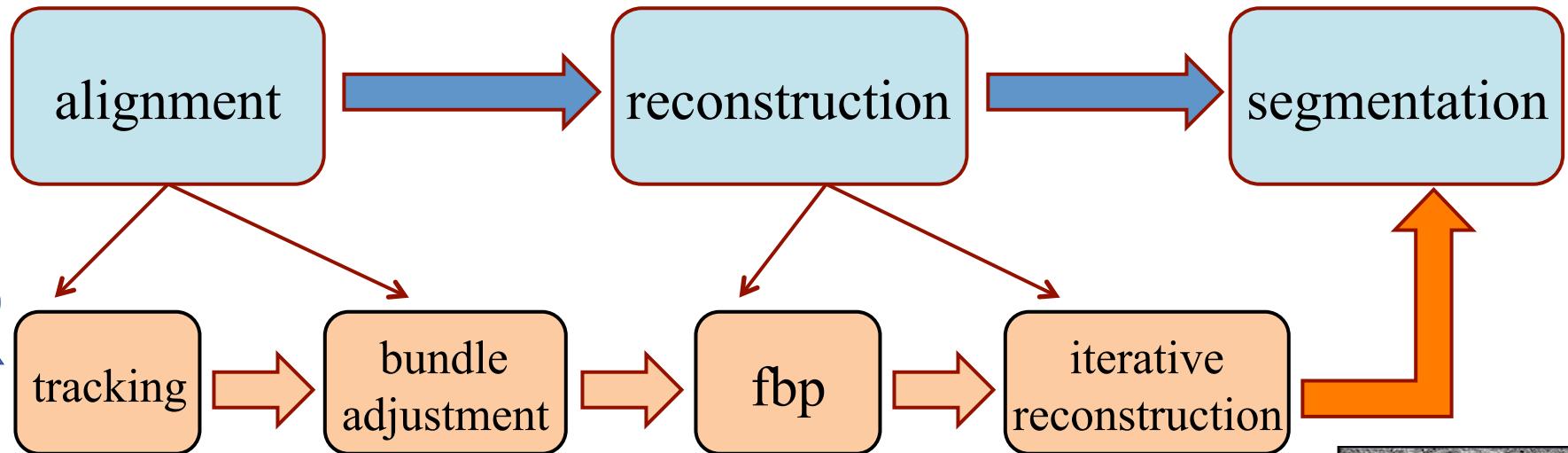
NBCR Workflow: EPiK

– ET reconstruction software in Kepler –

From Sample to Structure



DBPs: #5 Ting, Taylor; #6 Ross, Sejnowski; #7 Skupin, de Pillis; #8 Bers, Hoshijima

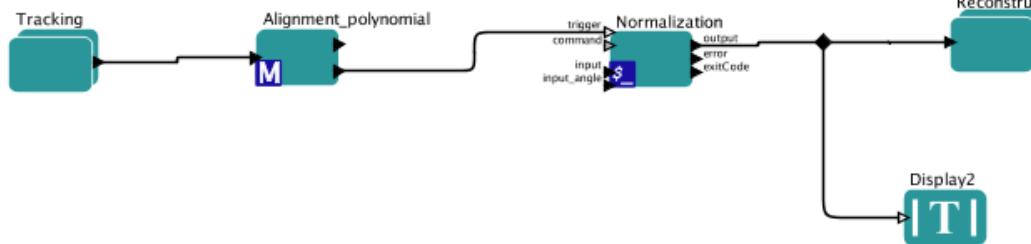


- Home: /Users/ruijuanchen
- WorkDir: \$Home/Documents/wxh_workflow
- dataDir: \$WorkDir/rawdata
- dataDir_normal: \$WorkDir/normalization
- inputFile_normal: \$dataDir/lewy_body.st
- angleFile: \$dataDir/lewy_body.rawtl
- upload_data: \$WorkDir/upload_data
- outputFile_normal: \$upload_data/lewy_body_normalized.st
- TargetHost: x5wan@rocce.ucsd.edu
- IdentityFile: \$Home/.ssh/id_rsa
- reconstruction_dir: /data/x5wan/kepler/reconstruction/iterative
- cmd_job: \$reconstruction_dir/run_ASART1.sh



- basename: \$dataDir/lewy_body
- lmodDir: /Applications/IMOD/bin/
- MFileDir: \$WorkDir/kepler_m_files
- BeadDiameter: 19.61
- xsize: 512
- ysize: 512

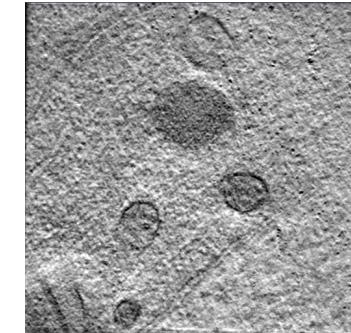
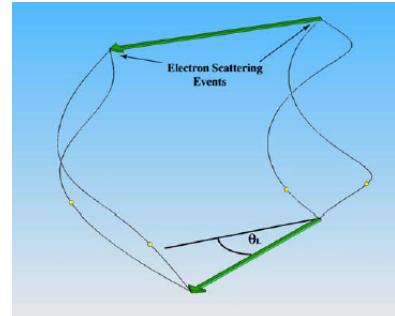
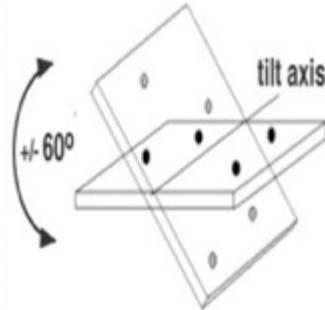
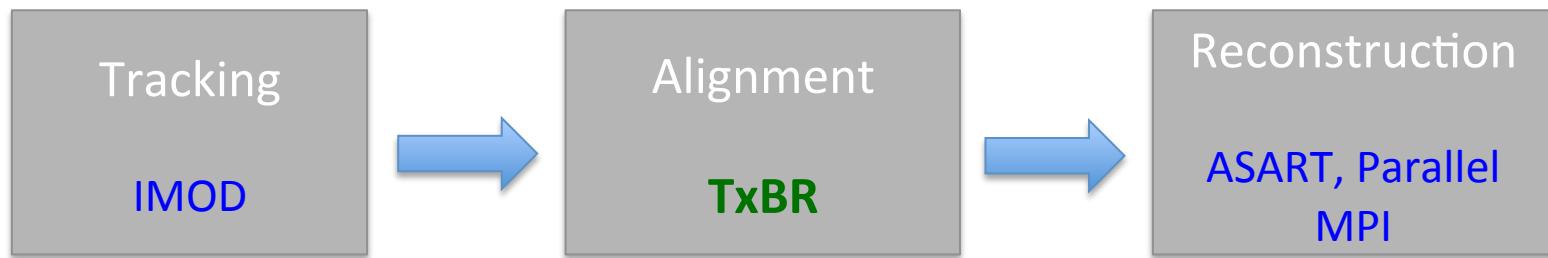
EPiK workflow in Kepler



BENEFITS:

- Increase reuse
- Standardize data interfaces
- Scale execution
- Compare methods
- Train students

Example: Integration of Software Tools for Iterative Reconstruction



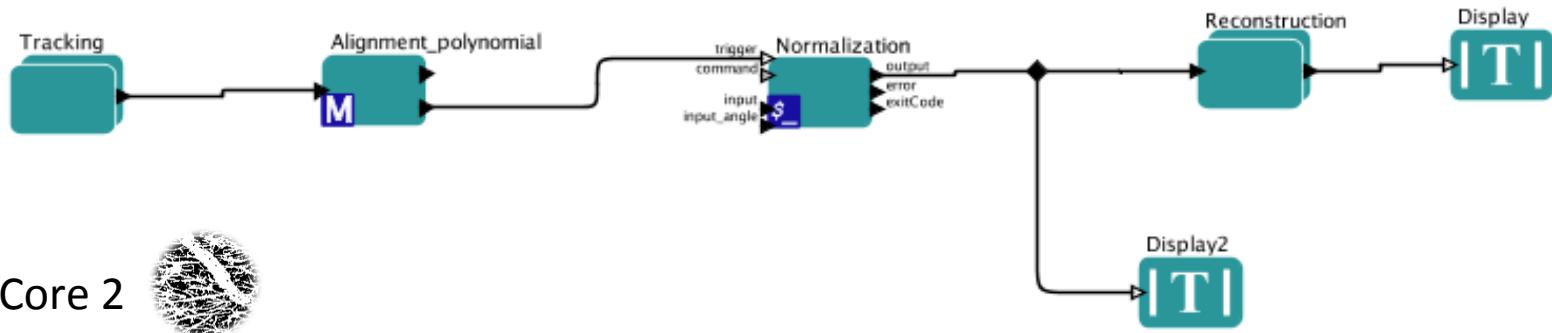
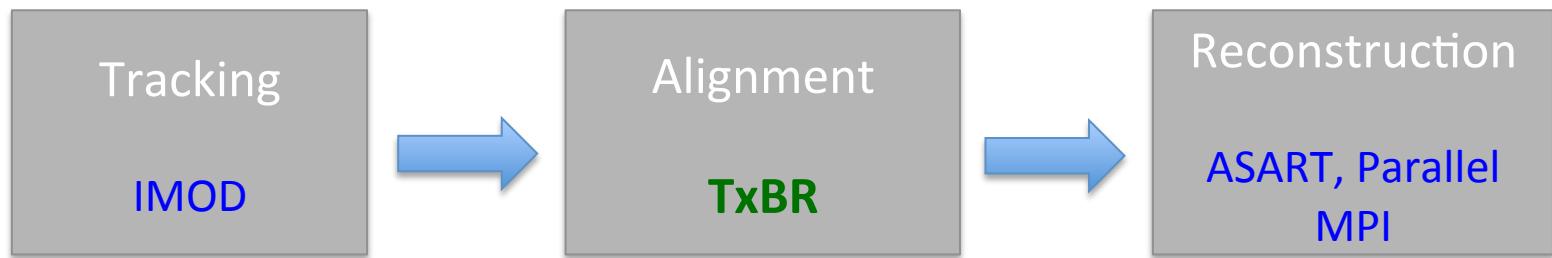
From “*Conceptual Steps*”

SDSC
SDO SUPERCOMPUTER CENTER

To *Integrated, Executable and Portable Workflows*

Community-developed open tools


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



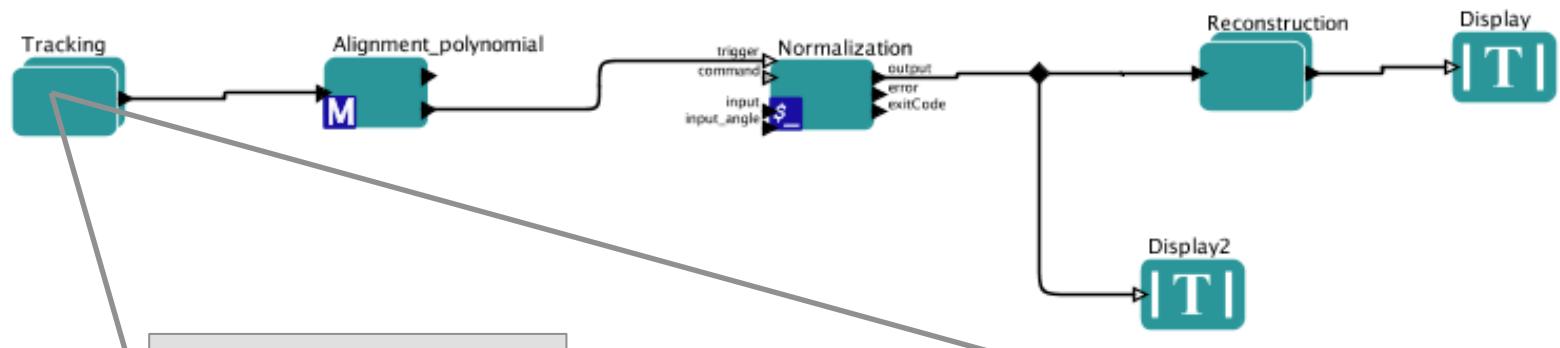
In Partnership with
Sun Yat Sen Foundation



BENEFITS:

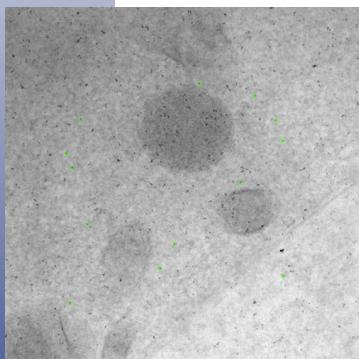
- Improved programmability
- Ability to use and compare multiple methods in one integrated workflow
- Reduction of complexity

Hiding Complexity and Facilitating Transparent Task Distribution in the EPiK Workflow

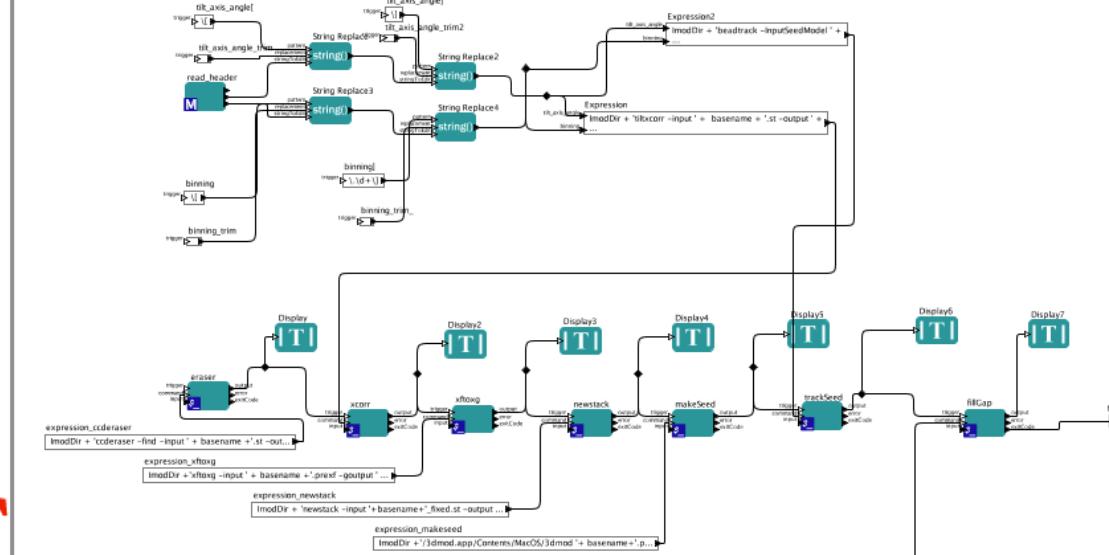
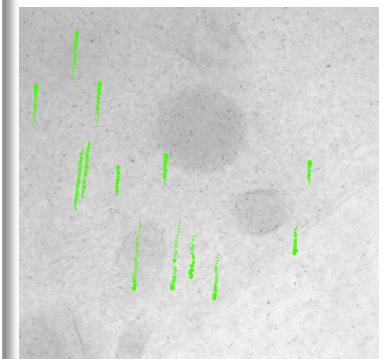


Tracking Actor

Input



Output



Discussion IV:

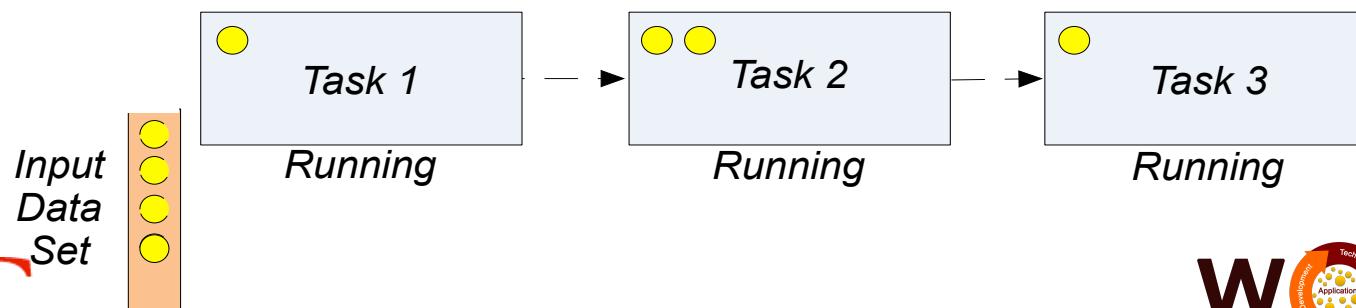
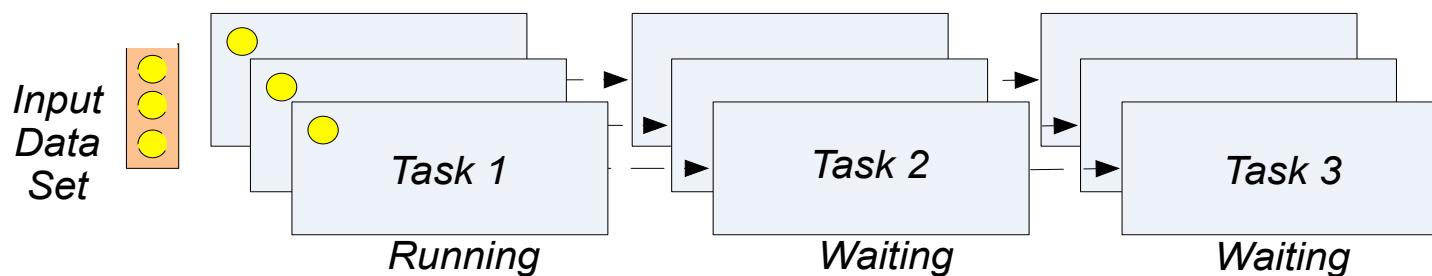
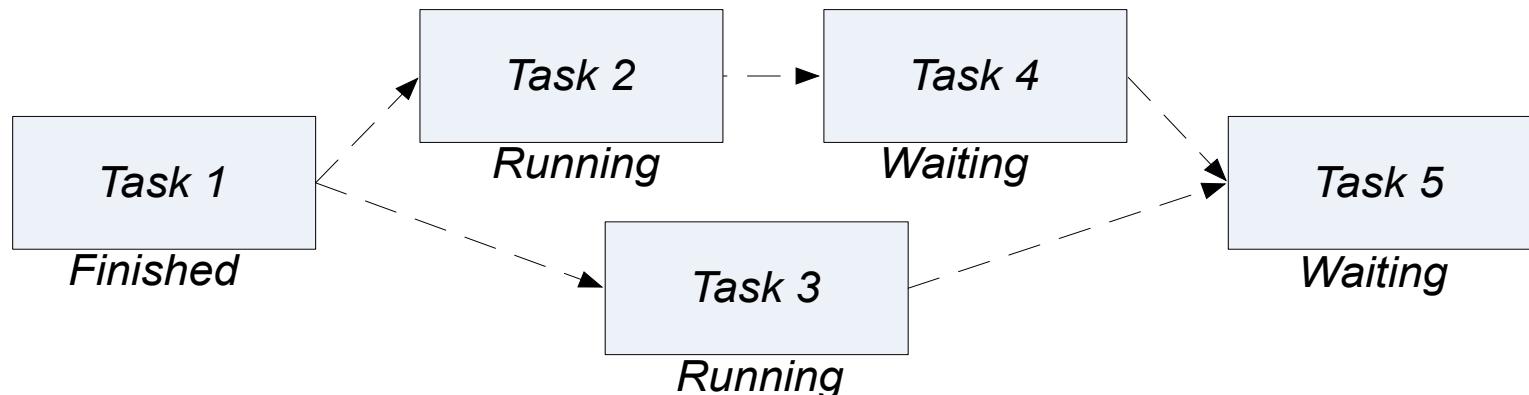
How do you define parallel execution?

Parallelization

**Multiple processes or threads
running at the same time**

- Execution environments
 - One machine
 - Distributed machines
- Parallelism Types
 - Computation/task parallelism
 - Data parallelism
 - Pipeline parallelism

There are different styles of parallelism!



Discussion V:

How do you apply different types
of parallelism while cooking?

The rest of this session...

- Execute legacy tools **locally and remotely on an HPC cluster**
 - Create a conceptual workflow
 - Map Kepler actors to analytical steps and customize if required
 - Local execution: on the Virtual Box VM
 - Remote execution: In the example workflow, Scheduler and TargetHost are made parameters that can be configured to schedule jobs on different cluster
 - Cluster – Gordon with PBS Scheduler and Comet with SLURM scheduler for GPUs
 - Demonstration:
 - Data-Parallel computing using Hadoop and Spark
 - Using iPython notebooks for workflow execution

HAPPY ENDING?

There are no happy endings.
Endings are the saddest part,
So just give me a happy middle
And a very happy start.

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