TYPES OF WORKFLOWS

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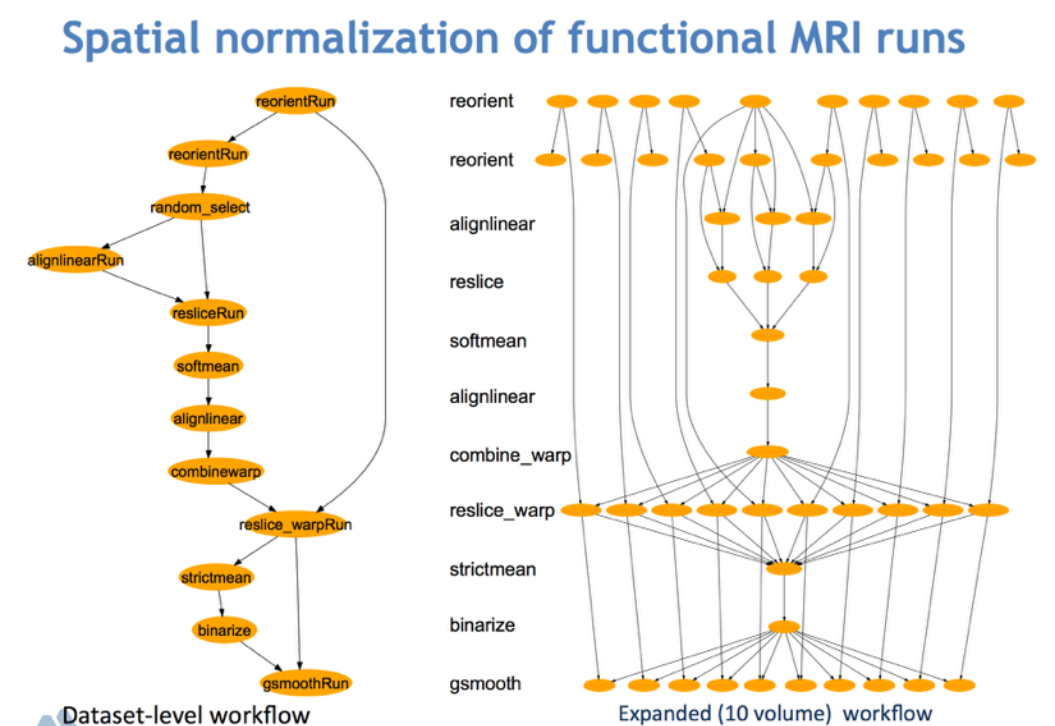
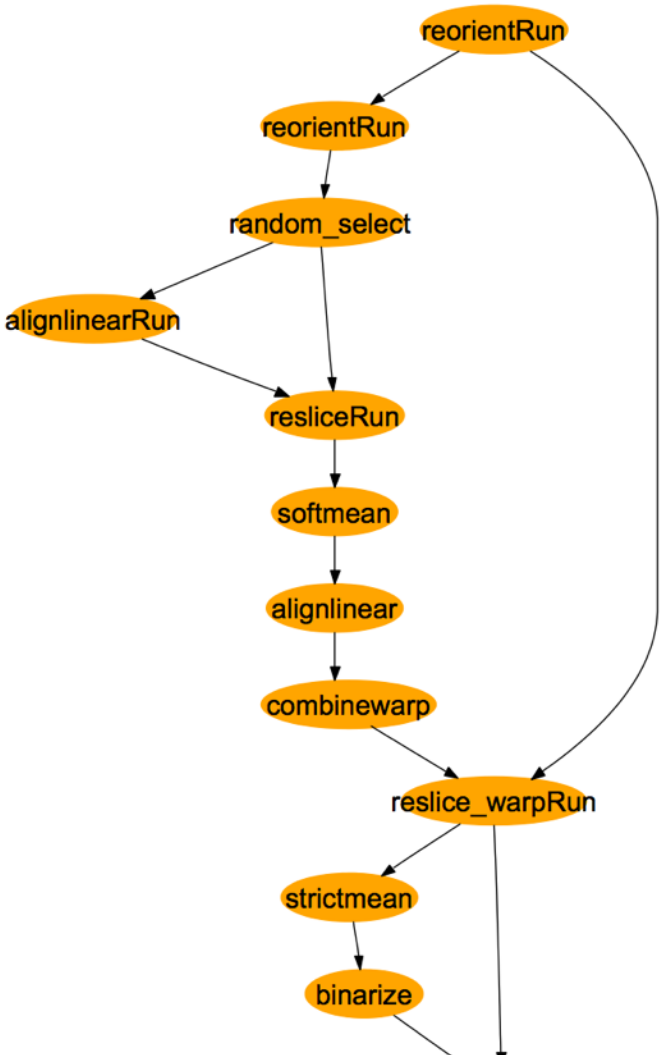
WHAT IS A WORKFLOW?

- A connected graph of application executions or phases
- Coupled together by data flow
- Phases can be distinguished by many factors
  - Configuration
  - Executable
  - Parallelism
  - Platform
  - Resource/Allocation



WHAT IS A WORKFLOW?

Spatial normalization of functional MRI runs



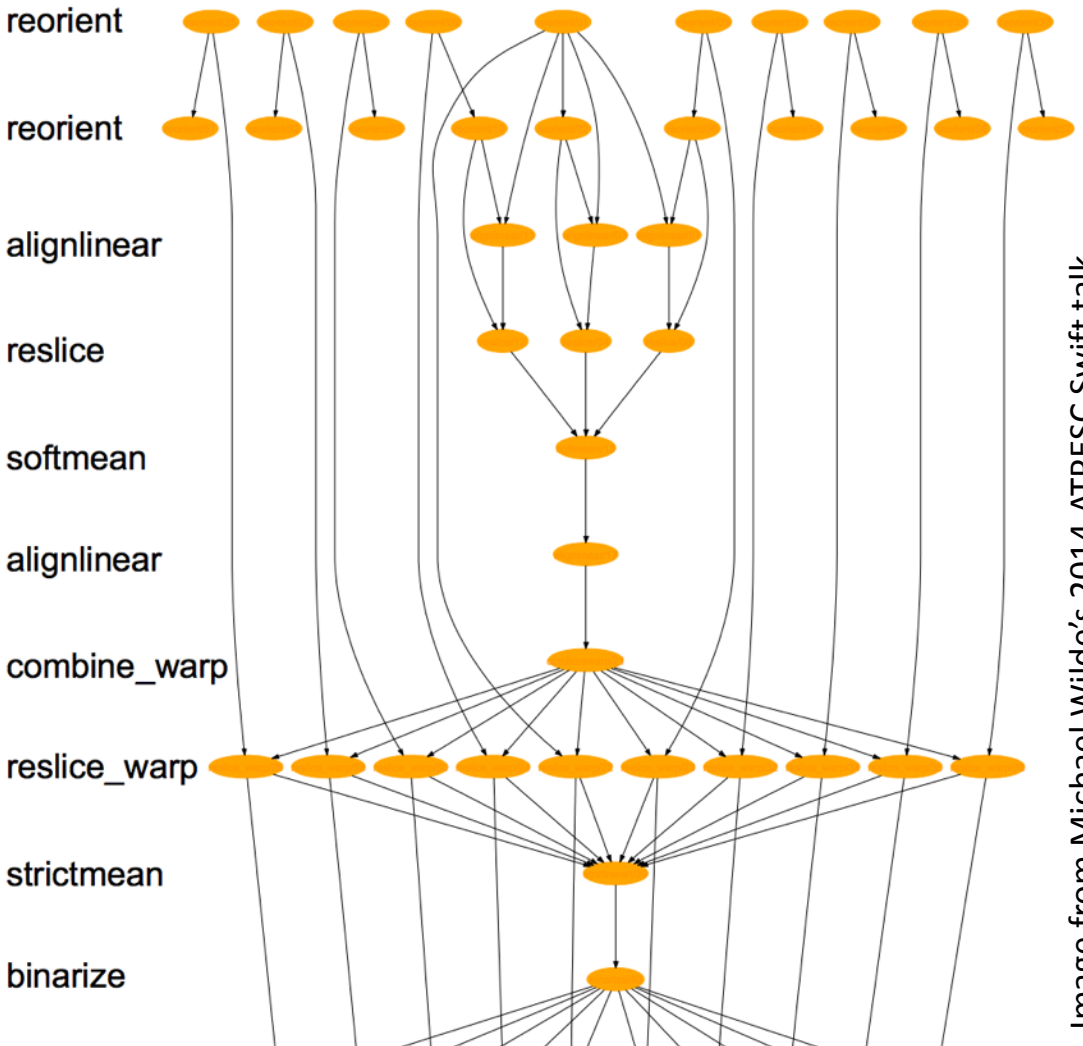
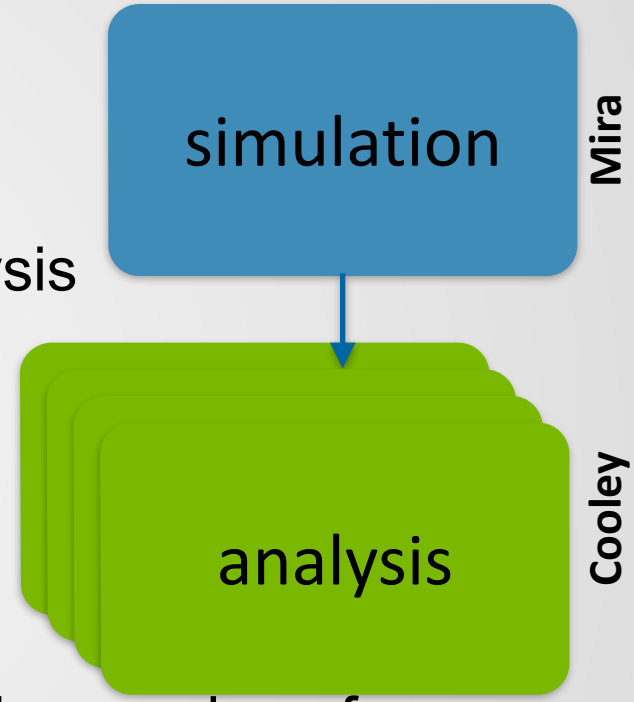


Image from Michael Wilde's 2014 ATPESC Swift talk

WHY DO WORKFLOWS ARISE?

- Complexity in Task Structure
  - Simulation -> Analysis
  - Multi-step Simulation -> Multi-step Analysis
  - Parameter Sweeps
- Compounded by multiple sites/resources
- Overall campaign management



Manual management of workflows gives the impression of ultimate control over the conducting of experiments, but is in fact tedious and error-prone, and is often counter to reproducibility (aka provenance)

WORKFLOW TOOLS

High throughput tools

- Cluster schedulers/local resource managers (PBS, SGE, Cobalt, LSF, LL, SLURM)
- Condor

Workflow task dependency managers

- DAGMan

Integrated dependency and data management

- Pegasus

Dataflow languages

- Dryad, Ciel, Swift

Big data solutions

- Hadoop, Spark, Zookeeper, Uzi

WORKFLOW TOOLS (CONT)

Multicore tools

- GNU Parallel, iPython parallel support

Interactive workflow frameworks

- Galaxy
- Taverna
- Kepler
- LONI Pipeline (neuroscience)
- Microsoft Workflow manager
- Apache Airavata

Science gateways

WHAT DO WORKFLOW TOOLS PROVIDE?

- High-throughput Computing (HTC)
- Many-task computing (MTC)
  - Parameter Sweeps
- Data Staging
- ~Portability
  - High-level flow control
- Error handling and recovery
- Monitoring
- Provenance: Details necessary to produce a given result (compiler, libraries, inputs, configuration, etc.)

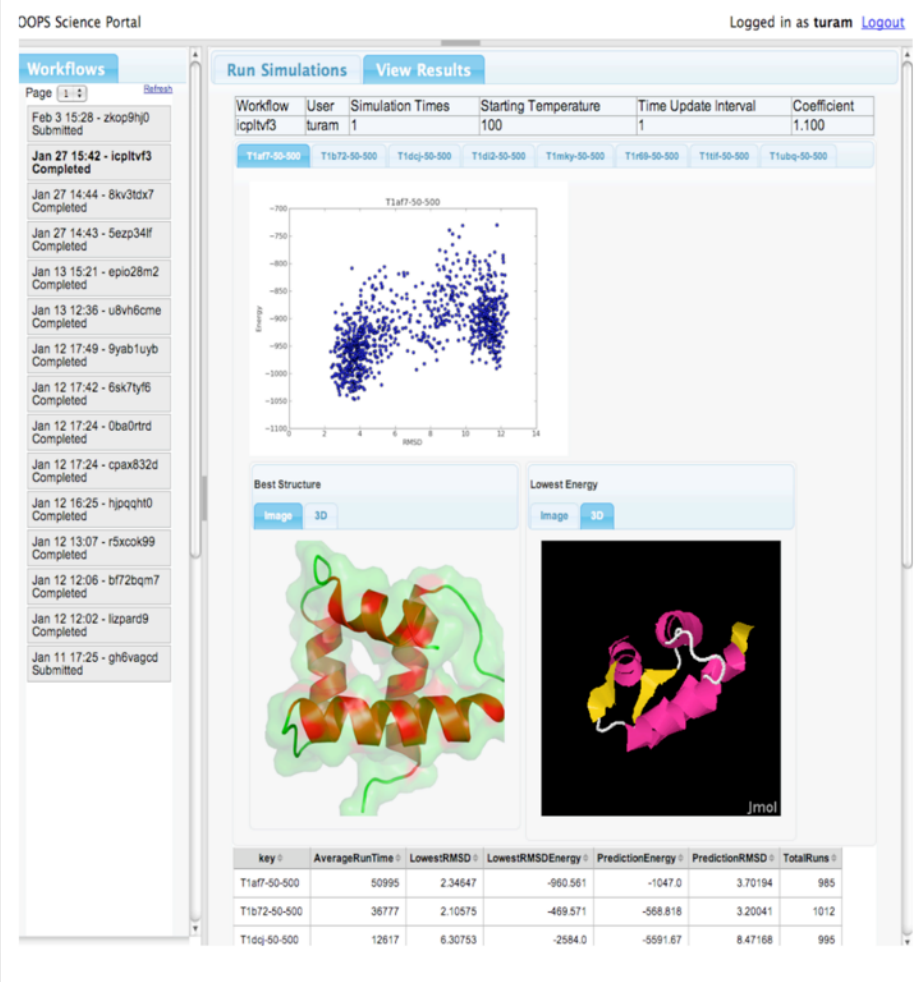
EXAMPLE: PROTEIN SIMULATION

```
main()
{
string plistfile=@arg("plist",""); // input protein
fasta file
string indir=@arg("indir","oops.input");
string outdir=@arg("outdir","output");
string nsims=@arg("nsims","1"); // simulation num
string st=@arg("st","100");     // start temperature
string tui=@arg("tui","100"); // time update interval
string coeff=@arg("coeff","0.1");

string plist[] = readData(plistfile);
RAMAIn ramain[]
 <ext;exec="RAMAInProts.map.sh",i=indir,p=plistfile>;
RAMAOut ramaout[][]
        <ext;exec="RandProtRadialMapper.py",
                o=outdir,p=plistfile,
                n=nsims,c=create>;
foreach sim in [ 0 : @toint(nsims) -1 ] {
  foreach prot,index in plist {
    ramaout[index][sim]
      =predictCf(prot,ramain[index],st,tui,coeff);
    VizOut outpng[] <ext; exec="pngmapper.py",
      o=metadir,
      p=@filename(ramaout[index][sim].pdb) >;
    outpng[0] = pngviz(ramaout[index][sim]);

  }
}
}
```

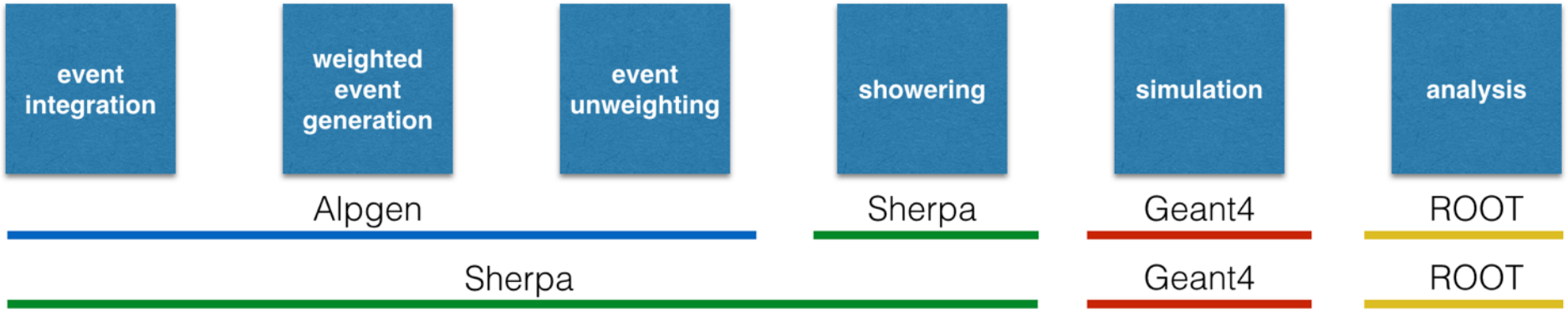
Swift script for protein folding workflow



Web interface for viewing workflow outputs

EXAMPLE: HEP EVENT SIMULATION

Workflow for simulating events such as occur in the ATLAS detector at the Large Hadron Collider



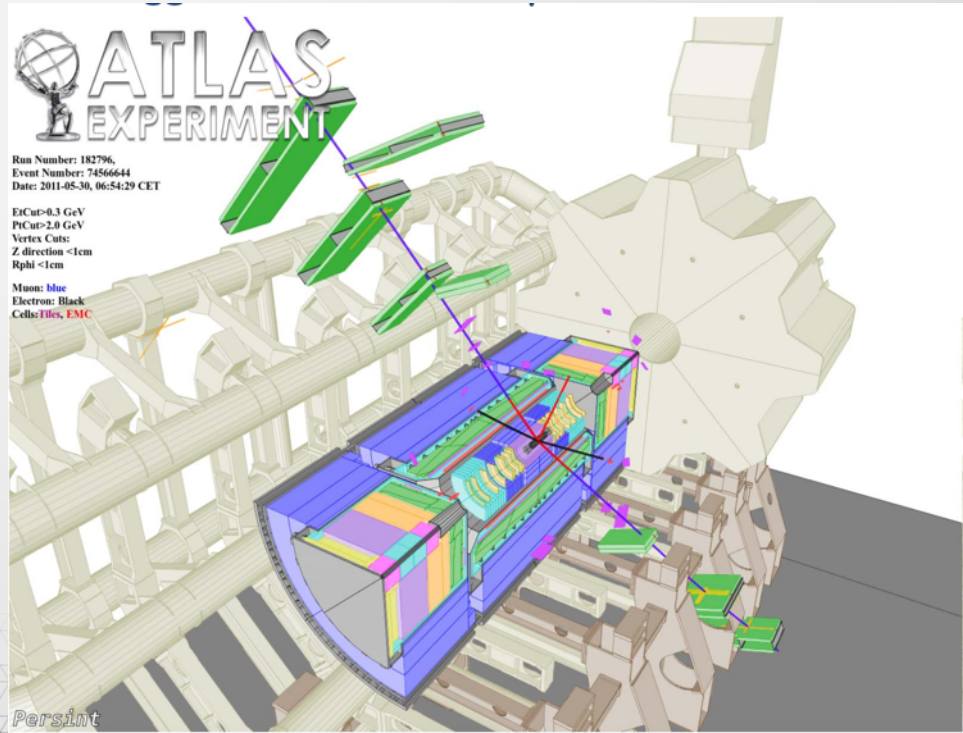
See Tom LeCompte's talk from Monday

EXAMPLE: HEP EVENT GENERATION

Monte Carlo-based generation of particle collision events such as occur in the ATLAS detector at the Large Hadron Collider, using Alpgen.

Consists of three stages:

1. Generation of integration grid
2. Generation of weighted events
3. Unweighting of events



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EXAMPLE: HEP EVENT GENERATION

Monte Carlo-based generation of particle collision events such as occur in the ATLAS detector at the Large Hadron Collider, using Alpgen.

Consists of three stages:

1. Generation of integration grid } serial
2. Generation of weighted events } independent, parallelizable
3. Unweighting of events

See Tom LeCompte's talk from Monday

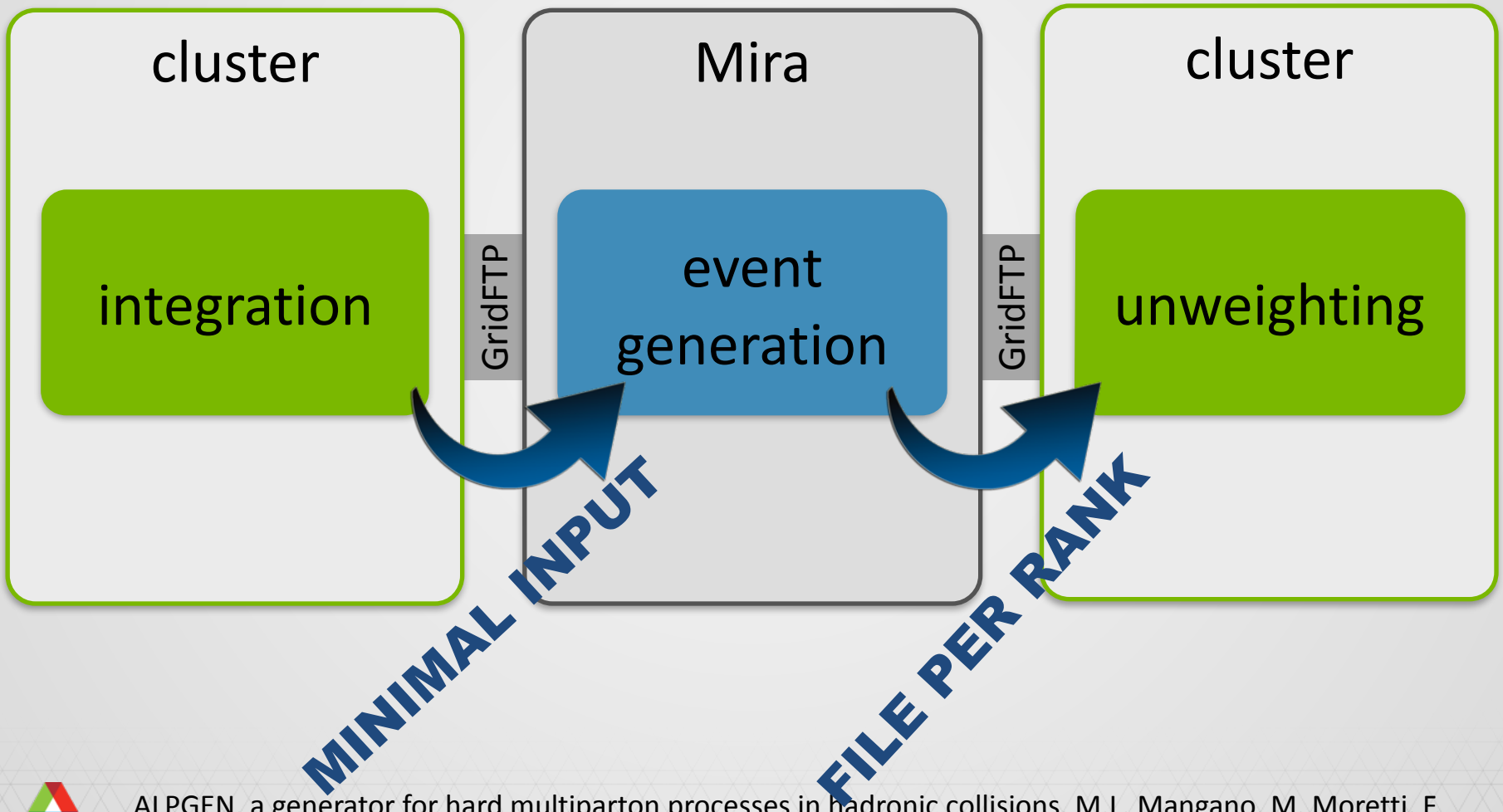
HEP EVENT GENERATION

General adaptations for event generation with Alpgen on Mira:

- Read input grid files and configuration files and distribute over MPI
- Use MPI to coordinate per-rank random seeds
- stdout/stderr from rank 0 only
- Reduced memory footprint to ~200MB
  - Removed unused proton models loaded into the data section of the executable
  - Allows us to run 64 ranks per node

ALPGEN, a generator for hard multiparton processes in hadronic collisions, M.L. Mangano, M. Moretti, F. Piccinini, R. Pittau, A. Polosa, JHEP 0307:001,2003

HEP EVENT GENERATION WORKFLOW



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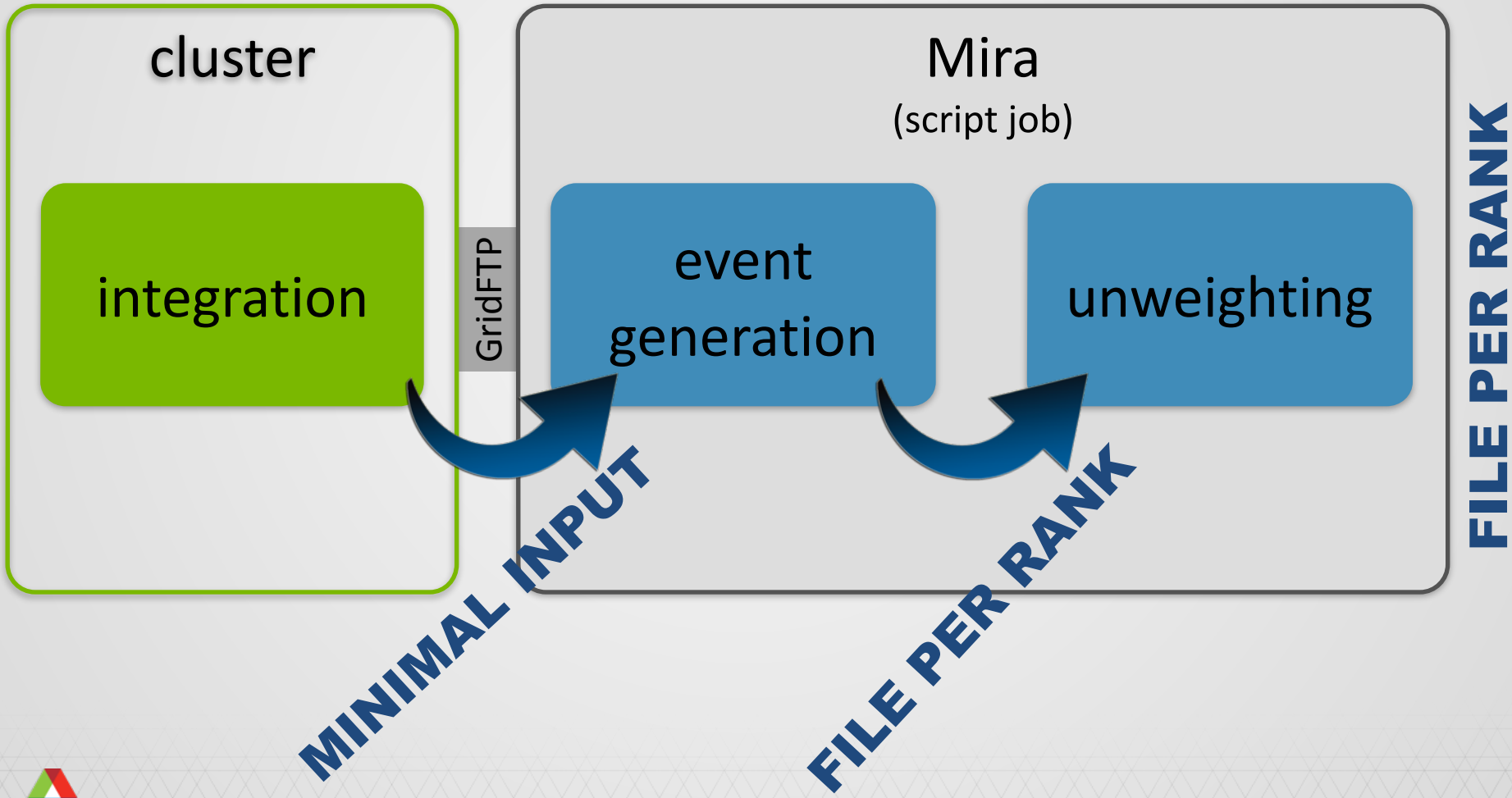
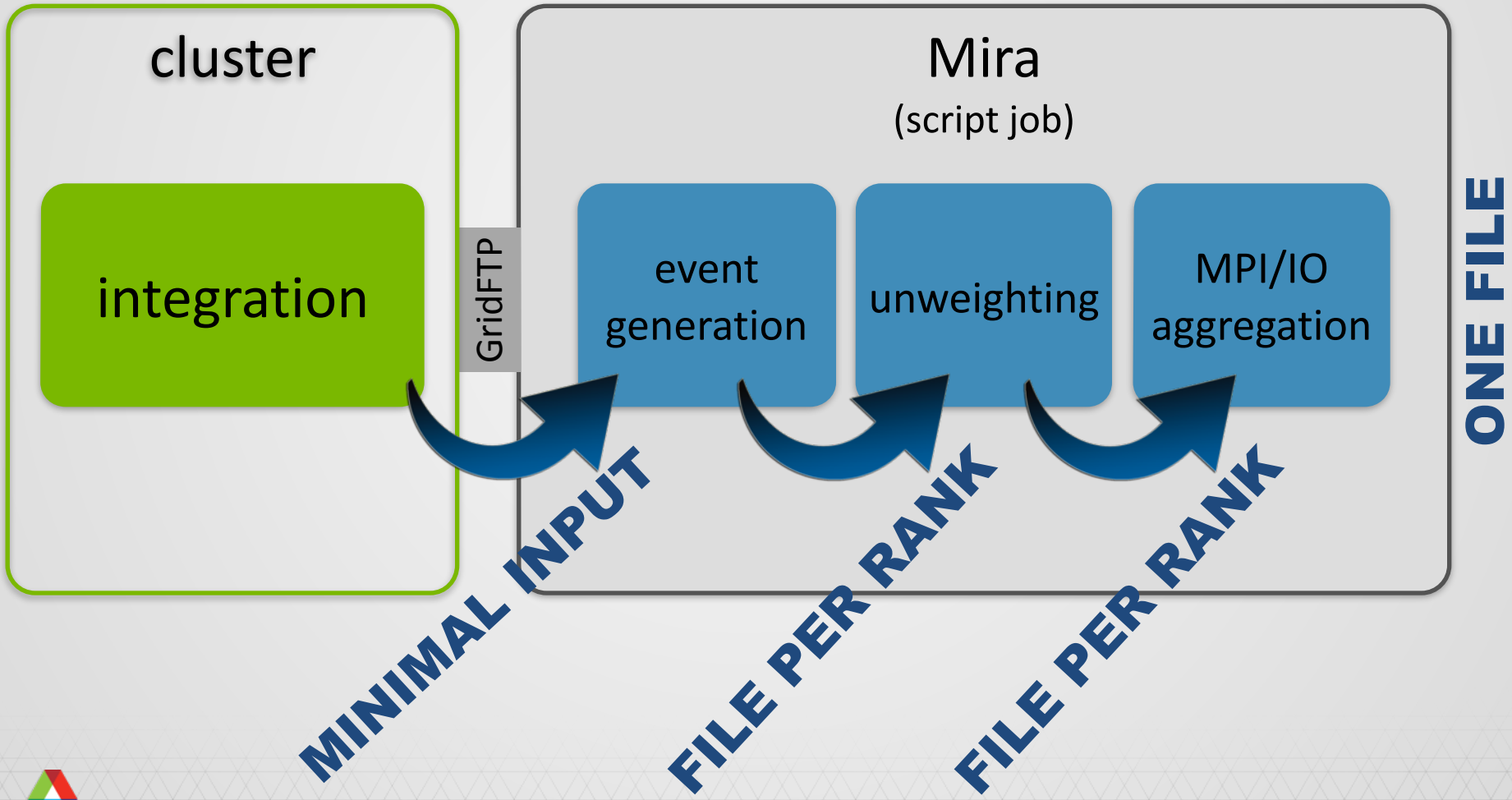


For info on script jobs: www.alcf.anl.gov/user-guides/running-jobs

HEP EVENT GENERATION WORKFLOW



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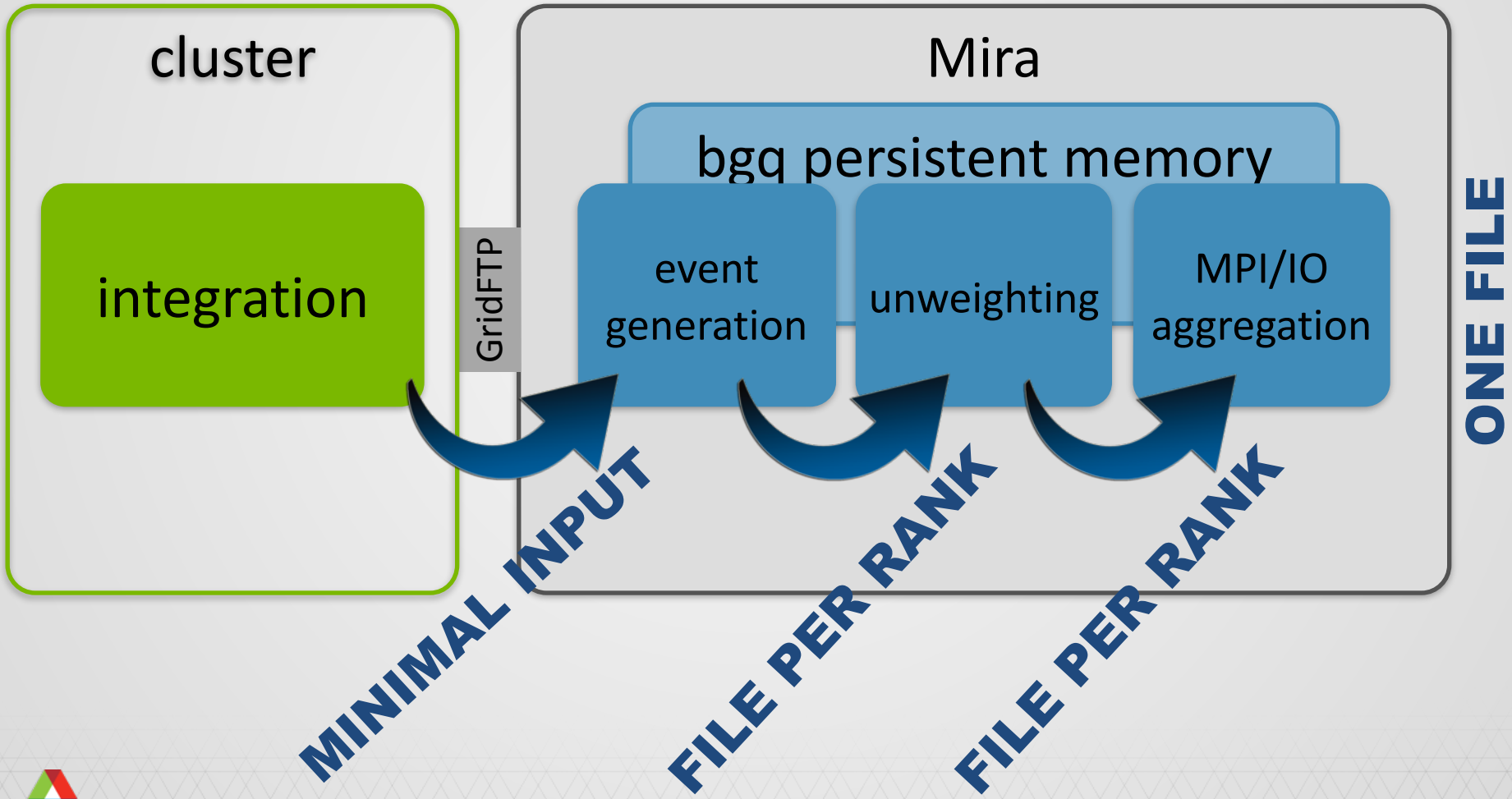

For info on BGQ persistent memory: www.redbooks.ibm.com/redbooks/pdfs/sg247948.pdf

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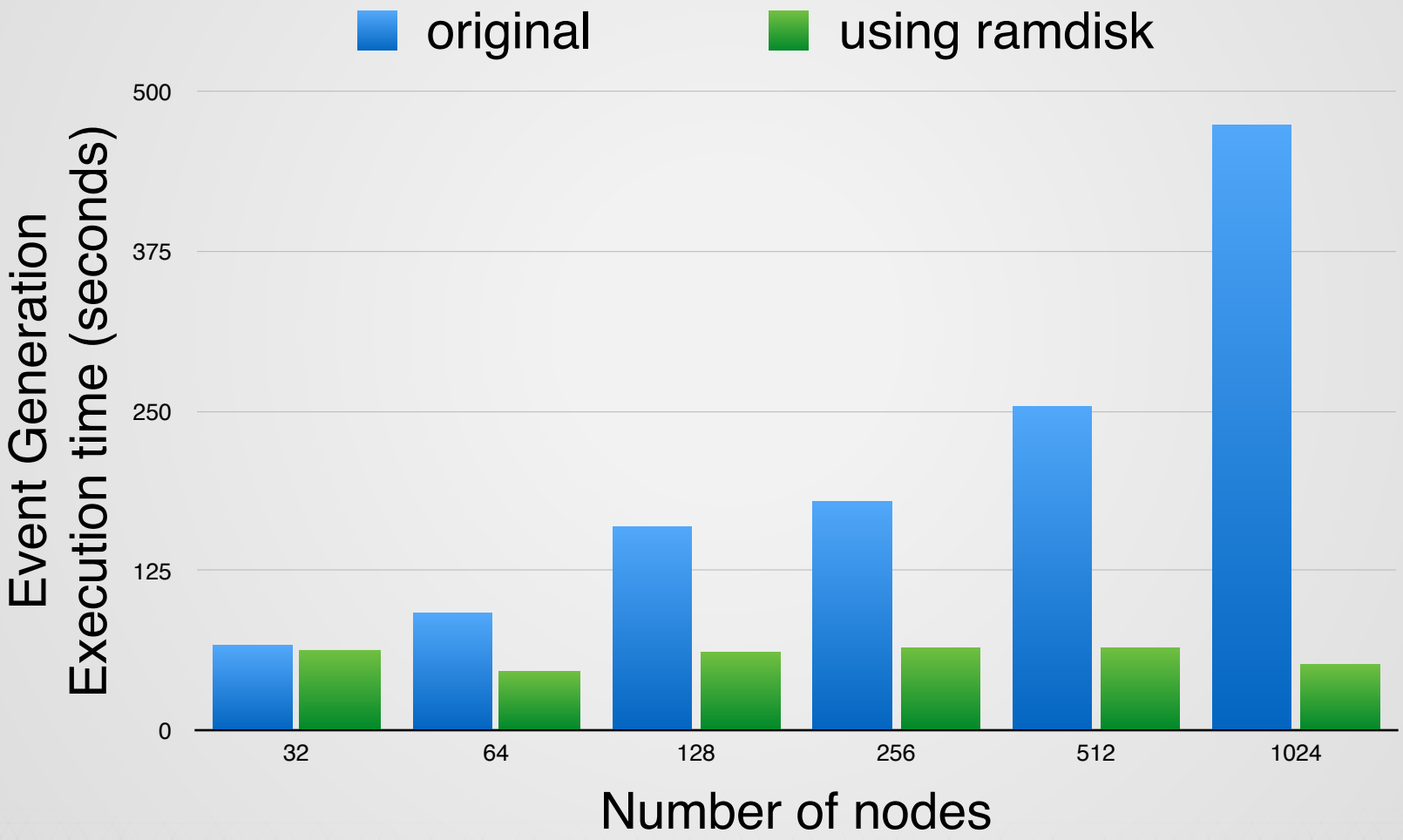

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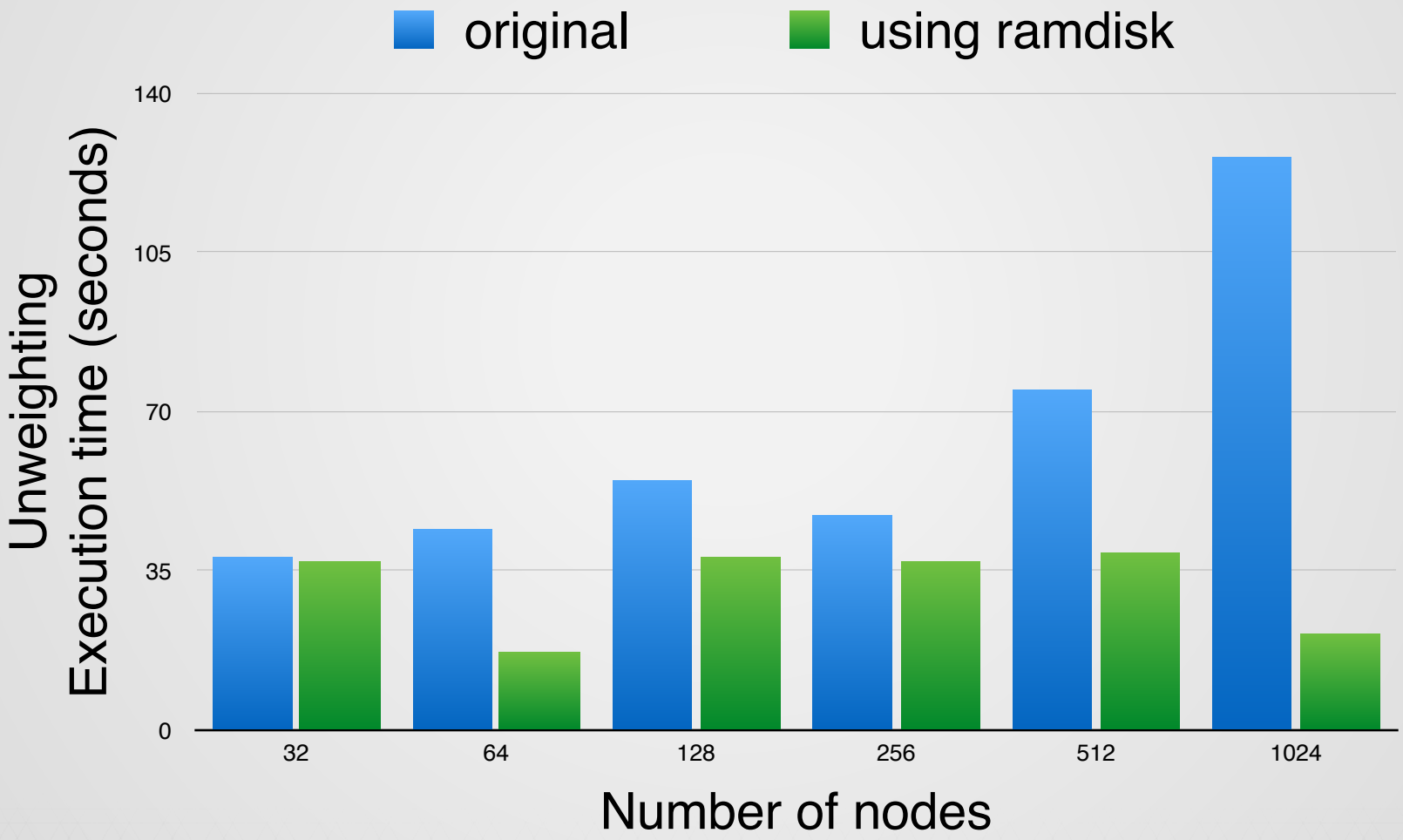
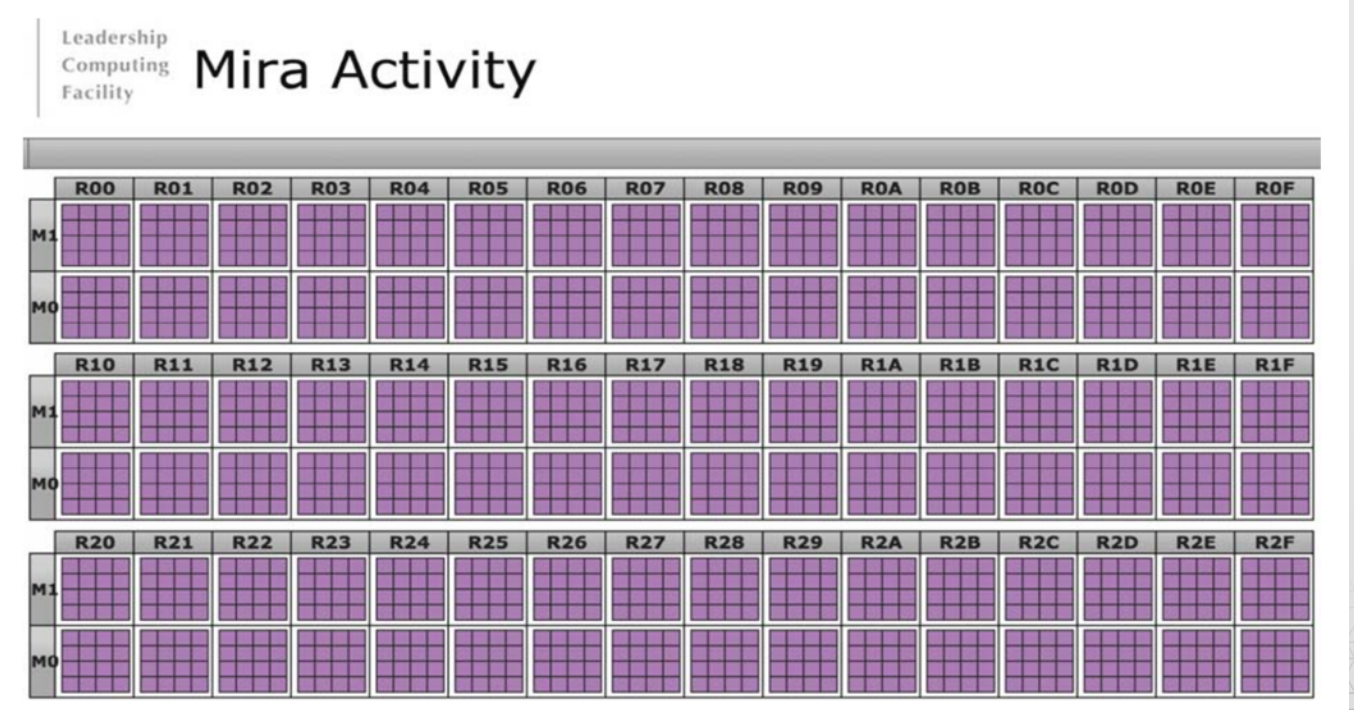


ALPGEN AT MIRA SCALE

- Alpgen running on 49,152 nodes of Mira
- Largest Alpgen job ever run: 786B W+5 jet events
- Running jobs at this scale has allowed us to run years of event generation jobs in a few weeks



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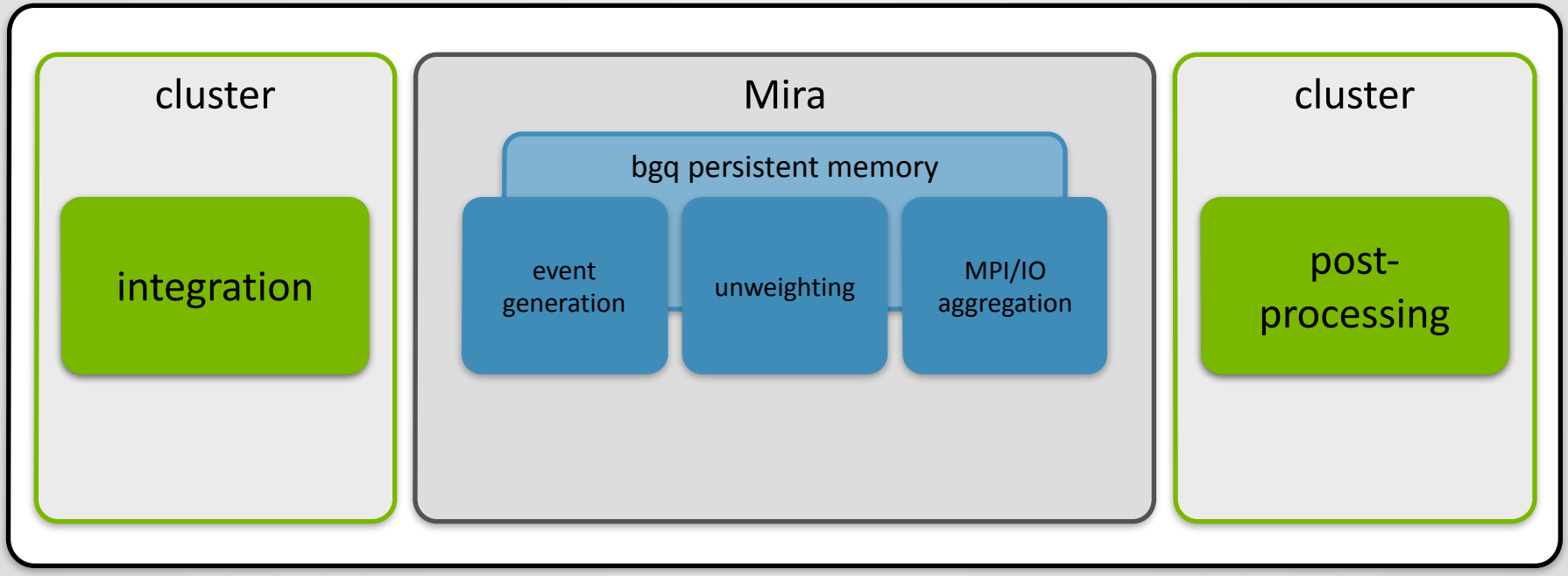
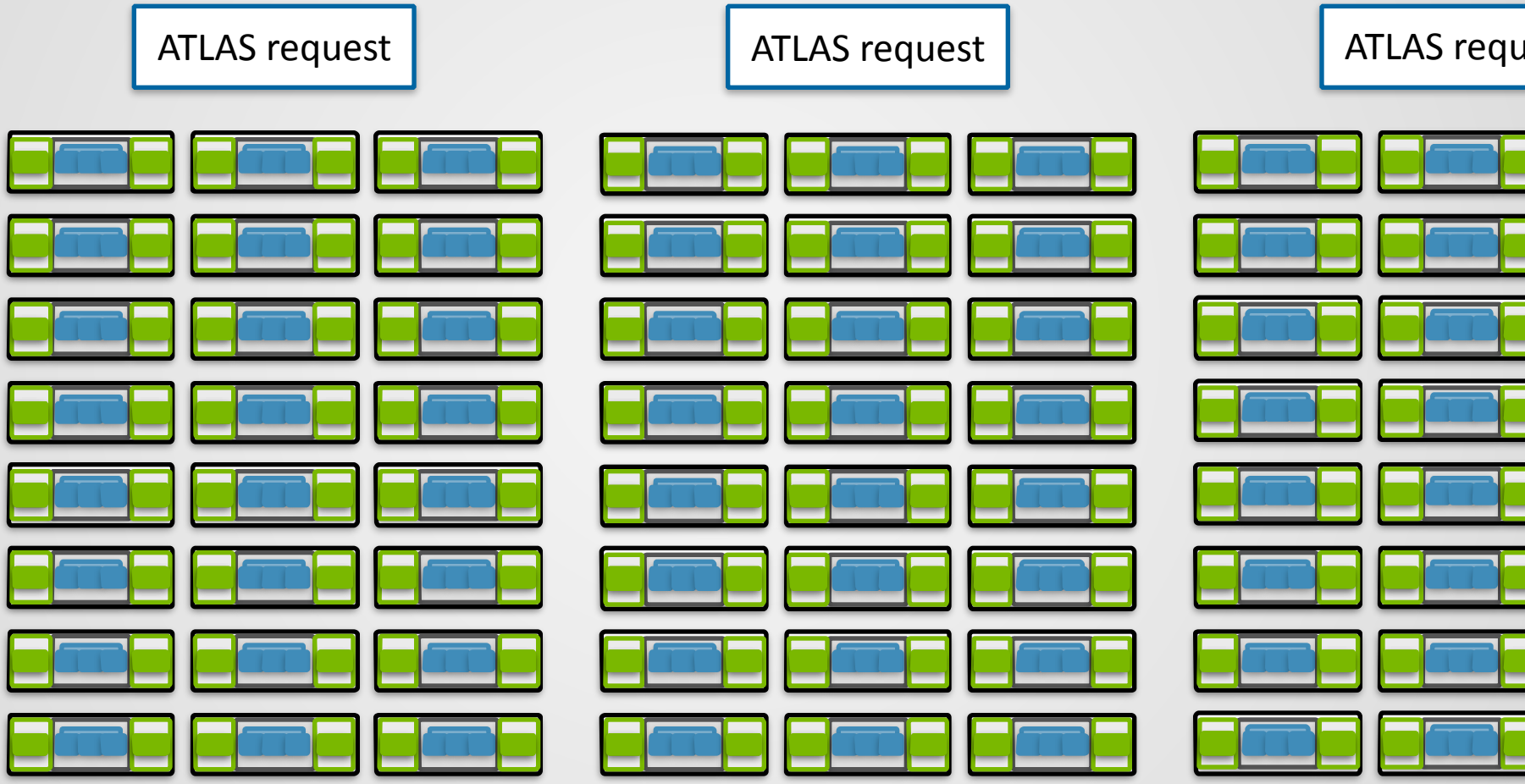
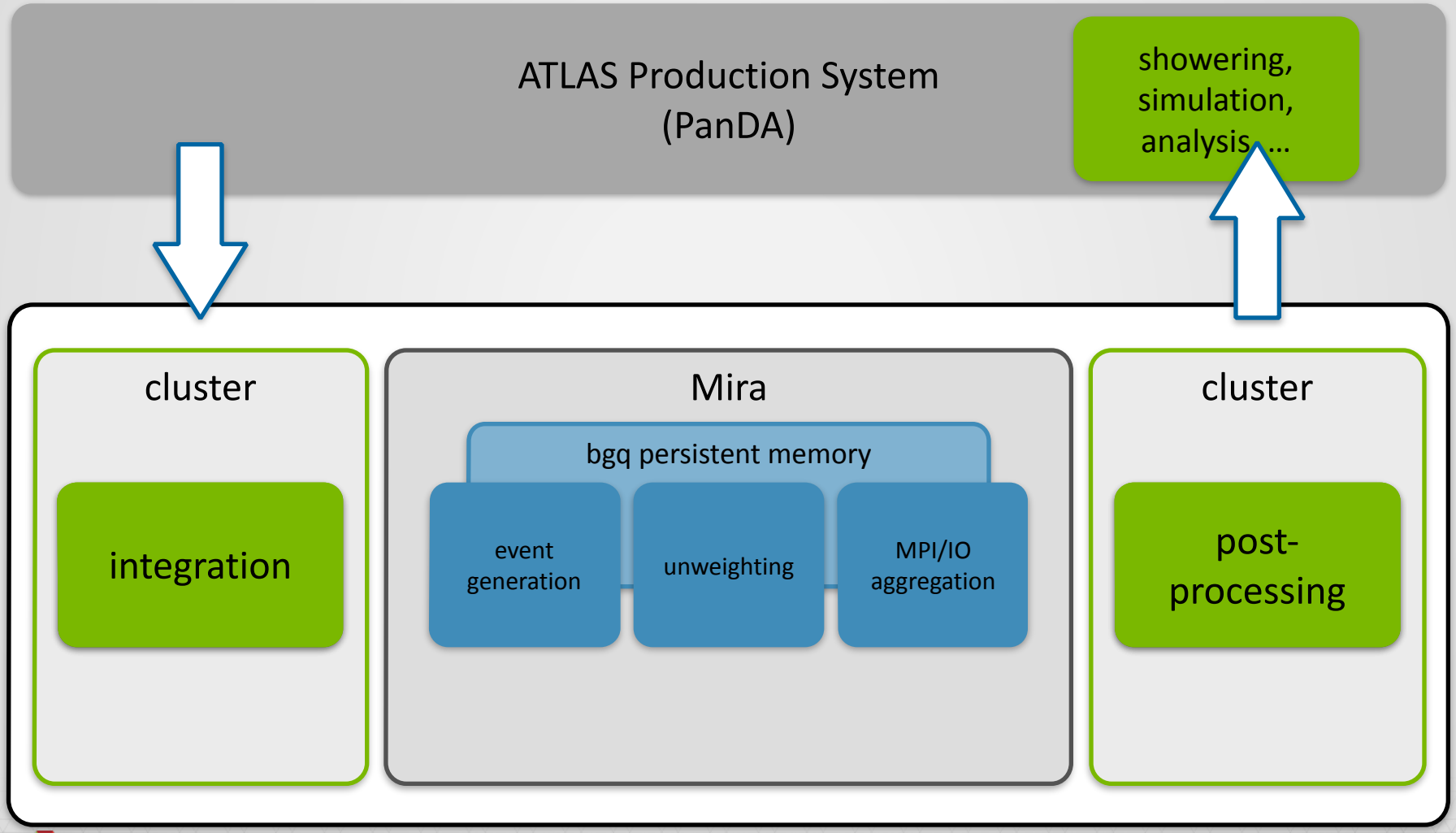


HEP EVENT GENERATION META WORKFLOW



HEP EVENT GENERATION META WORKFLOW

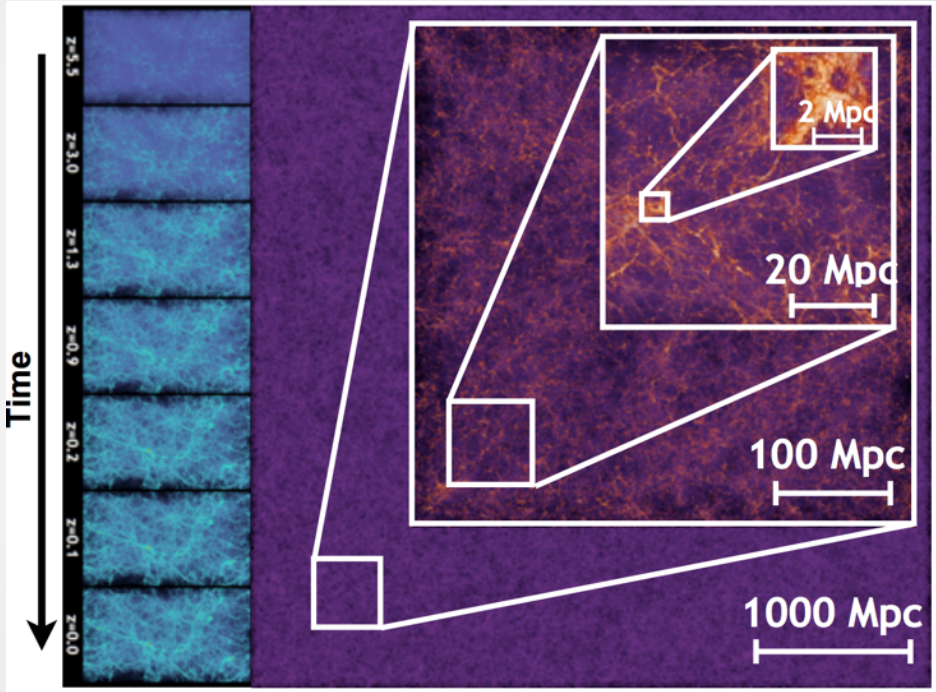


HACC SIMULATION AND ANALYSIS WORKFLOWS

- HACC is an nbody simulation code for cosmology
  - See Salman Habib's talk from Monday
- PDACS: Portal for Data Analysis services for Cosmological Simulations
  - Analysis workflow via a Galaxy-based web application
- CosmoTools
  - Analysis in-situ with simulation

HACC SIMULATION AND ANALYSIS WORKFLOWS

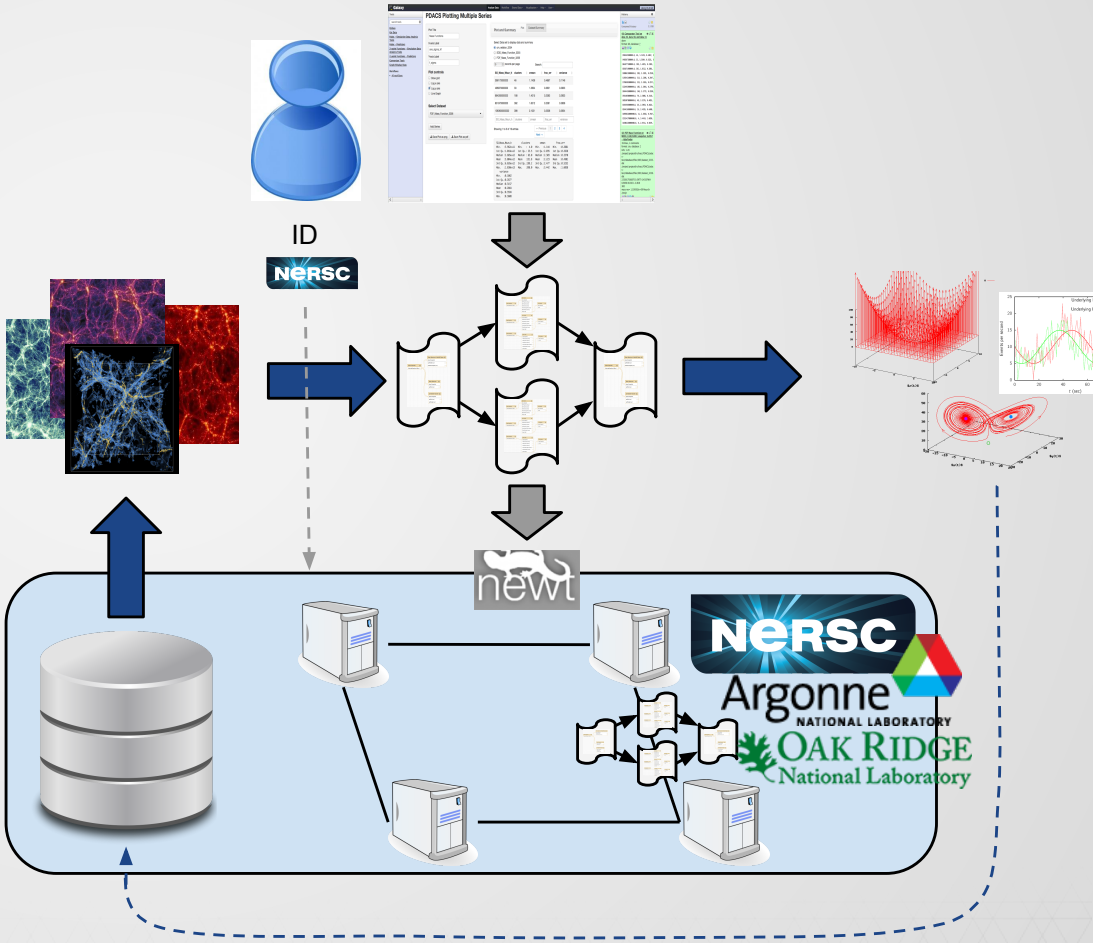
- HACC is a code for very large high-resolution cosmological simulations
  - First production science code to break 10PFlops (sustained)
  - See Salman Habib's talk from Monday



Gravitational Jeans Instability: 'Outer Rim' run with 1.1 trillion particles

HACC: PDACS WORKFLOWS

- Analysis tools wrapped as strongly-typed modules
- Users construct workflows from modules using a graphical tool
- Workflows are executed on resources according to underlying configuration
- PDACS instances running against resources at Argonne, Oak Ridge, and NERSC



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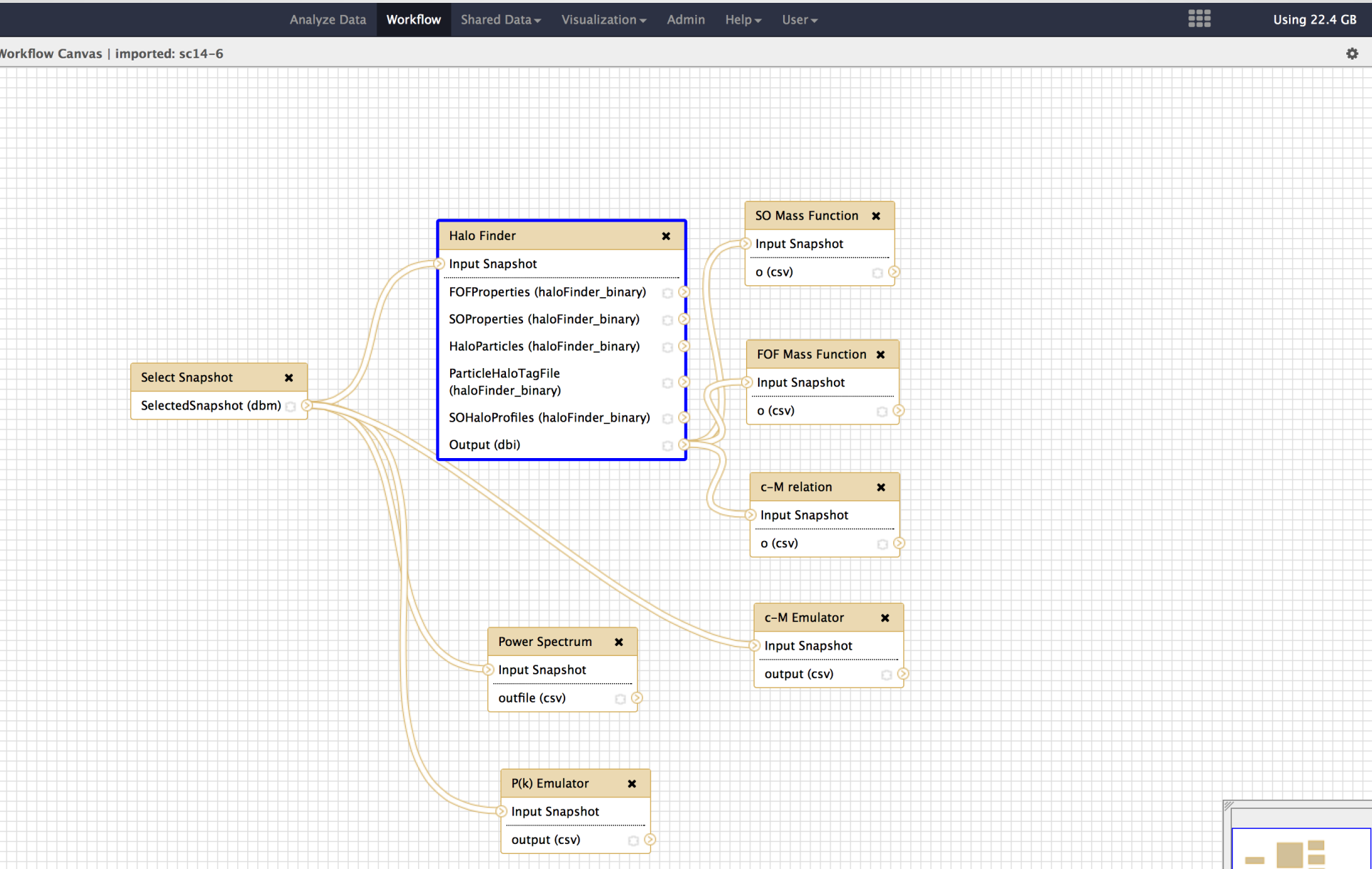

HACC: PDACS WORKFLOWS

Galaxy / PDACS

Analyze Data | Workflow | Shared Data | Visualization | Admin | Help | User

Using 8.1 GB

Tools

search tools

Get Data

- Upload File from your computer
- Upload Halo File into SciDB
- Select Snapshot from Coyote Universe Simulations
- DumpEnv Dump the environment variables

Halos - Simulation Data Analysis Tools

- Halo Finder FOF/SO Halo Finder
- c-M relation Measure c-M relation from the SO halo dataset
- FOF Mass Function Measure FOF mass function on FOF halo dataset
- SO Mass Function Measure SO mass function on SO halo dataset

Halos - Predictors

- c-M Emulator Predictor for the concentration-mass relation

2-point Functions - Simulation Data Analysis Tools

- Power Spectrum Measure matter power spectrum
- Power Spectrum in Redshift Space Measure matter power spectrum in redshift space
- Correlation Function Measure matter correlation function (FFT based)
- Correlation Function in Redshift Space Measure matter correlation function in redshift space (FFT based)

CAMB - tools

Cosmolike - tools

2-point Functions - Predictors

Conversion Tools

Query SciDB

Graph/Display Data

Workflows

- All workflows

```
# /global/project/projectdirs/hacc/PDACS/galaxy_dev_ravi/database/files/002/dataset_2362_files/dataset_2362.dat: 32 rank(s): 4x4x2
# physical coordinates: (0,0,0) -> (107.586,107.586,107.586)
# x variables: fof_halo_center_x [maybe ghost], fof_halo_mean_x [maybe ghost]
# y variables: fof_halo_center_y [maybe ghost], fof_halo_mean_y [maybe ghost]
# z variables: fof_halo_center_z [maybe ghost], fof_halo_mean_z [maybe ghost]
```

# fof_halo_count	fof_halo_tag	fof_halo_mass	fof_halo_center_x	fof_halo_center_y	fof_halo_center_z	fof_halo_mean_x	fof_halo_mean_y	fof_h
# rank 0: 0,0,0: 420 row(s)								
1790	9443857	1.985529e+12	5.086046e+00	3.098714e+00	5.199747e+00	5.095524e+00	3.105336e+00	5.1
997	7338515	1.105907e+12	3.779555e+00	5.599191e-01	4.801014e+00	3.741452e+00	4.712276e-01	4.7
1325	6037533	1.469736e+12	4.973934e+00	3.490682e+00	5.821113e+00	4.978521e+00	3.493268e+00	5.7
774	8653339	8.585474e+11	5.642964e+00	2.104293e+00	5.834346e+00	5.624816e+00	2.108796e+00	5.8
314	9973781	3.482996e+11	5.555581e+00	4.886257e+00	5.129282e+00	5.564182e+00	4.858309e+00	5.1
1979	4729363	2.195175e+12	4.974524e+00	4.822748e+00	5.003660e+00	4.958928e+00	4.802995e+00	5.0
427	8926225	4.736431e+11	5.339813e+00	4.871410e+00	4.551896e+00	5.322214e+00	4.875807e+00	4.5
874	4207120	9.694708e+11	3.844112e+00	5.341496e+00	5.516630e+00	3.855979e+00	5.350839e+00	5.4
326	8404524	3.616104e+11	4.362989e+00	5.412251e+00	1.021853e+01	4.349753e+00	5.403362e+00	1.0
546	13114922	6.056419e+11	6.715230e+00	3.700559e+00	1.000101e+01	6.692319e+00	3.697410e+00	1.0
503	13382205	5.579449e+11	6.705385e+00	4.437534e+00	1.352914e+01	6.705081e+00	4.453703e+00	1.3
783	11541572	8.685305e+11	6.738194e+00	3.621688e+00	1.356019e+01	6.729925e+00	3.641054e+00	1.3
1018	6821430	1.129200e+12	5.465863e+00	2.203966e+00	1.187279e+01	5.442614e+00	2.193952e+00	1.1
931	12848187	1.032697e+12	6.673181e+00	2.343091e+00	1.330826e+01	6.699861e+00	2.348076e+00	1.3
314	9177152	3.482996e+11	6.370151e+00	1.868648e+00	1.277165e+01	6.356579e+00	1.840329e+00	1.2
344	13369403	3.815766e+11	6.703818e+00	1.679048e+00	1.326414e+01	6.676252e+00	1.708056e+00	1.3
535	5770817	5.934403e+11	3.738639e+00	1.446123e+00	1.161667e+01	3.713626e+00	1.464892e+00	1.1
1541	7340601	1.709330e+12	4.266432e+00	1.170475e+00	1.122371e+01	4.261847e+00	1.176999e+00	1.1
487	8912960	5.401971e+11	6.267961e+00	7.298886e-01	1.247528e+01	6.232492e+00	7.394629e-01	1.2
414	10485314	4.592230e+11	6.449651e+00	1.066418e+00	1.294445e+01	6.412864e+00	1.047645e+00	1.2
306	9181737	3.394257e+11	5.146138e+00	2.849011e+00	9.293453e+00	5.130563e+00	2.841170e+00	9.3
564	12076051	6.256082e+11	8.641116e+00	5.911632e+00	3.646091e+00	8.654634e+00	5.903877e+00	3.6
485	13380113	5.379786e+11	7.939690e+00	5.496223e+00	3.655312e+00	7.932212e+00	5.495975e+00	3.6
908	13644798	1.007185e+12	8.101008e+00	5.688502e+00	3.014820e-01	8.108429e+00	5.685754e+00	2.8
372	13385734	4.126352e+11	8.465195e+00	5.629597e+00	1.517687e+00	8.475306e+00	5.610163e+00	1.5
452	9977347	5.013739e+11	7.348852e+00	5.343278e+00	9.729415e-01	7.346080e+00	5.333977e+00	9.6
469	11543056	5.202309e+11	7.010191e+00	3.567172e+00	3.136586e+00	7.035797e+00	3.590554e+00	3.1
339	14951434	3.760304e+11	1.027589e+01	4.206992e+00	2.426530e+00	1.027426e+01	4.187965e+00	2.4
364	18098193	4.037613e+11	1.221137e+01	4.765515e+00	2.899142e+00	1.221687e+01	4.772936e+00	2.8
411	11296797	4.558953e+11	8.606277e+00	9.387453e+00	6.617541e+00	8.561678e+00	9.388859e+00	6.6
307	13131288	3.405349e+11	9.014297e+00	9.553939e+00	6.650502e+00	8.973190e+00	9.589107e+00	6.6
355	16277547	3.937782e+11	1.125426e+01	1.069792e+01	1.060614e+01	1.125834e+01	1.069577e+01	1.0
360	18114092	3.993243e+11	1.282260e+01	1.047128e+01	1.036338e+01	1.282386e+01	1.043926e+01	1.0
313	14181924	3.471903e+11	9.623220e+00	1.018634e+01	7.423010e+00	9.626452e+00	1.015729e+01	7.4
308	6049833	3.416442e+11	3.796223e+00	7.432703e+00	9.375122e+00	3.773252e+00	7.397883e+00	9.4
485	1592858	5.379786e+11	1.712599e+00	8.739969e+00	7.021303e+00	1.701178e+00	8.743618e+00	7.0
1119	2640943	1.241233e+12	2.566047e+00	8.470745e+00	1.161239e+01	2.554385e+00	8.473631e+00	1.1
346	2126892	3.837951e+11	8.282121e-01	1.151152e+01	1.076415e+01	8.105011e-01	1.151360e+01	1.0
1257	1864226	1.394307e+12	3.346745e-01	1.177479e+01	9.089565e+00	3.685234e-01	1.175060e+01	9.1
603	4488229	6.688683e+11	1.854487e+00	1.248918e+01	8.865780e+00	1.854900e+00	1.249672e+01	8.8
324	6844939	3.593919e+11	4.726613e+00	1.302508e+01	2.578389e+00	4.746942e+00	1.302327e+01	2.5
946	1859578	1.049336e+12	2.360930e+00	1.061170e+01	8.192973e-01	2.337552e+00	1.058146e+01	8.5
627	5288466	6.954899e+11	3.620457e+00	1.989519e+01	3.070848e+00	3.615792e+00	1.987287e+01	3.0

History

Copy of 'for Tom' shared by 'madduri@nersc.gov' (active items only)

771.7 MB

- 16: P(k) Emulator
- 15: P(k) Emulator
- 13: FOF Properties.ascii
- 12: cm-relation on M001_L180_G001_snapshot_0.2857 - HaloFinder
- 11: SOD Mass Function on M001_L180_G001_snapshot_0.2857 - HaloFinder
- 10: Particle and Halo Tags.ascii
- 9: FOF Mass Function on M001_L180_G001_snapshot_0.2857 - HaloFinder
- 8: c-M Emulator on data

HACC - COSMOTOOLS IN-MEMORY WORKFLOWS

- Configurable in-situ analysis framework
- Simulation configuration specifies analyses that should be performed between time steps during the simulation, and their parameters
- On execution, particles are passed from the simulation to analysis routines for processing
- When finished, the simulation proceeds to the next timestep
- Leverages in-memory data
  - before data reduction, potentially the only opportunity to analyze this data
  - efficient: avoids the need to subsequently load data from disk
- Delivers analysis results during (long) simulation run

WHY USE WORKFLOWS?

- Simplifies computational campaigns
  - Job scheduling
  - Data management
- Improves error handling and recovery (retries)
- Provides provenance/reproducibility

QUESTIONS?