The Flux framework: overcoming scheduling and management challenges of exascale workflows

RADIUSS Tutorial on AWS
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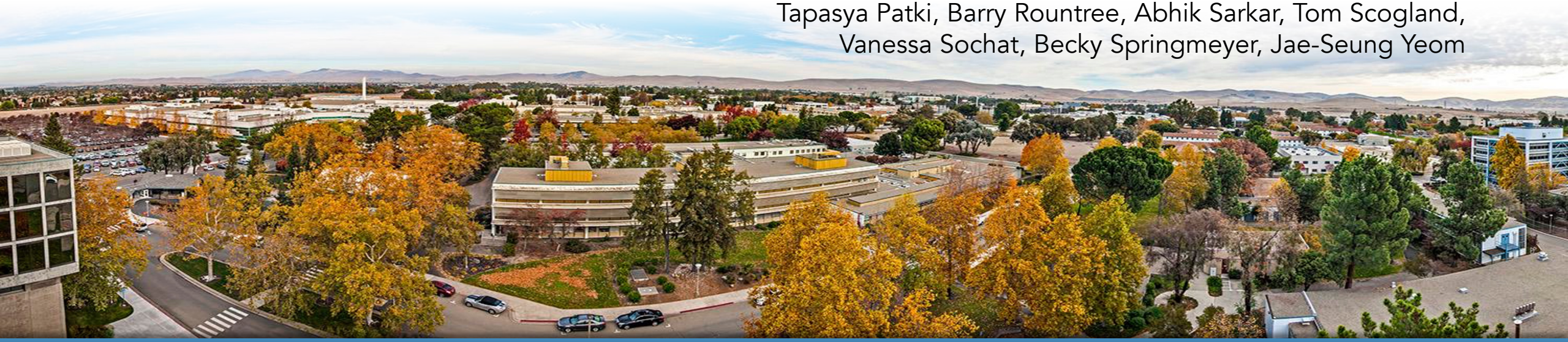

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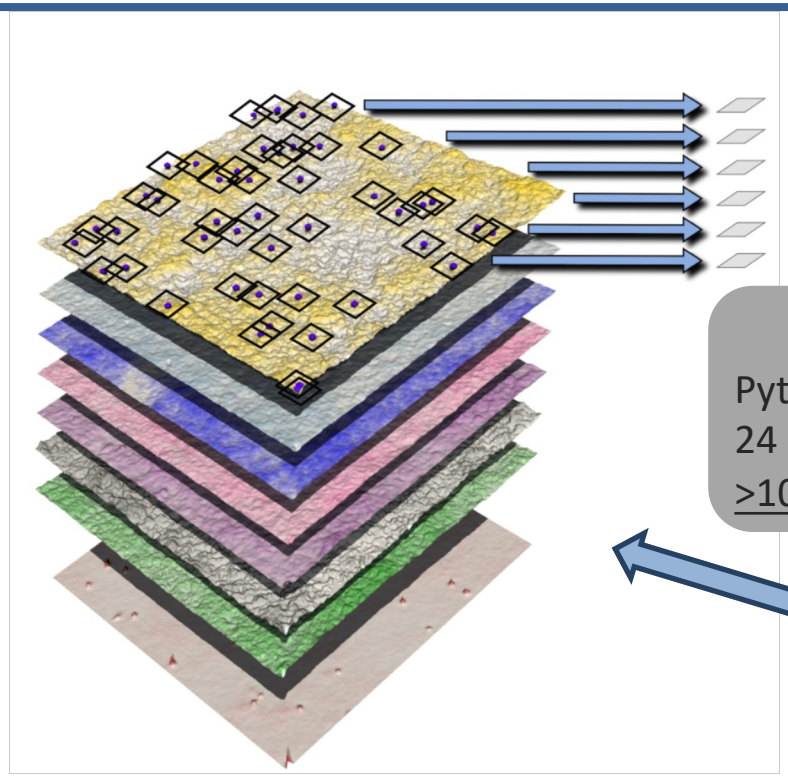
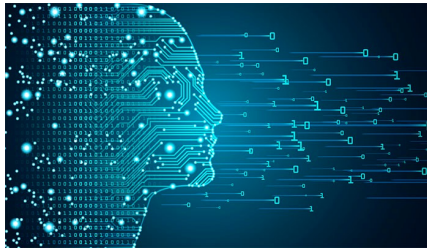
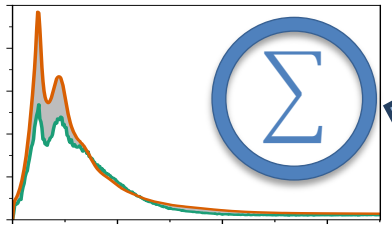
Sierra pre-exascale system is a wakeup call (MuMMI).

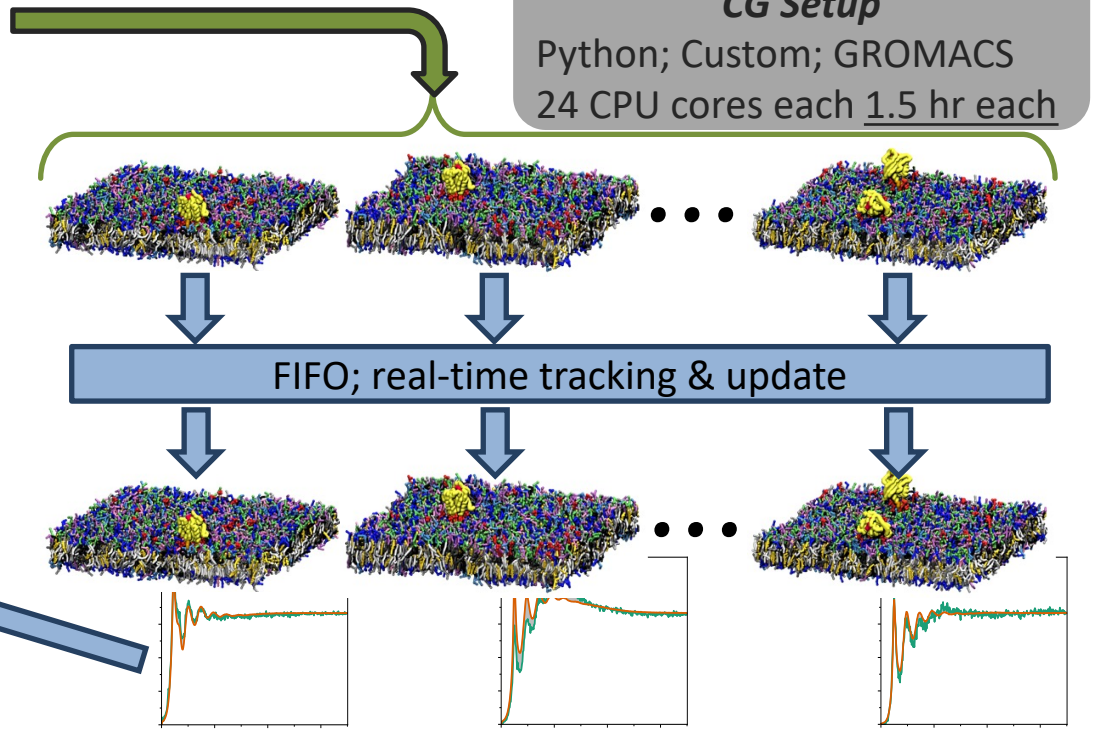




ML-based Selection
Python; ML frameworks; FAISS
24 CPU cores
>1000 decisions per minute



CG Setup
Python; Custom; GROMACS
24 CPU cores each 1.5 hr each



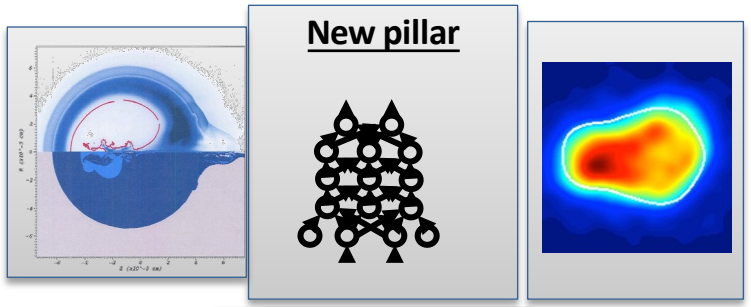
Single Macro Simulation
C++ (with MPI); MOOSE; ddcMD
24 CPU cores/node; 2400 MPI tasks
242 GB per day

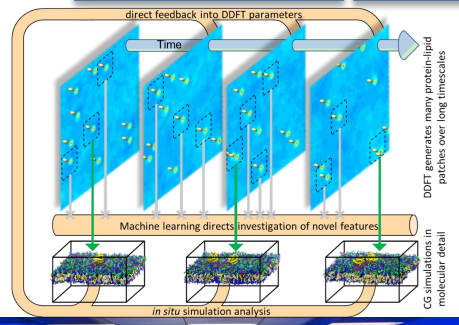
Analysis Aggreg. & Feedback
Python; Custom
24 CPU cores
120,000 reads per cycle

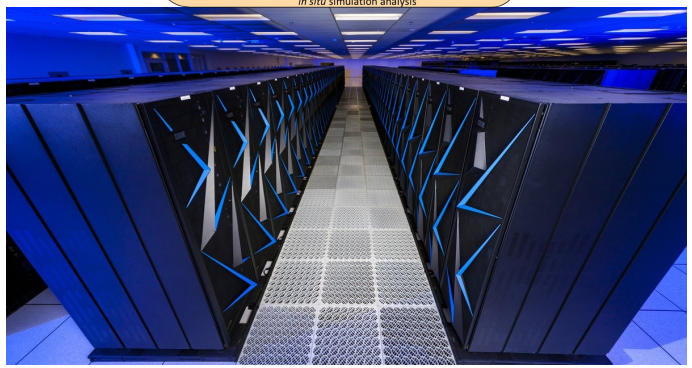
CG Simulation
C++ (with CUDA); ddcMD
1 GPU + 1 CPU core each
1.04 μs and ~6.5 GB per day

In situ CG Analysis
Python; Custom
3 CPU cores each
>2K frames per day

Trends towards complex workflows, extreme resource heterogeneity, and converged computing render traditional workload managers increasingly ineffective.

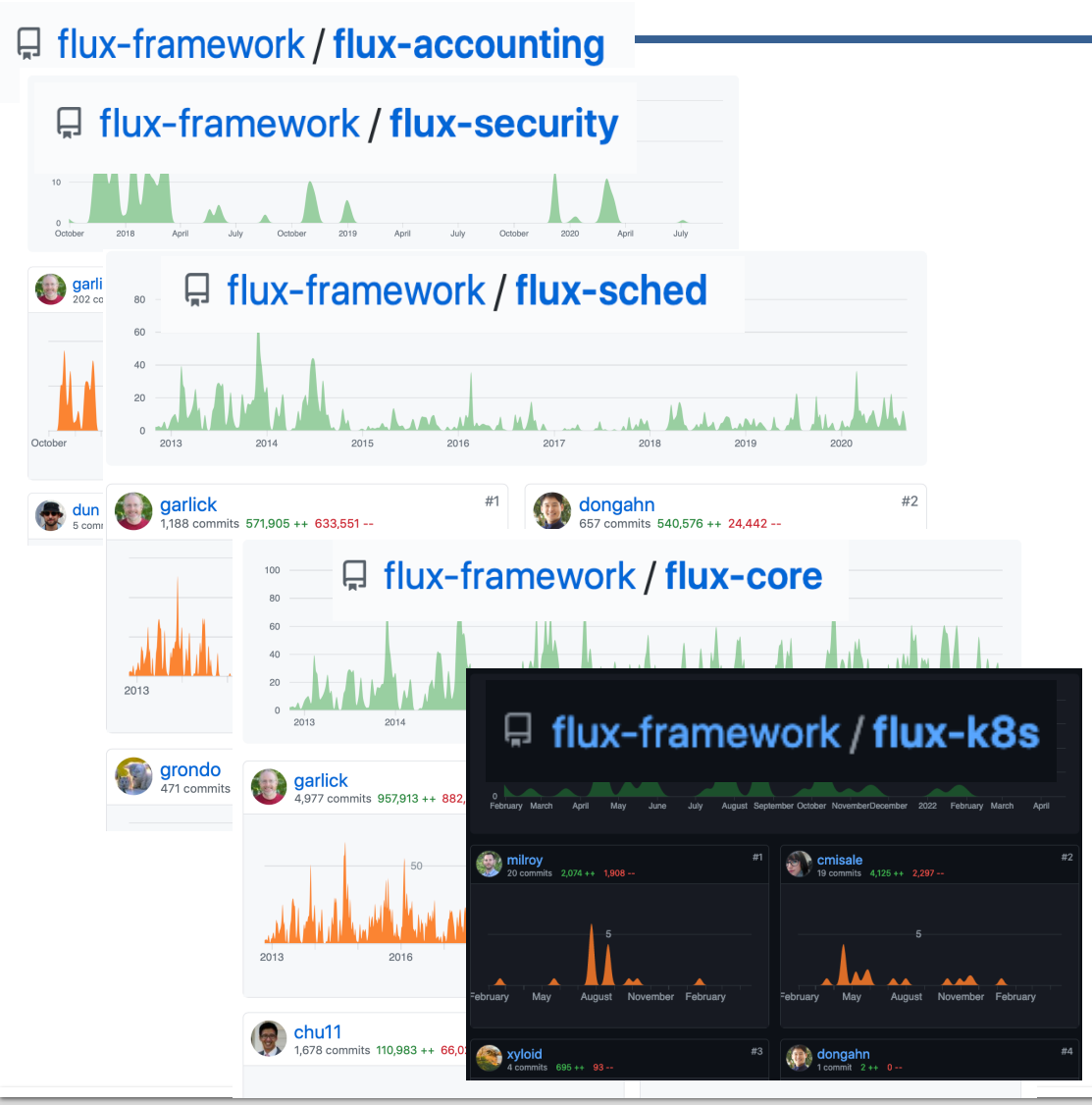






- Co-scheduling
- Job throughput
- Job communication/coordination
- Portability
- Extremely heterogenous resources

Flux solves key technical problems that emerge from these trends.

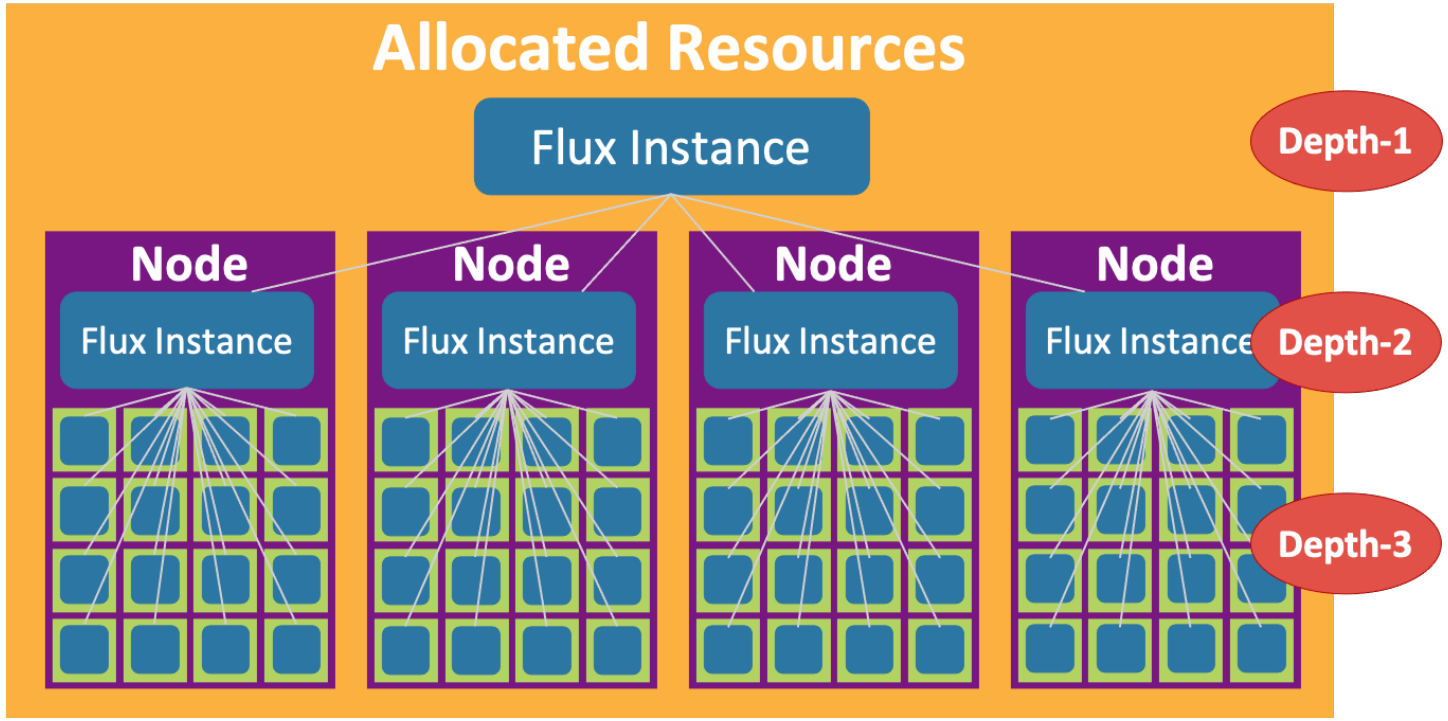


- Open-source project in active development at flux-framework GitHub organization
  - Multiple projects: flux-core, -sched, -security, -accounting, -k8s etc.
  - Over 15 contributors including some principal engineers behind Slurm
- Single-user and System instance modes
  - Single-user mode in production for about 4 years
  - Multi-user mode debuting on LLNL Linux clusters
- Plan of record for **LLNL El Capitan** exascale system

flux

2021 R&D 100 WINNER

Flux's fully hierarchical resource management solves primary deficiencies of the conventional approach.

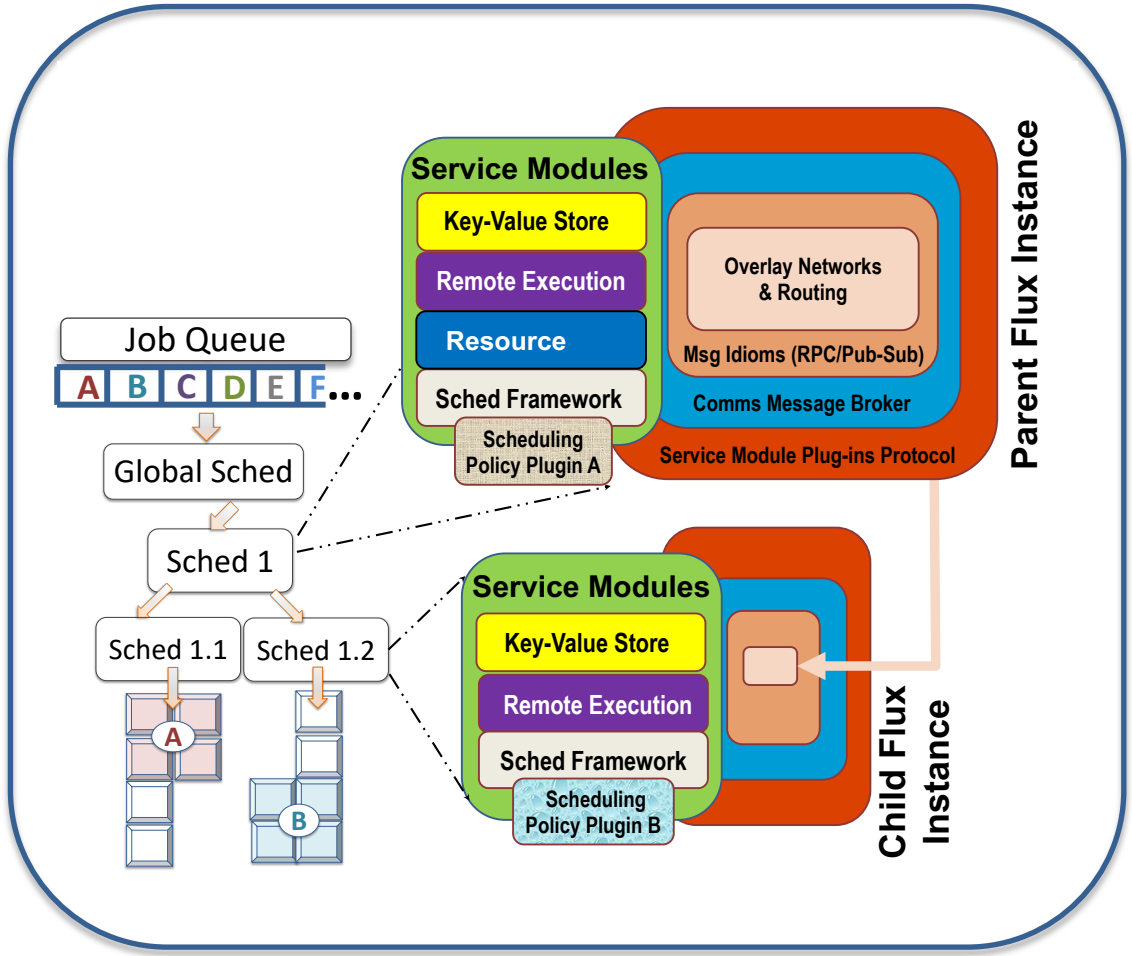


"Fractal scheduling" mitigates centralized scheduler bottleneck

- handles high throughput
- job steps needn't hit central sched

- Full workflow-enablement support
  - Via hierarchical resource subdivision
  - Sub-resource manager per subdivision with service specialization
  - E.g., at LLNL: MuMMI, AHA MoleS, UQP
- Capable of managing resources from almost anywhere
  - Bare metal resources, virtual machines in the cloud, HPC resources allocated by another workload manager
  - Workflows only need to program to Flux
- Provide rich and well-defined interfaces
  - Facilitate communications and coordination among tasks within a workflow
  - CLI, Python, C

Flux is architected to embody our fully hierarchical scheduling model.



Flux framework

Techniques

Scheduler Specialization

Scheduler Parallelism

Rich API set

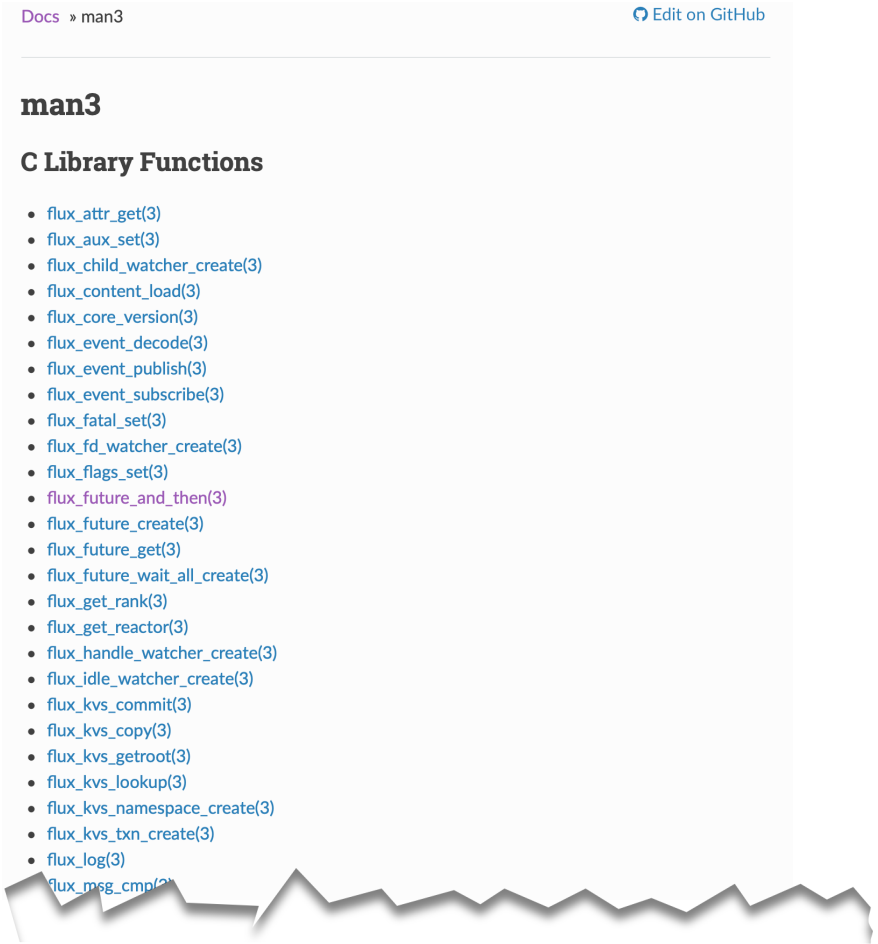
Consistent API set

Challenges

- Co-scheduling challenge
- Job throughput challenge
- Job communication/coordination challenge
- Portability challenge

A rich set of well-defined APIs enables easy job coordination and communication.

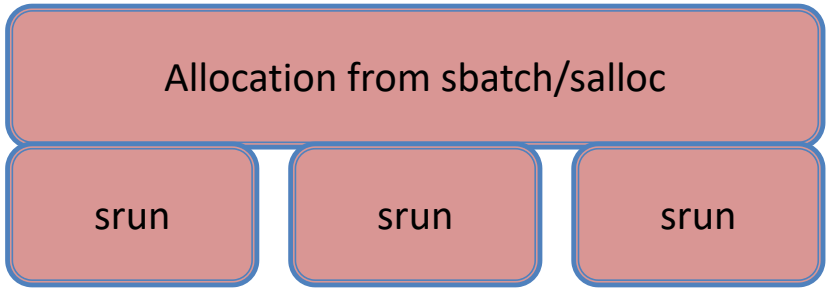
- Jobs in ensemble-based simulations often require close coordination and communication with the scheduler as well as among them.
  - Traditional CLI-based approach can be slow and cumbersome.
  - Ad hoc approaches (e.g., many empty files) can lead to many side effects.
- Flux provides well-known communication primitives.
  - Pub/sub, request-response, and send-recv patterns
- High-level services
  - Key-value store (KVS) API
  - Job API (submit, wait, state change notification, etc)
- Flux's APIs are consistent across different platforms



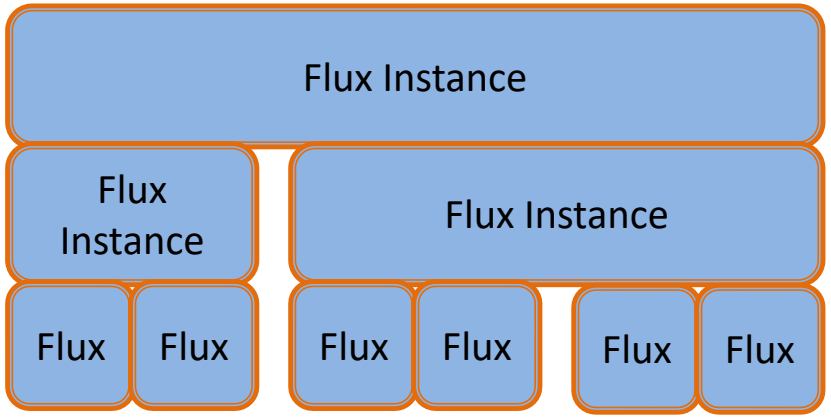
https://flux-framework.readthedocs.io/projects/flux-core/en/latest/index.html

Flux's hierarchical scheduling makes managing and scheduling complex allocations easier.

- Significant start-up cost for running on new resource manager (portability)
  - Learn to use the manager
  - Translate batch script logic
- Traditional resource managers can't subdivide allocations (hierarchy)
  - Slurm has two levels: **`sbatch`** creates allocation, **`srun`** launches parallel task
  - **`sbatch`** from inside an allocation starts a separate allocation
- Flux's hierarchical scheduling provides a natural solution
  - Request one large allocation and partition schedulable resource subgroups



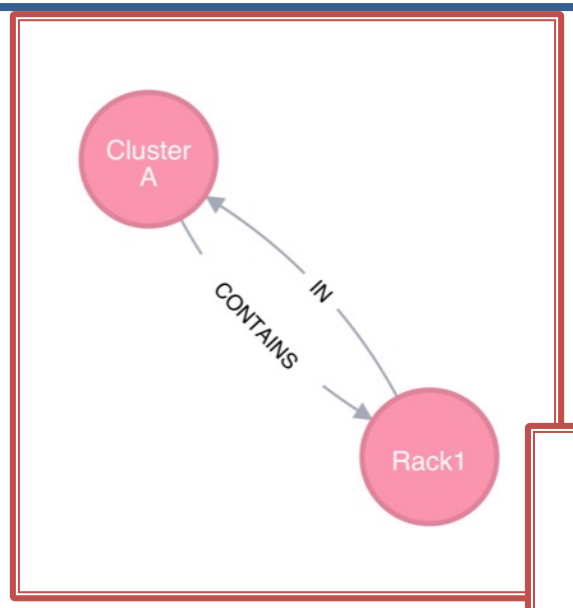
The Slurm hierarchy



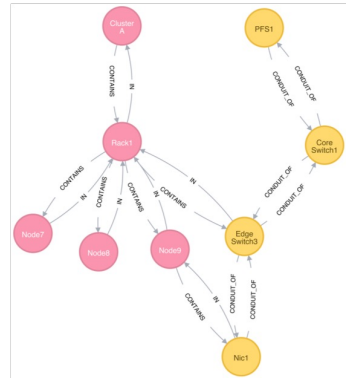
One possible Flux hierarchy

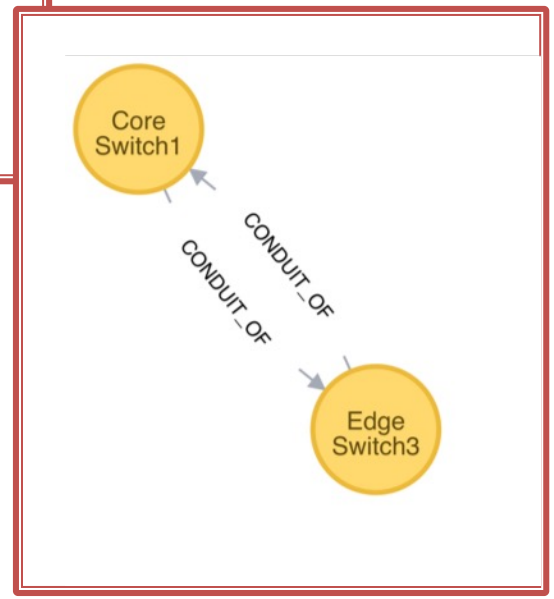
Flux pioneers and uses graph-based scheduling to manage complex combinations of extremely heterogenous resources.

- Traditional resource data models are largely ineffective for resource heterogeneity
  - designed when systems were simpler
  - node-centric models
- Elevate resource relationships (edges) to an equal footing with resources (vertices)
- Complex scheduling can be expressed without changing the scheduler code
- Rich and well-defined C and C++ API for graph traversal and allocation



Containment subsystem





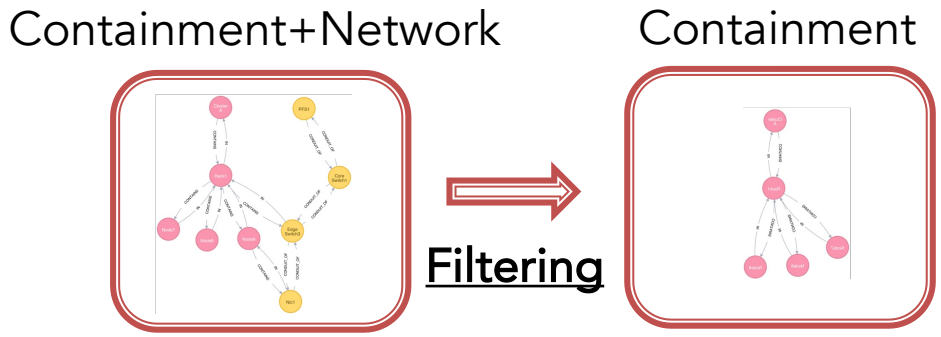
Network connectivity subsystem

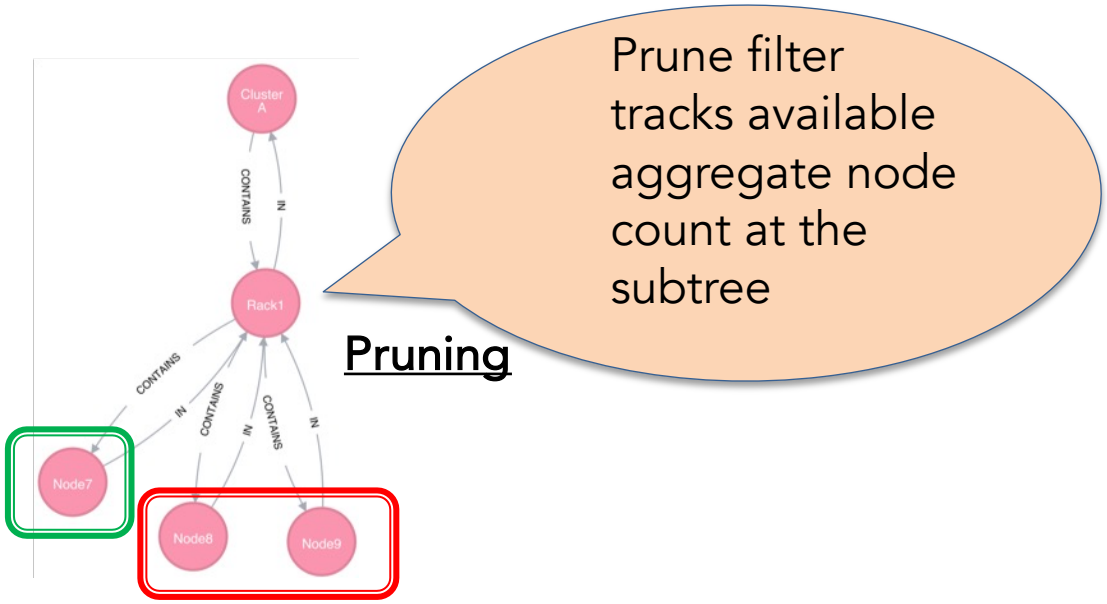
We use graph filtering and pruned searching to manage the graph complexity and optimize our graph search.

- The total graph can be quite complex
  - Two techniques to manage the graph complexity and scalability

1. Filtering reduces graph complexity
   - The graph model needs to support schedulers with different complexity
   - Provide a mechanism by which to filter the graph based on what subsystems to use

2. Pruned search increases scalability
   - Fast RB tree-based planner is used to implement a pruning filter per each vertex.
   - Pruning filter keeps track of summary information (e.g., aggregates) about subtree resources.
   - Scheduler-driven pruning filter update



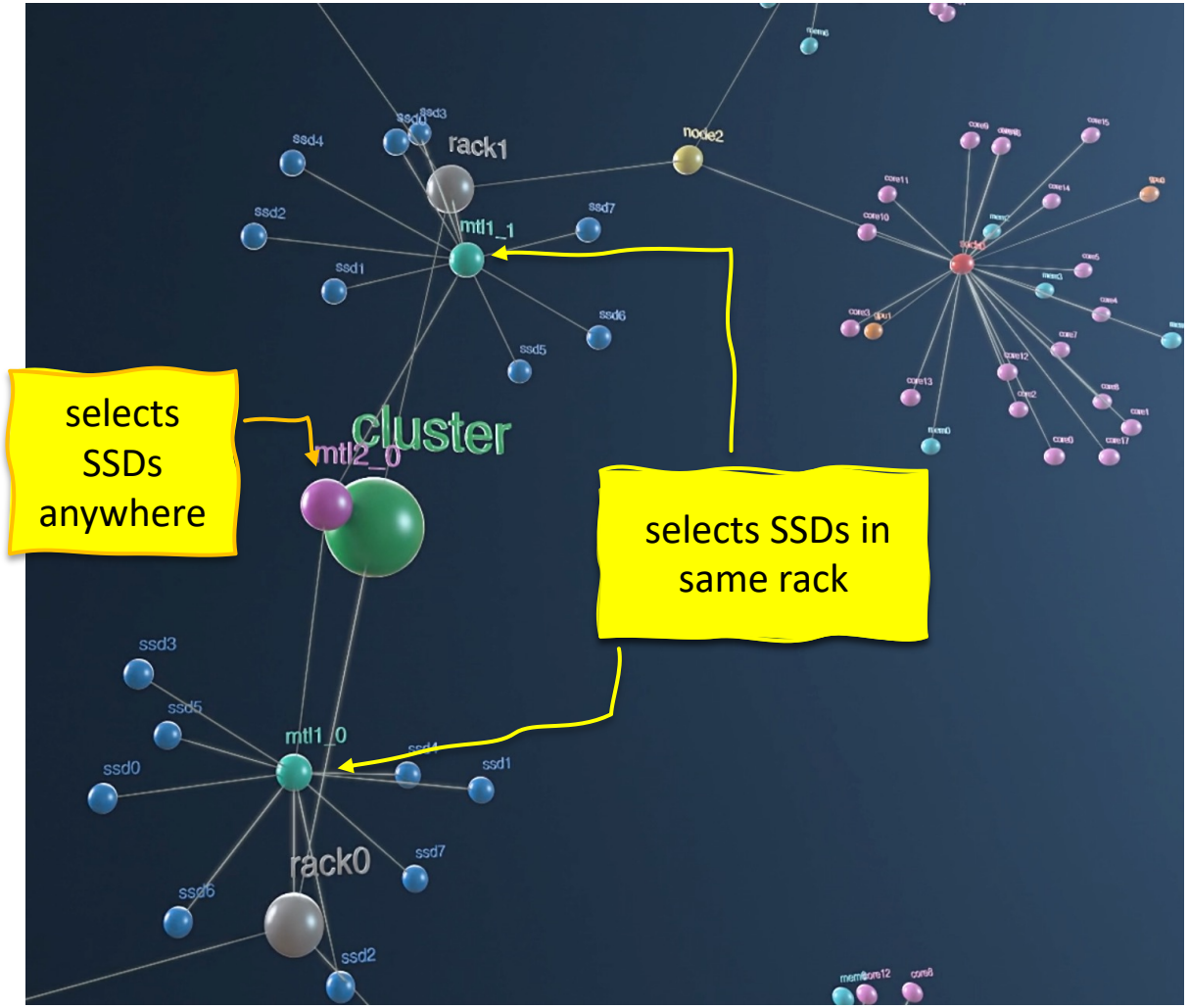


Flux's graph-oriented canonical jobspec allows for a highly expressive resource request specification.

- Graph-oriented resource requirements
  - Express the resource requirements of a program to the scheduler
  - Express program attributes such as arguments, runtime, and task layout to the execution service
- cluster→ rack[2]→slot[3]→node[1]→socket[2]→core[18]
- ***slot*** is the only non-physical resource type
  - Represent a schedulable place where program processes will be spawned and contained
- Tasks section references slot and defines command

```
1  version: 1
2  resources:
3    - type: cluster
4      count: 1
5      with:
6        - type: rack
7          count: 2
8          with:
9            - type: slot
10             label: myslot
11             count: 3
12             with:
13               - type: node
14                 count: 1
15                 with:
16                   - type: socket
17                     count: 2
18                     with:
19                       - type: core
20                         count: 18
21
22 # a comment
23 attributes:
24   system:
25     duration: 3600
26 tasks:
27   - command: app
28     slot: myslot
29     count:
30       per_slot: 1
```

Fluxion graph approach solves the critical scheduling need for El Capitan's Rabbit multi-tired storage.

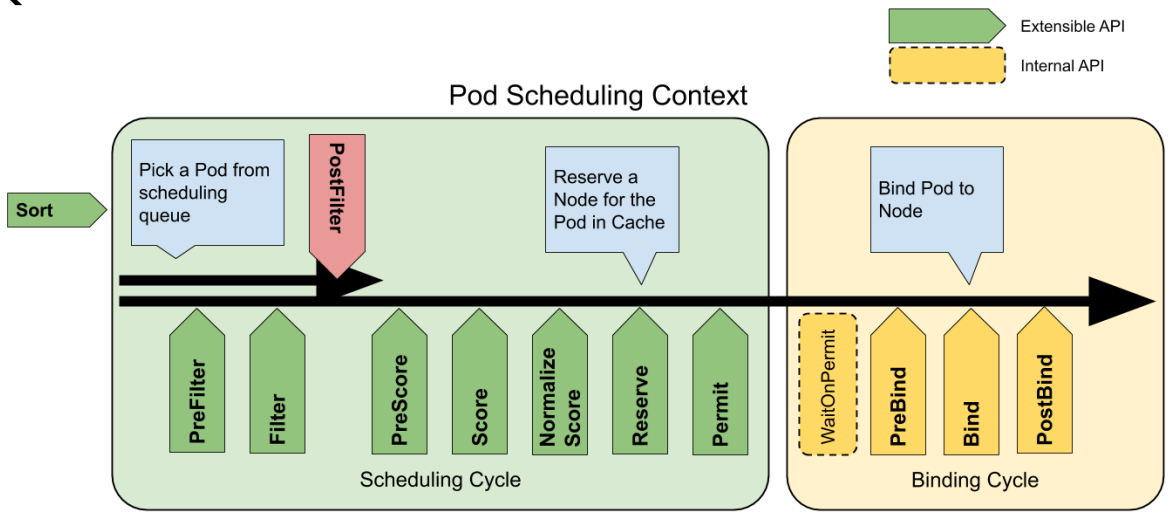


- Schedule SSDs in each rack
  - mount as node-local storage to compute in same rack
  - used to build ephemeral Lustre
  - deemed too difficult for traditional schedulers
- Easily enabled by Fluxion; no code change
- End-to-end job state transition
  - DataWarp/Rabbit mock service containers by HPE
  - Uses Kubernetes CRD

Team formed industry collaborations to tackle converged computing challenges and contribute to community.

We bring complementary backgrounds in HPC, cloud, and performance-oriented orchestration

- LLNL LDRD team
- **IBM T.J. Watson Research Center**: T. Elengikal, M. Drocco, C. Misale, Y. Park
- **Red Hat**: E. Arango Gutierrez
- Newly added **AWS**: E. Bollig, M. Hugues, H. Poxon, L. Wofford
- **Integrate Fluxion into Kubernetes via** KubeFlux



Accessing the hands-on tutorial

- Using our EC2 instance at **https://tutorial.flux-framework.org**
  - Choose a unique username (if not, you'll be sharing with someone else)
  - Password: **<password>**
  - Double-click **radiuss-aws-flux.ipynb** to start
    - To execute a cell in JupyterLab: **Shift+Enter**
  - It's a shared instance- please don't run computationally demanding tasks in your container
  - The instance will disappear shortly after the tutorial
- Running locally with Docker:
  - **git clone https://github.com/flux-framework/Tutorials.git**; README in the 2022-RADIUSS-AWS directory