# Using Pilot Systems to Execute Many Task Workloads on Supercomputers

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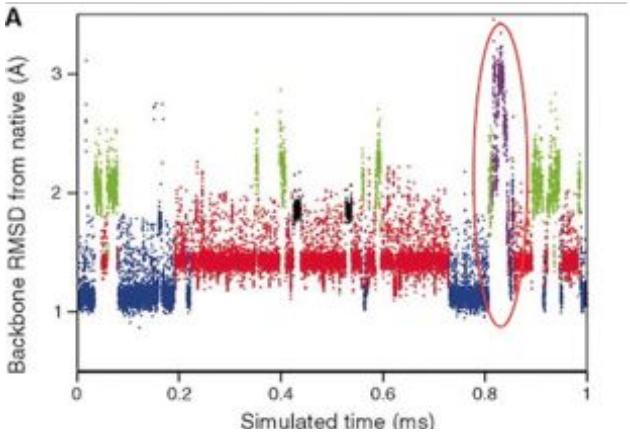
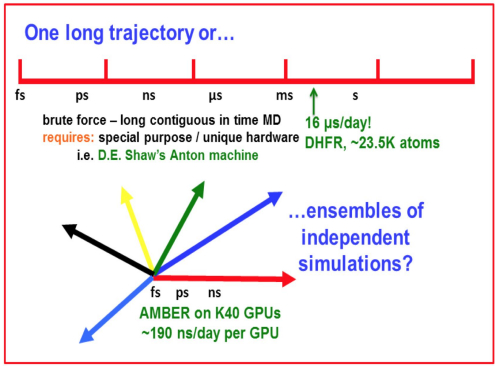
# Outline

- Why Execute Many Task Workloads?
  - Importance of applications with “more than a single task” (workflows)
  - Workflows aren’t what they used to be!
- Building Blocks approach to Workflow Middleware
  - What is a Pilot System?
  - Pilot Abstraction (P* Model)
- RADICAL-Pilot: A Pilot-System for HPC Workflows
  - Programming and Execution Model
  - Implementation on Cray systems
  - Performance characterisation

# Biomolecular (MD) Simulations: Context

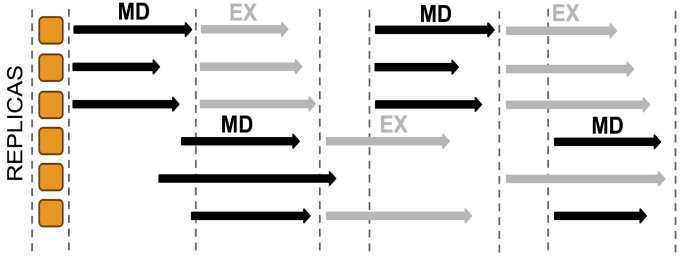
- Larger biological systems
  - Requires **weak** scaling
- Long time scale problem
  - Requires **strong** scaling
  - DE Shaw special purpose computer (Anton)
- Gap between weak and strong scaling will grow
  - Scaling challenges > than either single-partition strong and weak scaling.
  - Ensemble simulations
- **Ensemble-based Adaptive Algorithms:**
  - Intermediate data used to determine next stages
  - Improved simulation efficiency (MSM: $10^3$)

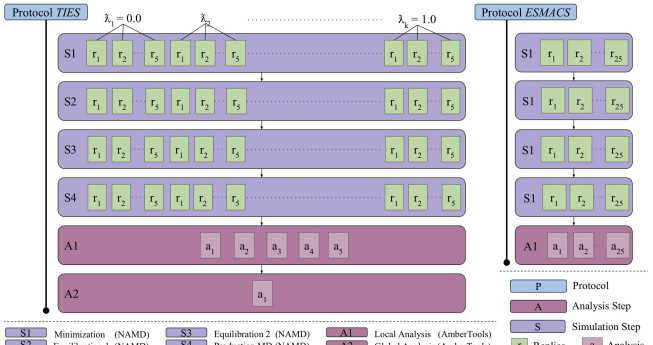


# Biomolecular Adaptive Algorithms

- Many biomolecular **sampling algorithms** formulated as adaptive algorithms/methods:
  - Replica-exchange
  - Expanded Ensemble
  - …
- Types of Adaptivity:
  - Task parameter(s), order, …
  - Task count, iteration count, ….
- **Adaptive logic separate from the MD code**
  - Each task is an independent simulation
  - Task often interact (not a “bag-of-tasks”); degrees and levels of coupling

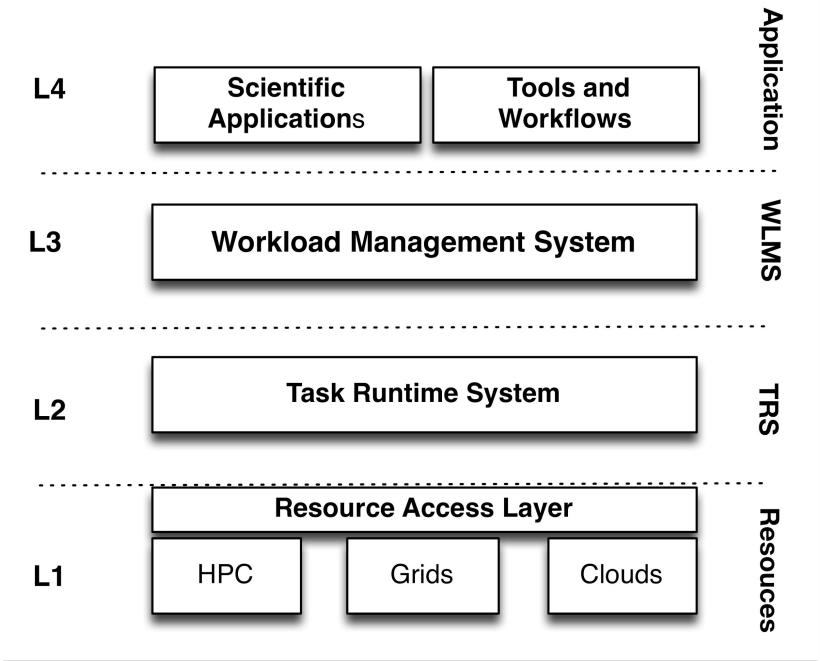


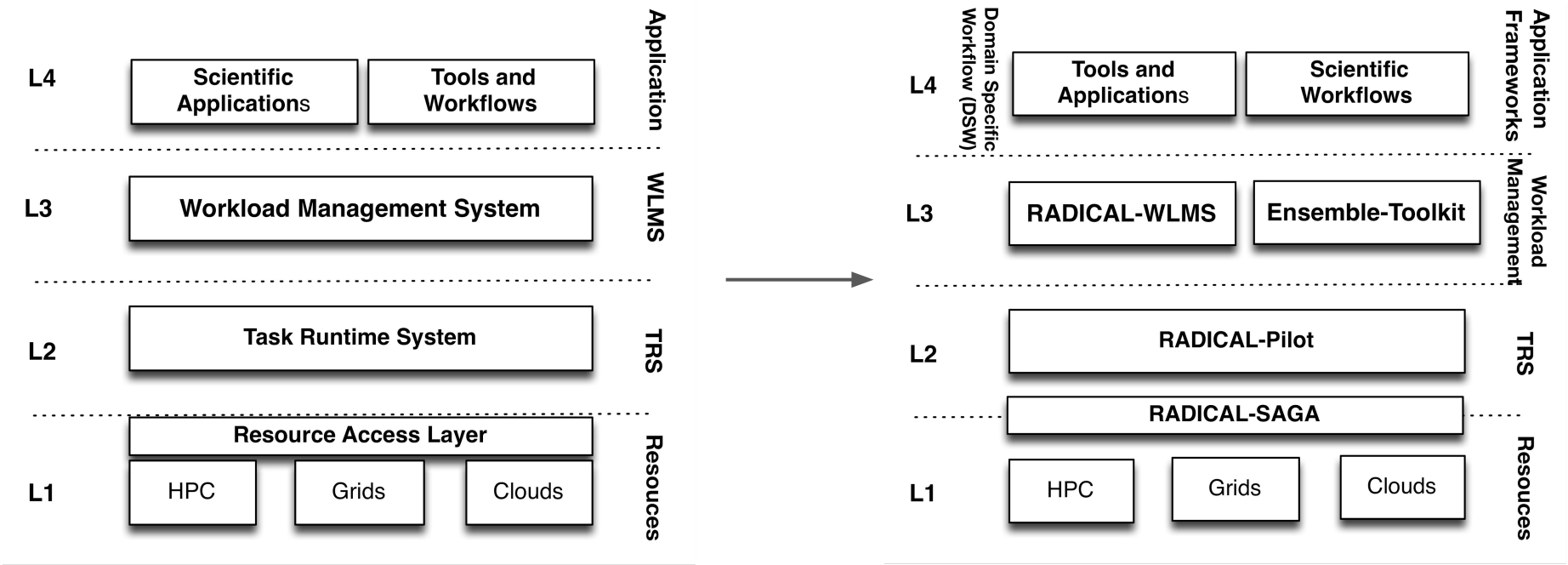
# Why a “Fresh Perspective” to Workflows?

- Initially “Monolithic” Workflow systems with “end-to-end” capabilities
  - Workflow systems were developed to support “big science” projects.
  - Software infrastructure was “fragile”, unreliable, missing services
- Workflows aren’t what they used to be!
  - More pervasive, sophisticated but no longer confined to “big science”
  - Prevent vendor lock-in
  - **Extend traditional focus from end-users to workflow tool developers!**
- Building Blocks (BB)  permit workflow tools and applications can be built
  - Diverse “design points”; unlikely “one size fits all”
  - Last mile distinction → proliferation of workflow systems vs single system

# Developing Workflow Tools Using Building Blocks



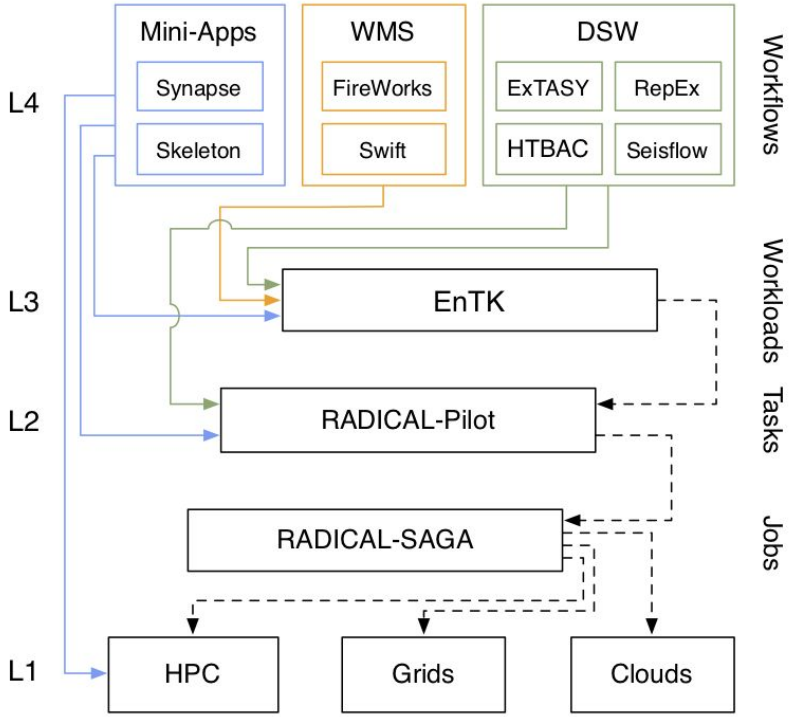
# RADICAL-Cybertools: Building Blocks for Workflows




- BB to support workflows, and the development of workflow tools
- A “laboratory” for testing ideas, support production science
- Stand alone, as well as vertical integration and horizontal extensibility

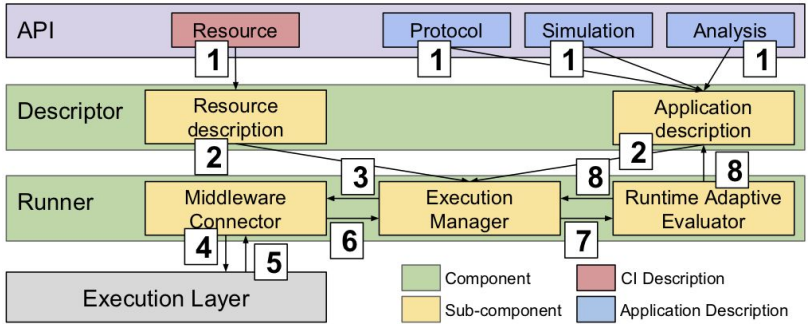
# RADICAL-Cybertools: Building Blocks for Workflows

- A “laboratory” while supporting production grade workflows **and** workflow tools.
  - Consistent with HPC & scale
- **Integrate with existing tools:**
  - Swift, Fireworks, PanDA, Binding Affinity Calculator (BAC)
  - Distinct points of integration, vertical integration and horizontal extensibility
  - Need “faster” start, “scalable” (more tasks) and “better” (resource utilization)
- **Novel tools and libraries:**
  - ExTASY, RepEx, **HTBAC**, Seisflow,..



# HTBAC: High-throughput Binding Affinity Calculator

- Python library for defining and executing ensemble-based biosimulation protocols
  - Protocols expressed and implemented using HTBAC's API
  - HTBAC utilizes RADICAL-Cybertools: **EnTK and RP**
- Implemented ESMACS and TIES protocols at scale
- Define additional adaptivity parameters that are passed down to the underlying runtime system.

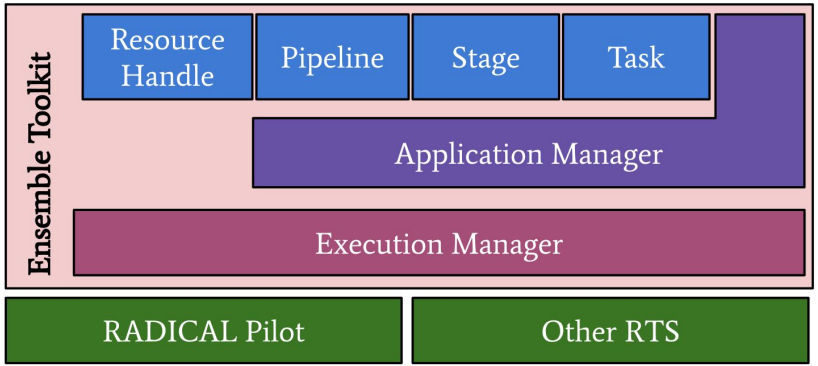



(1) **TIES** (alchemical **protocol**) employs enhanced sampling at each lambda window to yield reproducible, accurate and precise relative binding affinities.

(2) **ESMACS** (endpoint **protocol**) is a computationally cheaper, but less rigorous method, it is used to directly compute the binding strength of a drug to the target protein from MD simulations (as opposed to differences in affinity).

# RADICAL-EnTK: Building Blocks for Workflows

- **Ensemble Toolkit (EnTK):** Toolkit to manage complexity of resource acquisition and task execution for ensemble based applications.
- **Design:**
  - User facing components (blue)
  - Workflow management components (purple) to manage the execution order of the individual tasks of the application
  - Workload management components (red) to manage resources and task execution via a runtime system (green)
- **Integrated with other tools:**
  - HTBAC, Replica-Exchange, ...



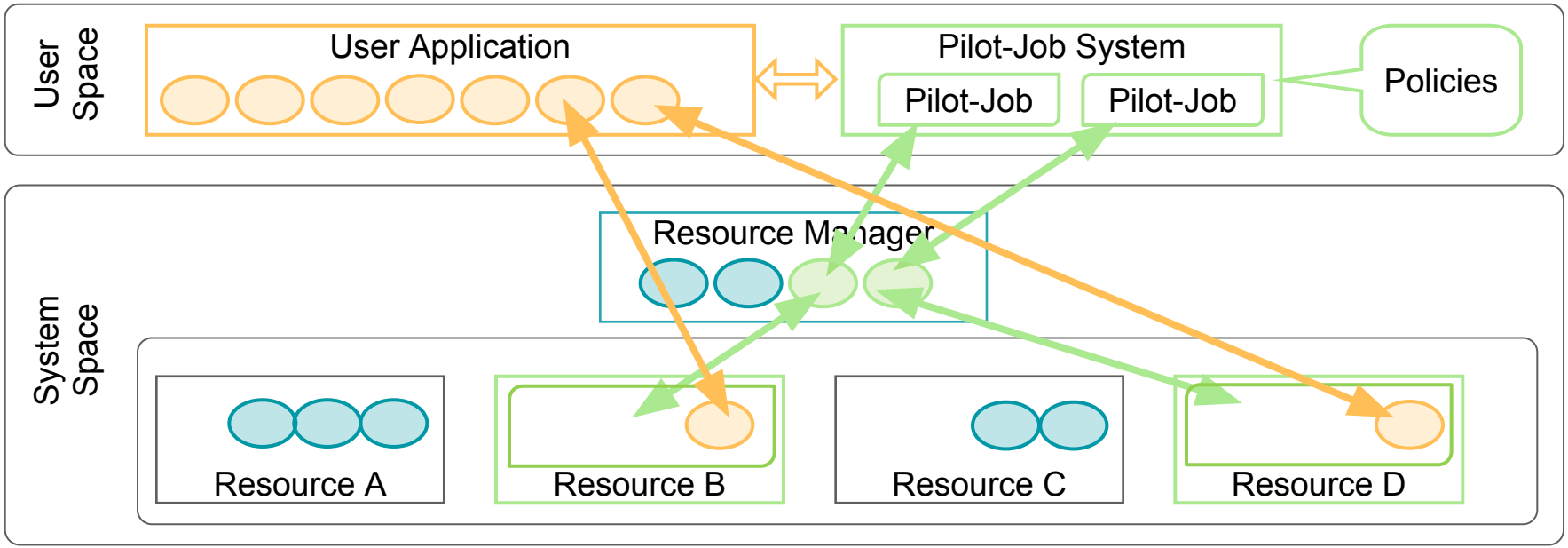

```
# Add post-exec to the Stage
p = Pipeline()
s1 = Stage()
...     # Define tasks and add them
...     # to Stage 's1'
s1.post_exec = {
                    # 'func_condition' operates on
                    # intermediate results to produce a
                    # boolean output
                    'condition': func_condition,

                    # 'func_on_true' is executed when the
                    # condition is True, e.g., adds another
                    # Stage 's2' to Pipeline 'p'
                    'on_true': func_on_true,

                    # 'func_on_false' is executed when the
                    # condition is False, e.g., returns
                    # without any adaptation
                    'on_false': func_on_false
                }    # Add Stage 's1' to Pipeline 'p'
```

Listing 1: Example of the enhanced EnTK API with post-execution properties to describe the adaptation to be performed after the execution of a Stage

# Pilot Abstraction: Schematic

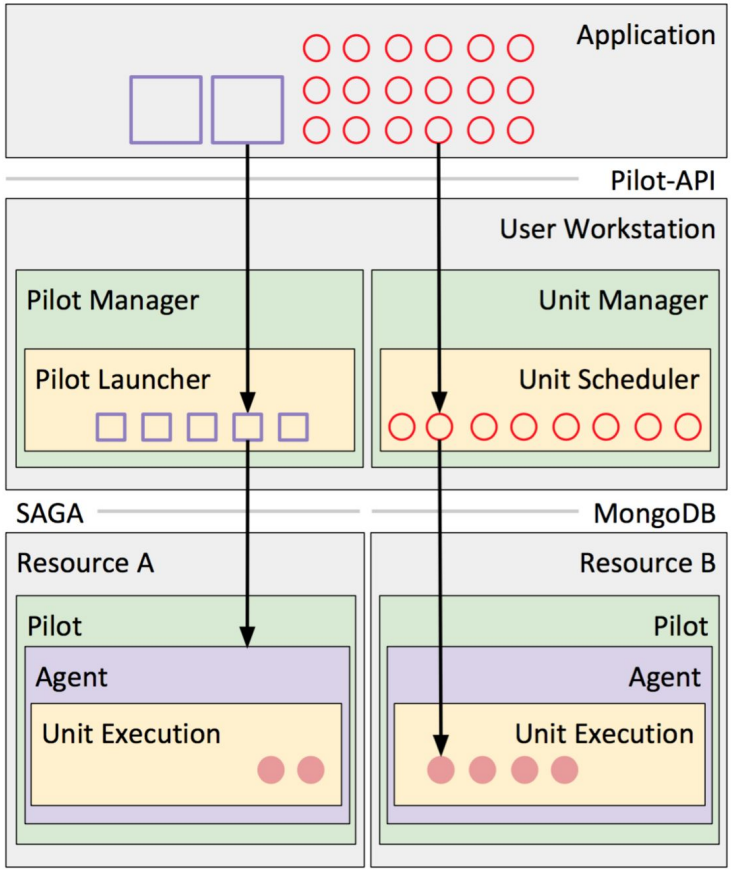
A system that generalizes a placeholder job to allow application-level control of acquired resources via a scheduling overlay.

- Decouples workload from resource management
- Enables the fine-grained “slicing and dicing” of resources
- Build higher-level frameworks without explicit resource management.



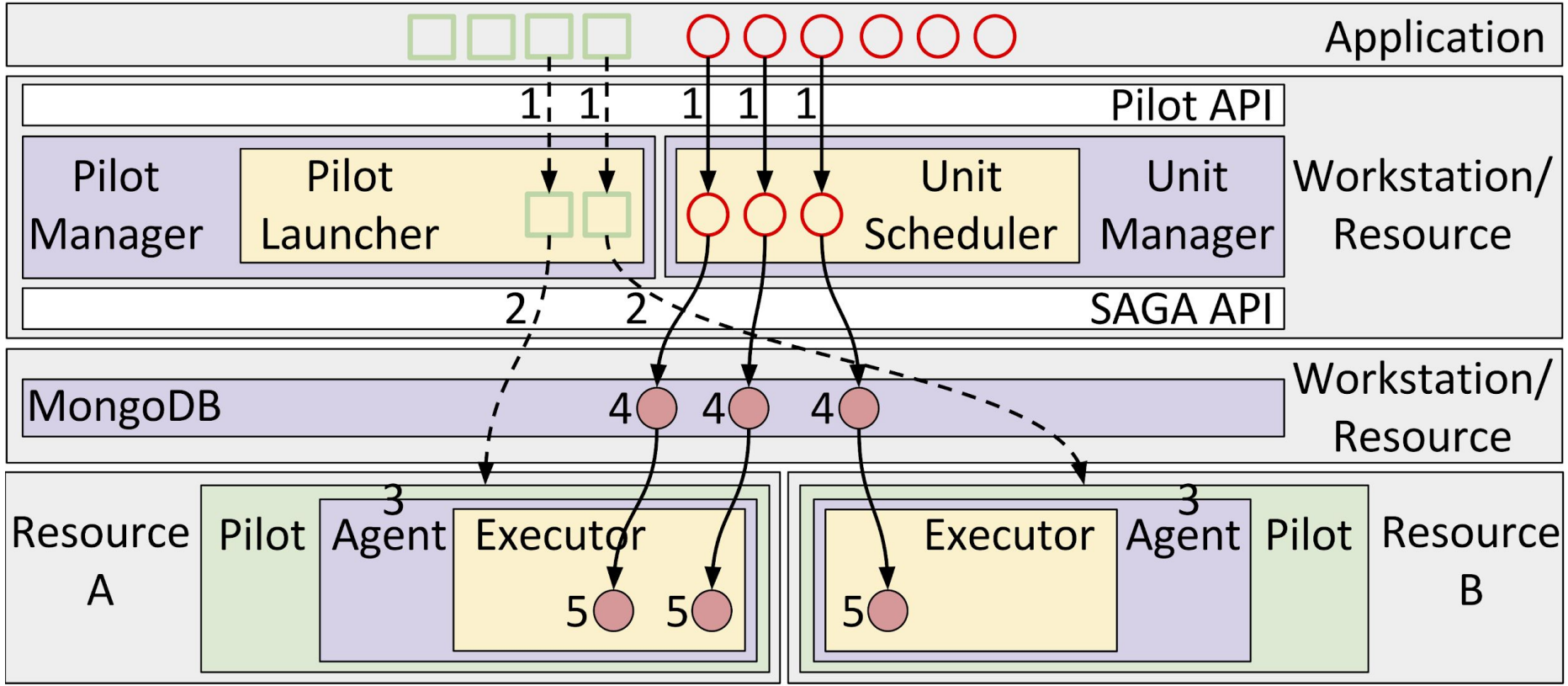
# RADICAL-Pilot: Implementation of Pilot-Abstraction

- *".. a scheduling overlay which generalizes the recurring concept of utilizing a placeholder as a container for compute tasks"*
- Decouples workload from resource management
- Enables the fine-grained spatio-temporal control of resources
- Build higher-level frameworks without explicit resource management
- Provides building block for late-binding of workloads on HPC

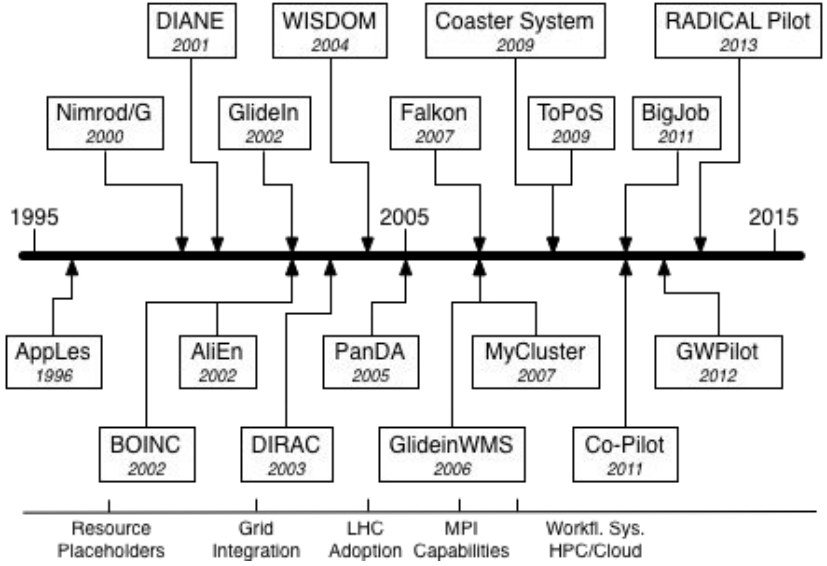


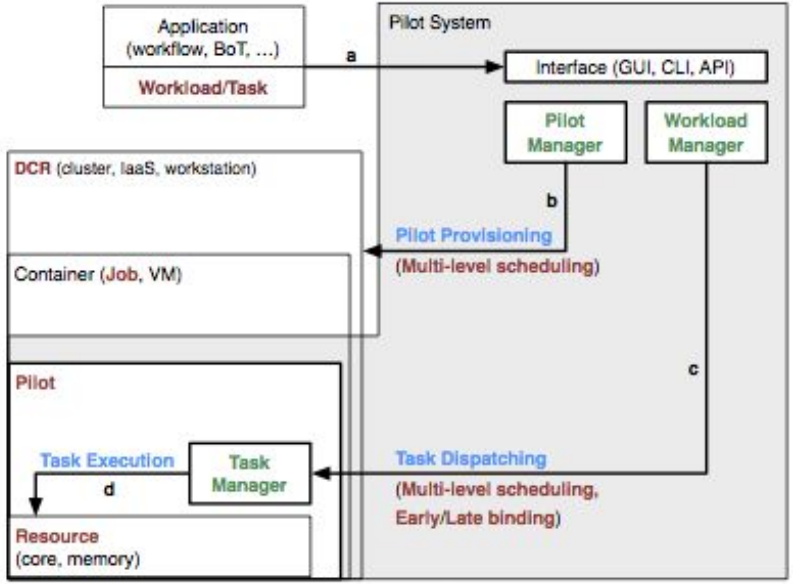

*Comprehensive Perspective on Pilot-Job Systems, ACM Computing Surveys (2018)*

# RADICAL-Pilot: Execution Model



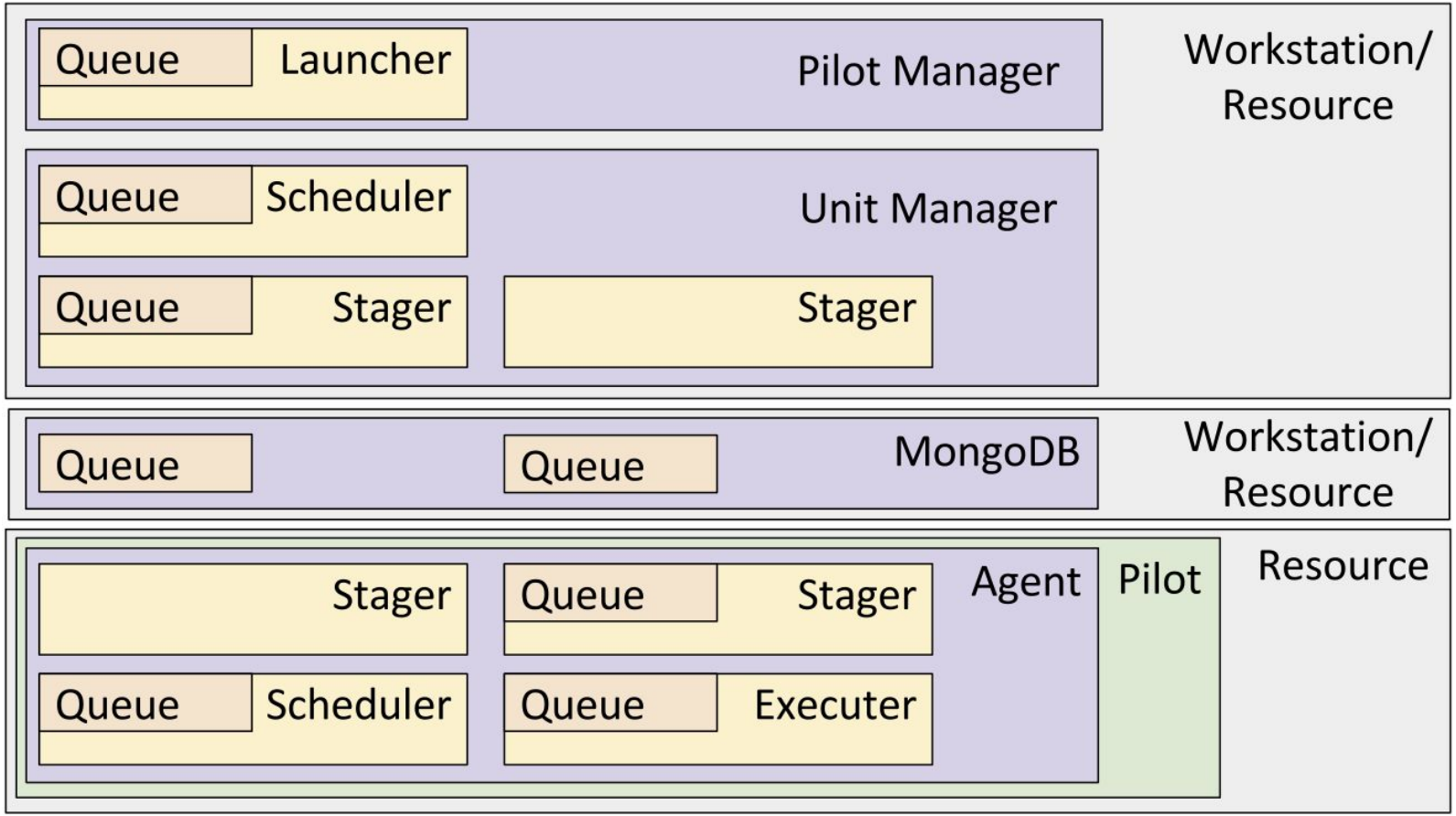
# Pilot Jobs: Many Variations on a Theme



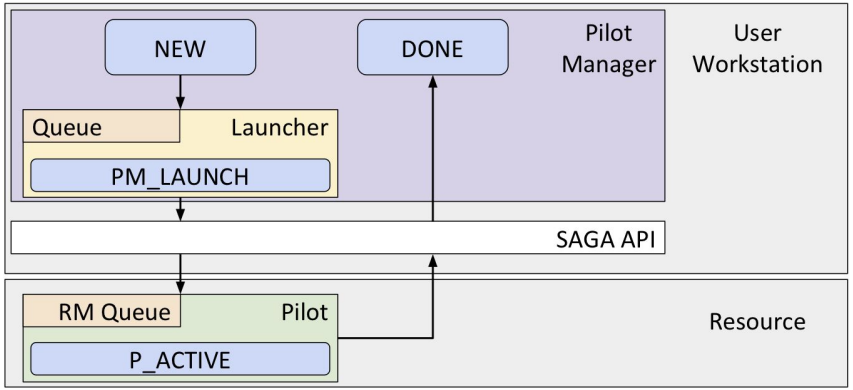



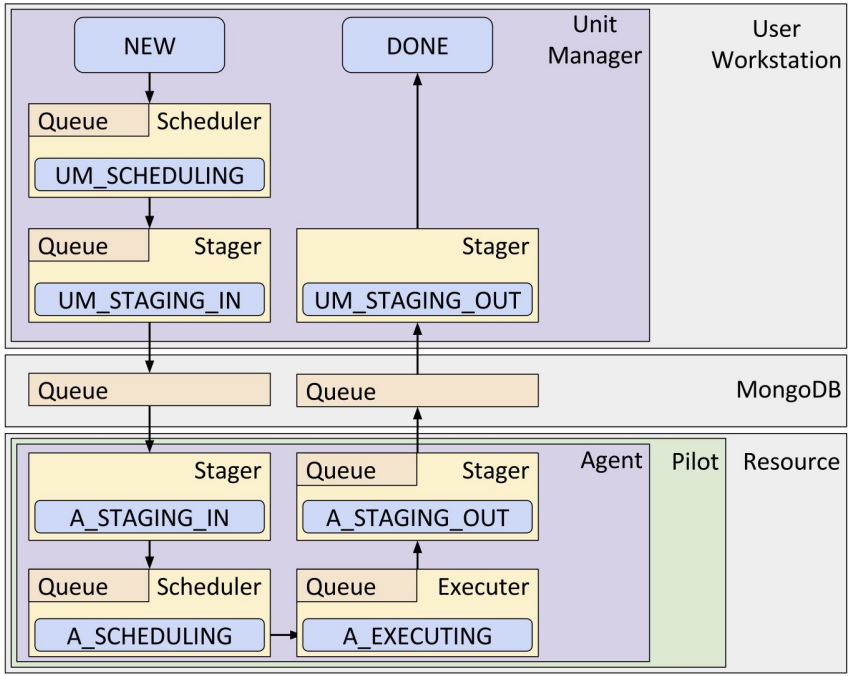

- "P*: A Model of Pilot-Abstractions", *8th IEEE International Conference on e-Science (2012)*
- *A Comprehensive Perspective on Pilot-Jobs* http://arxiv.org/abs/1508.04180 *(ACM Computing Surveys, 2018)*

# RADICAL-Pilot: Overall Architecture



# RADICAL-Pilot: State Model




- Pilot State Model:
  - 4 states, over client & server
- Unit State Model
  - 9 states, spread over 3 components

# RADICAL-Pilot: Programming Model

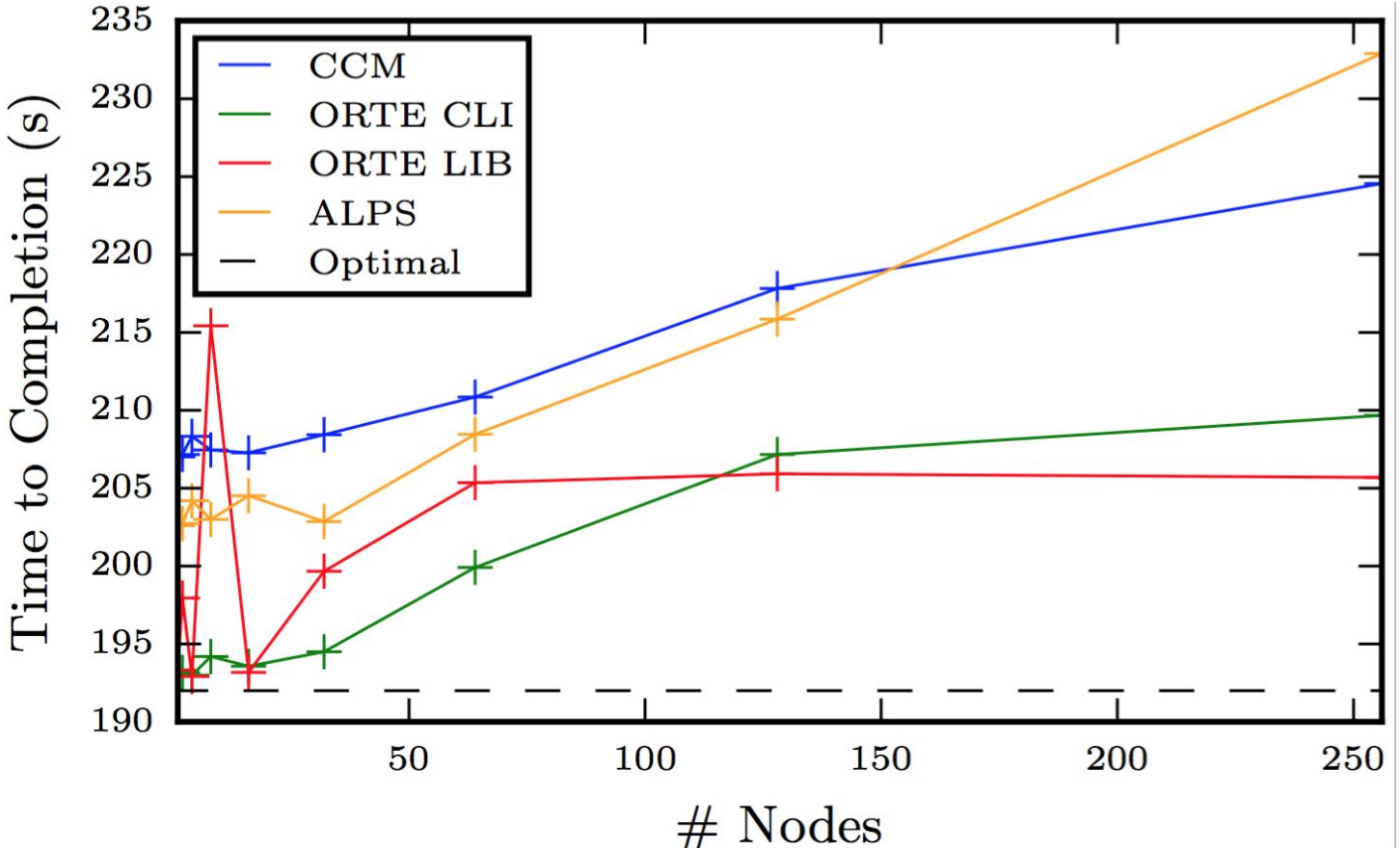
```
# Declare a 64-core pilot that will
# be available for 10 minutes.
pdesc = rp.ComputePilotDescription({
        'resource' : ncsa.bw,
        'cores'    : 64,
        'runtime'  : 10,
        'queue'    : 'debug',
        'project'  : 'gkd'
    })

# Submit the pilot for launching.
pilot = pmgr.submit_pilots(pdesc)

# Make the pilot resources available
# to a unit manager.
umgr.add_pilots(pilot)
```

```
# Number of units to run.
cuds = []
for i in range(0,42):
    # create a new CU description,
    # and fill it.
    cud = rp.ComputeUnitDescription()
    cud.executable = '/bin/date'
    cuds.append(cud)

# Submit units.
umgr.submit_units(cuds)

# Wait for the completion of units.
umgr.wait_units()

# Tear down pilots and managers.
session.close()
```

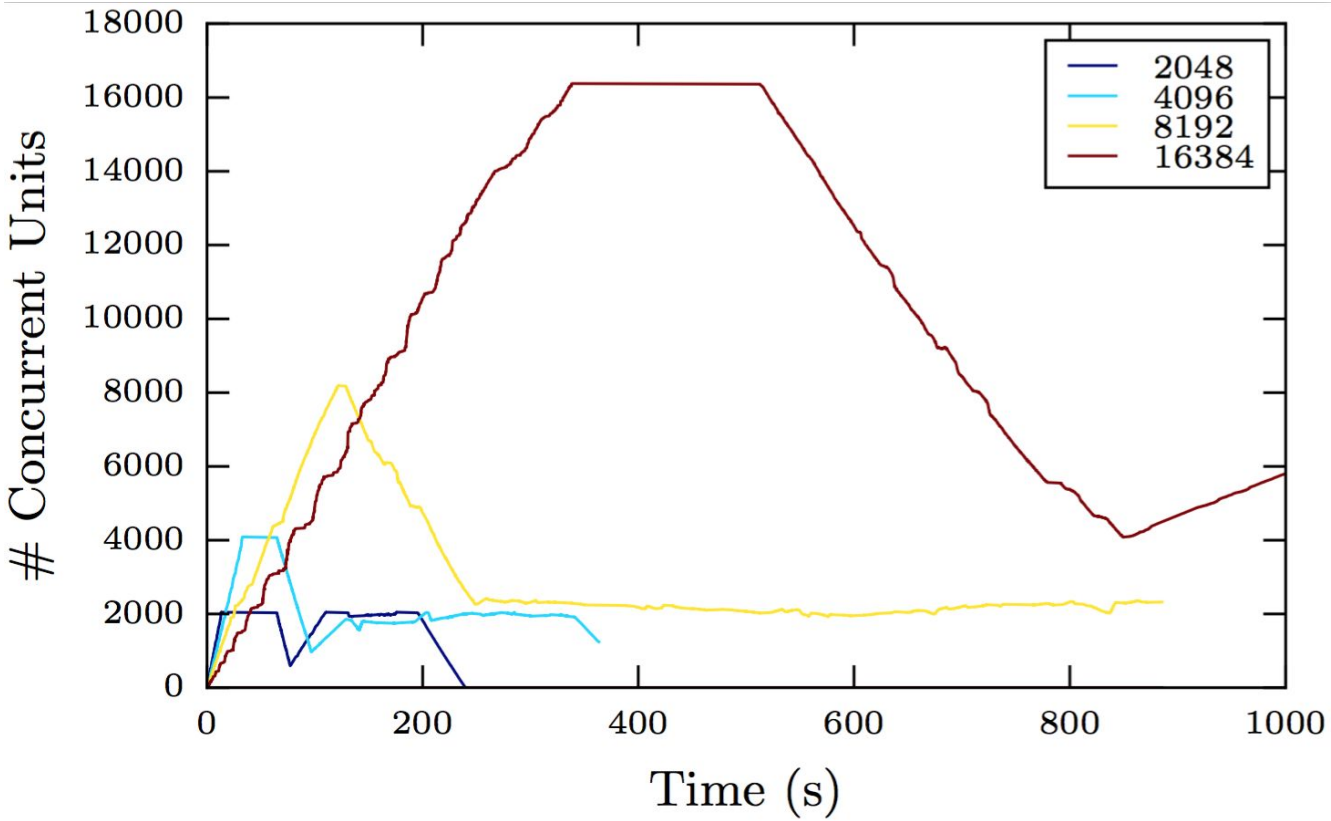
# Execution: (Why not) RADICAL-Pilot + APRUN

- RP Agent runs on MOM node
- Uses aprun to launch tasks onto the worker nodes
- Low throughput (ALPS not designed for short/small tasks)
- Limit on total concurrency (1000 aprun instances)
  - Less than 1000 on other CRAYS
- Maximum of one task per node

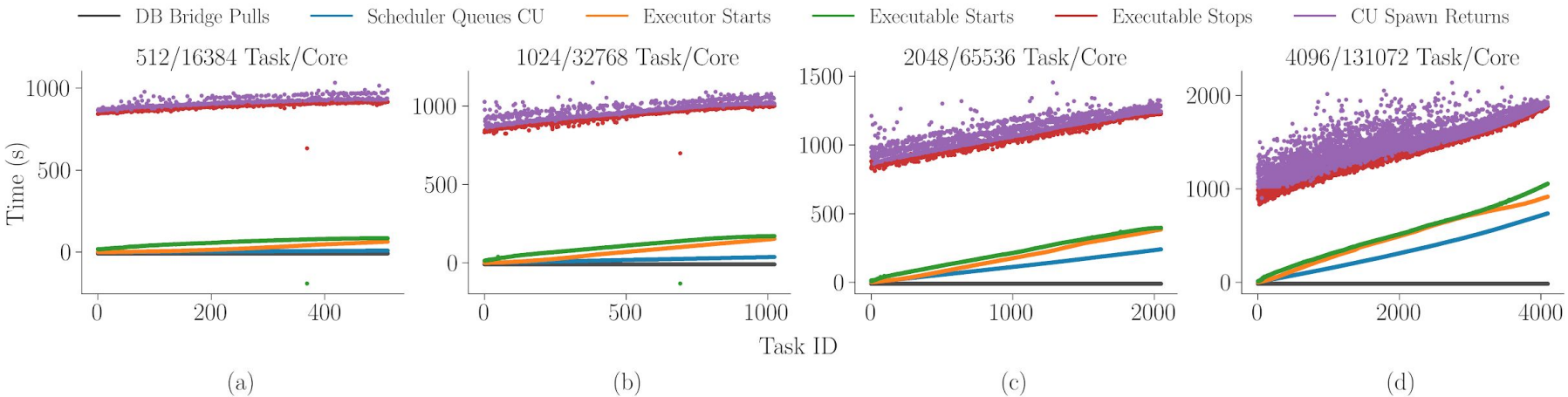
# Agent Performance: Full Node Tasks (3 x 64s)



# Agent Performance: Concurrent Units (3x)

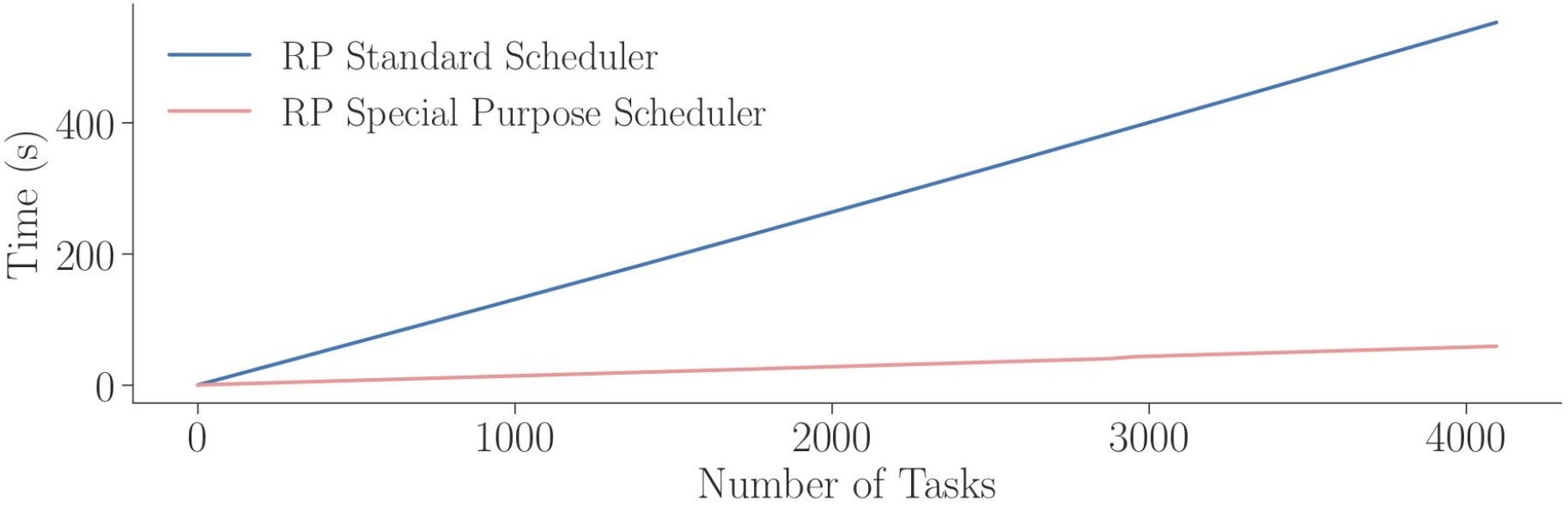


# RADICAL-Pilot: Weak Scaling Performance (Titan)



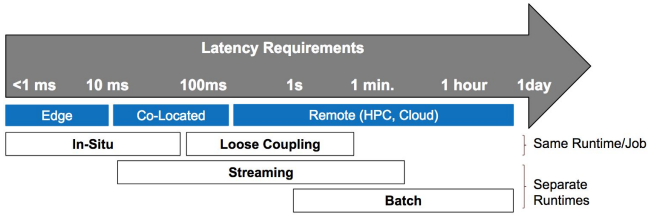
# RADICAL-Pilot: Resource Utilization Performance (Titan)

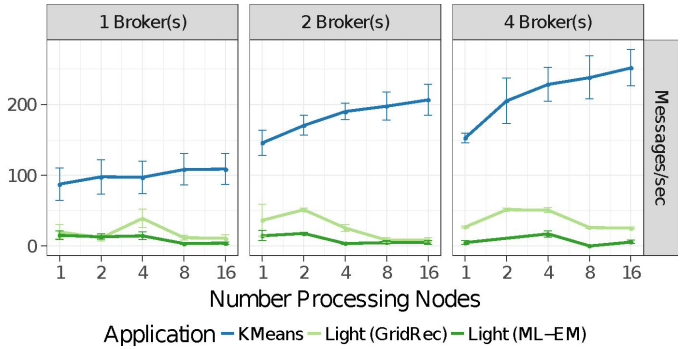
# RADICAL-Pilot: Price of Heterogeneity



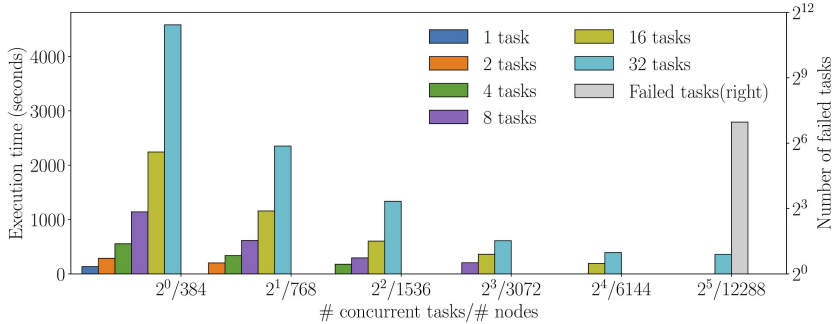
# RCT BB: From Streaming to Seismic Data

- Design HPC stream processing systems
  - Resource contention limits scalability of reconstruction algorithms
  - *Pilot-Streaming: Streaming Processing for HPC https://arxiv.org/pdf/1801.08648.pdf*

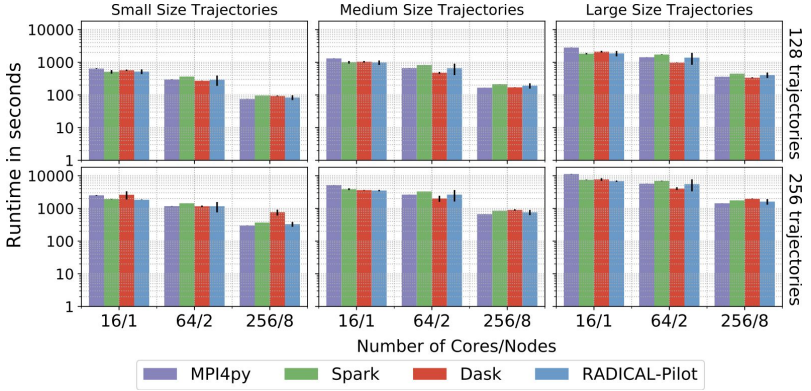



- Supporting Seismic Physics Workflows




- Task Parallel Analysis for Trajectory Data



# Summary

- **Importance and diversity of “workflows” set to increase**
  - Proliferation of middleware systems for “workflows” unsustainable
  - Substitute discussions of software with **abstractions & execution models**
- **Building blocks approach to workflows**
  - Focussed, principled design and development of middleware systems
  - Each building block has well defined performance characterization
- **RADICAL-Pilot: Implementation of Pilot abstraction**
  - Engineered to support heterogeneous workloads and resources
  - Investigated implementation and performance on Cray (Titan and Blue Waters)
- **Results:**
  - (i) ~O(10K) MPI simulations and tasks; (ii) Price for heterogeneity (generality); (iii) Ready for scheduling optimization; (iv) O(100K): When we overcome the scheduling challenges, message subsystem will hit!

# Thank You!