

# RADICAL-Cybertools: Abstractions-based Tools for Large-Scale Data-Intensive Applications

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# Outline: Part I (Lecture)

- A broad perspective on data-intensive science
  - Rich and diverse landscape of data-intensive architectures, applications and software systems
  - Need for Balanced, Interoperable and Federated CI
    - Architectures for data-intensive applications
    - HPC vs Grids vs Clouds?
- A Tale of Two Data Intensive Paradigms
  - BigData Ogres (mini-app, macro/micro patterns, skeleton)
    - Variations of "task level" parallelism and variants, Kmeans
  - HPC vs Hadoop/Apache Big Data stack (ABDS)
    - Convergence? Consilience between HPC and Apache/Hadoop?
- Introduction to RADICAL-Cybertools
  - Abstractions-based tools for interoperable extensible "task-level parallelism"



# Outline: Part II (Hands On)

- RADICAL Cybertools:
  - RADICAL-SAGA Interoperability Layer
    - Basics
    - Tutorial
    - Side detour: SAGA-Hadoop
  - RADICAL-Pilot
    - Basics
    - Tutorial
  - Kmeans redux
    - Multiple Kmeans concurrently
    - Trade-off: number vs size
    - Kmeans Map Reduce



## **Exponential Growth of High-end Computing**



#### HW: Think about the implications of this graph.

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Compute & Data: Two sides of the same coin An Interesting Observation



RUTGERSThink about the implications of this graph.

## **Data-intensive Sciences**



High Energy Physics:

- LHC at CERN produces petabytes of data per day.
- Data is processed and distributed across Tier 1 and 2 sites.



Astronomy:

- Sloan Digital Sky Survey (80 TB over 7 years).
- LSST will produce 40 TB per day (for 10 years).



#### Geonomics:

- Data volume increasing with every new generation of sequence machine. A machine can produce TB/day.
- Costs for Sequencing are decreasing.

#### WLCG: Worldwide LHC Computing Grid The First "Small" BigData Problem



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# ATLAS Project: Setting the Scale





- ATLAS one of the LHC experiments responsible for discovery of Higgs
  - Relies heavily on DCI for all computing needs
- PANDA: WMS for ATLAS. 1.2 Exabytes processed in 2013!!
- Current scale:
  - 25M jobs completed every month at > O(100) sites
  - ~O(10<sup>9</sup>) CPU hours a year!
- Scale and complexity of computing will increase by factor of O(10)
- Example of Big Data before it was "Big"!
- Using RADICAL Cybertools (SAGA) to manage access to supercomputers



# Data Lifecycle and Challenges



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# Diversity of Data-Intensive Applications [COURTERSY GCF]

- <a href="http://bigdatawg.nist.gov/usecases.php">http://bigdatawg.nist.gov/usecases.php</a>
- 51 Detailed Use Cases: Contributed July-September 2013 Covers goals, data features such as 3 V's, software, hardware
- Government Operation(4): National Archives and Records Administration, Census
  Bureau
- **Commercial(8):** Finance in Cloud, Cloud Backup, Mendeley (Citations), Netflix, Web Search, Digital Materials, Cargo shipping (as in UPS)
- **Defense(3):** Sensors, Image surveillance, Situation Assessment
- Healthcare and Life Sciences(10): Medical records, Graph and Probabilistic analysis, Pathology, Bioimaging, Genomics, Epidemiology, People Activity models, Biodiversity
- **Deep Learning and Social Media(6):** Driving Car, Geolocate images/cameras, Twitter, Crowd Sourcing, Network Science, NIST benchmark datasets
- The Ecosystem for Research(4): Metadata, Collaboration, Language Translation, Light source experiments
- Astronomy and Physics(5): Sky Surveys including comparison to simulation, Large Hadron Collider at CERN, Belle Accelerator II in Japan



# Towards Balanced, Interoperable, Federated DCI

- What is Federation?
  - Federation is the collective and concurrent utilization of DCI
    - Integration and interoperability are necessary conditions
- Why Federate DCI?
  - Effective application-resource mapping
    - Application characteristics and sophistication increase
  - Application scalability
    - Peak (time) and steady-state demand, heterogeneous workload
  - Resource utilization efficiency
    - Exploit diversity, yet preserve specificity
- How to Federate?
  - Three Architectures:
    - "Grid" vs "Cloud" vs "Hybrid"
  - Types and levels of Federation



#### A Tale of Two Data-Intensive Pardigms: Architectures, Applications and Abstractions

Collaboratinon with Geoffrey Fox http://arxiv.org/abs/1403.1528



#### **Data-Intensive Application Pattern (or Structure)**

- Capture "essence of these use cases".. Classify applications into patterns, "small" kernels, mini-apps
  - Focus on cases with detailed analytics
  - Use for benchmarks of computers and software
- In parallel computing, this is well established
  - Linpack for measuring performance to rank machines in Top500
  - NAS Parallel Benchmarks (originally a pencil and paper specification to allow optimal implementations; then MPI library)
  - Other specialized Benchmark sets keep changing and used to guide procurements
    - Last 2 NSF hardware solicitations had NO preset benchmarks perhaps as no agreement on key applications for clouds and data intensive applications
  - Berkeley dwarfs capture different structures that any approach to parallel computing must address
  - Templates used to capture parallel computing patterns



# **HPC Benchmark Classics**

- Linpack or HPL: Parallel LU factorization for solution of linear equations
- NPB version 1: Mainly classic HPC solver kernels
  - MG: Multigrid
  - CG: Conjugate Gradient
  - FT: Fast Fourier Transform
  - IS: Integer sort
  - EP: Embarrassingly Parallel
  - BT: Block Tridiagonal
  - SP: Scalar Pentadiagonal
  - LU: Lower-Upper symmetric Gauss Seidel



# 7 Original Berkeley Dwarfs (Colella)

- 1. Structured Grids (including locally structured grids, e.g. Adaptive Mesh Refinement)
- 2. Unstructured Grids
- 3. Fast Fourier Transform
- 4. Dense Linear Algebra
- 5. Sparse Linear Algebra
- 6. Particles
- 7. Monte Carlo

Note "vaguer" than NPB



# **13 Berkeley Dwarfs**

- Dense Linear Algebra
- Sparse Linear Algebra
- Spectral Methods
- N-Body Methods
- Structured Grids
- Unstructured Grids
- MapReduce
- Combinational Logic
- Graph Traversal
- Dynamic Programming
- Backtrack and Branch-and-Bound
- Graphical Models
- Finite State Machines

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First 6 of these correspond to Colella's original.

Monte Carlo dropped N-body methods are a subset of Particle

Note a little inconsistent in that MapReduce is a programming model and spectral method is a numerical method

Need multiple facets!

## **Distributed Computing MetaPatterns I**

Jha et al, 1532-0634, 2012. DOI: 10.1002/cpe.2897CCPE

Application example	execution unit	Communication (data exchange)	Coordination	Execution environment
Montage	Multiple sequential and parallel executables	Files	Dataflow (DAG)	Dynamic process creation, workflow execution, file transfer
NEKTAR	Multiple concurrent instances of single executable	Messages	SPMD	MPI, coscheduling
Coupled fusion simulation	Multiple concurrent parallel executables	Stream-based	Dataflow	Coscheduling, data streaming, async. data I/O
Asynchronous replica-exchange	Multiple sequential and/or parallel executables	Pub/sub	Dataflow and events	Decoupled coordination and messaging, dynamic task generation
ClimatePrediction.net (generation)	Multiple sequential executables, distributed data stores	Files and messages	Master/ worker, events	At-Home (BOINC)
ClimatePrediction.net (analysis)	A sequential executable, multiple sequential or or parallel executables	Files and messages	Dataflow (Forest)	Dynamic process creation, workflow execution
SCOOP	Multiple different parallel executables	Files and messages	Dataflow	Preemptive scheduling, reservations

Table I. Characteristics of the set of applications arranged according to the identified vectors.

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#### **Distributed Computing MetaPatterns II**

Jha et al

Table IV. Applications and their pattern usage. A '-' indicates that no pattern can be identified, not that the application does not have any communication, coordination, or deployment.

Application example	Coordination	Deployment
Montage	Task farm, data processing pipeline	-
NEKTAR	-	Co-allocation
Coupled fusion simulation	Stream	Co-allocation
Async RE	Pub/sub	Replication
ClimatePrediction (generation)	Master/worker, AtHome	Consensus
ClimatePrediction (analysis)	MapReduce	
SCOOP	Master/worker, data processing pipeline	-



#### **Distributed Computing MetaPatterns III**

Jha et al

Pattern	Tools that support the pattern				
Master/Worker-Task farm	Aneka, Nimrod, Condor, Symphony, SGE, HPCS				
Master/Worker-BagOfTasks	Comet-G, TaskSpace, Condor, TSpaces				
All-Pairs	All-Pairs				
Data processing pipeline	Pegasus/DAGMan				
MapReduce	Hadoop, Twister, Pydoop				
AtHome	BOINC				
Pub-Sub	Flaps, Meteor, Narada, Gryphon, Sienna				
Stream	DART, DataTurbine				
Replication	Giggle, Storm, BitDew, BOINC				
Co-allocation	HARC, GUR				
Consensus	BOINC, Chubby, ZooKeeper				
Brokers	GridBus, Condor matchmaker				

Table V. Tools and libraries that support patterns identified in Sections 3.1 and 3.2.

## **Comparison of Data Analytics with Simulation -- I**

- Pleasingly parallel often important in both
- Both are often SPMD and BSP
- Non-iterative MapReduce is major big data paradigm
  - not a common simulation paradigm except where "Reduce" summarizes pleasingly parallel execution
- Big Data often has large collective communication
  - Classic simulation has a lot of smallish point-to-point messages
- Simulation dominantly sparse (nearest neighbor) data structures
  - "Bag of words (users, rankings, images..)" algorithms are sparse, as is PageRank
  - Important data analytics involves full matrix algorithms

# **Comparison of Data Analytics with Simulation - II**

- There are similarities between some graph problems and particle simulations with a strange cutoff force.
  - Both Map-Communication
- Note many big data problems are "long range force" as all points are linked.
  - Easiest to parallelize. Often full matrix algorithms
  - e.g. in DNA sequence studies, distance  $\delta(i, j)$  defined by BLAST, Smith-Waterman, etc., between all sequences *i*, *j*.
  - Opportunity for "fast multipole" ideas in big data.
- In image-based **deep learning**, neural network weights are block sparse (corresponding to links to pixel blocks) but can be formulated as full matrix operations on GPUs and MPI in blocks.
- In HPC benchmarking, Linpack being challenged by a new sparse conjugate gradient benchmark HPCG, while we use **non- sparse conjugate gradient solvers** in clustering and Multi-dimensional scaling.

# **Big Data Ogres and Their "Facets"**

- The first Ogre Facet captures different problem "architecture". Such as (i) Pleasingly Parallel – as in Blast, Protein docking, imagery (ii) Local Machine Learning – ML or filtering pleasingly parallel as in bio-imagery, radar (iii) Global Machine Learning seen in LDA, Clustering etc. with parallel ML over nodes of system (iv) Fusion: Knowledge discovery often involves fusion of multiple methods. (v) Workflow
- The second Ogre Facet captures source of data (i) SQL, (ii) NOSQL based, (iii) Other Enterprise data systems (10 examples at NIST) (iv)Set of Files (as managed in iRODS), (v) Internet of Things, (vi) Streaming and (vii) HPC simulations.
- Before data gets to compute system, there is often an initial data gathering phase which is characterized by a block size and timing. Block size varies from month (Remote Sensing, Seismic) to day (genomic) to seconds (Real time control, streaming)
- There are storage/compute system styles: Dedicated, Permanent, Transient
- Other characteristics are need for permanent auxiliary/comparison datasets and these could be interdisciplinary implying nontrivial data movement/replication

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# **Detailed Structure of Ogres**

- The third Ogre Facet is distinctive system features such as (i) Agents, as in epidemiology (swarm approaches) and (ii) GIS (Geographical Information Systems).
- The fourth Ogre Facet captures Style of Big Data applications. (i) Are data points in metric or non-metric spaces (ii) Maximum Likelihood, (iii)  $\chi^2$ minimizations, and (iv) Expectation Maximization (often Steepest descent)
- The fifth Facet is Ogres themselves classifying core analytics kernels (i) Recommender Systems (Collaborative Filtering) (ii) SVM and Linear Classifiers (Bayes, Random Forests), (iii) Outlier Detection (iORCA) (iv) Clustering (many methods), (v) PageRank, (vi) LDA (Latent Dirichlet Allocation), (vii) PLSI (Probabilistic Latent Semantic Indexing), (viii) SVD (Singular Value Decomposition), (ix) MDS (Multidimensional Scaling), (x) Graph Algorithms (seen in neural nets, search of RDF Triple stores), (xi) Learning Neural Networks (Deep Learning), and (xii) Global Optimization (Variational Bayes).
- Flops per byte and Communication Interconnect requirements characterize fifth facet

## "Many Tasks" Pathway to Extreme Scale

- Problems in computational science *naturally* amenable to "task level" parallelism model of computing:
  - "Embarrassingly Parallel" data-intensive applications
  - Many free energy calculations, enhanced sampling problems.
  - Many multi-physics simulations are also multi components.
- Single "application" might be broken into many smaller simulations
- This is not *just* HTC or HPC, but complex application objectives
  - Isn't about just peak perf, nor maximal throughput
  - Given access to X cores/ nodes – slice/dice or distribute as needed



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#### From Many Tasks to Complex Applications

- Starting from uncoupled heterogeneous simulations, varying levels of coordination and dependency can be gradually added and "tuned"
- Depending upon the above properties, the importance and feasibility of distribution varies





Scalable Online Comparative Genomics of Mononucleosomes.

"Scalable Online Comparative Genomics of Mononucleosomes: A BigJob", *Proceedings of Conference on XSEDE*, 2013.



Asynchronous Replica-Exchange: Advanced Algorithms for enhanced sampling.

"A Framework for Flexible and Scalable Replica-Exchange on Production Distributed CI", *Proceedings* of Conference on XSEDE, 2013.

#### The Case for an Integrating Apache/Hadoop Big Data Stack with HPC



C	Orchestration & Workflow Oozie, ODE, Airavata and OODT (Tools) NA: Pegasus, Kepler, Swift, Taverna, Trident, ActiveBPEL, BioKepler, Galaxy																							
	Cross Cutting Data Analytics Libraries: Capabilities Machine Learning Statistics Riginformatics Imageny Linear Algebra																							
٢					Machine LearningStatistics, BioinformaticsImageryMahout , MLlib , MLbaseR, Bioconductor (NA)ImageJ (NA)Sca							Algebra , PetSc (NA)												
	Monitoring		tribut	Message		High Level (Integrated) Systems for Data Processing																		
	Message Protocols Distributed Coordination Monitoring					Hive (SQL on Hadoop)	H catalo Interfac	es (Pro		Shark (SQL on park, NA)	(SQL	MRQL on Hadoop, na, Spark)	Impala (NA) Cloudera	Swazall (Log Files Google NA)										
			latio	S		Para	llel horizo	ntally sca	lable Data	Processin	g													
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	Ambari	S				-		— Bat	ch —			— Stream -	<b>→</b>	Graph										
	ari	e c				ABDS	Inter-proc	ess Comn	nunication		HPC	Inter-proces	s Communicatio	on										
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		a				NoSQL: [	Document		1. See	NoSQL:	Key Va	lue (all NA)	-											
		c y			R	MongoDB (NA)	CouchDB	Luce		erkeley DB	Azur Tabl			Voldemort ~Dvnamo										

Orchestration & Workflow Oozie, ODE, Airavata and OODT (Tools) NA: Pegasus, Kepler, Swift, Taverna, Trident, ActiveBPEL, BioKepler, Galaxy



Enhanced Apache/Hadoop Big Data Stack (ABDS)

- ~120 Capabilities
- >40 Apache
- Green layers have strong HPC Integration opportunities
- Goal
  - Functionality of ABDS
  - Performance of HPC

Extraction Tools SQL			_	SciDB	NoSQL: C	Solandra				
UIMA (Entities) (Watson)	Tika (Content)	MySQL (NA)	Phoenix (SQL on HBase)	(NA) Arrays, R,Python	HBase (Data on HDFS)	Accumulo (Data on HDFS)	Cassandra (DHT)	(Solr+ Cassandra) +Document		
NoSQL: [	Documen	t		NoSQL:	Key Value	(all NA)				
MongoDB (NA)	B Luce Sol		erkeley DB	Azure Table	Dynamo Amazon	Riak ~Dynamo	Voldemort ~Dynamo			
No SQL: Ge	eneral Gra	aph	NoSQL: T	ripleSto	File Aanagement					
Java Gnu Com		cdata mercial NA)	Jena	Sesam (NA)			A RDF on ccumulo	iRODS(NA)		
ABD	ABDS Cluster Resource Management HPC Cluster Resource Management									
	Mesos, Yarn, Helix Condor, Moab, Torque(NA)									
ABDS File S	systems	Use	r Level		HPC File	Systems (N	A)			
HDFS,      Swift, Ceph      FUSE(NA)      Gluster, Lustre, GPFS, GFFS        Object Stores      POSIX Interface      Distributed, Parallel, Federated										
Interoperability Layer Whirr / JClouds OCCI CDMI (NA) DevOps/Cloud Deployment Puppet/Chef/Boto/CloudMesh(NA)										
laaS Platfo OpenStack	-		n Source alyptus, C	oudStack	Commerci , vCloud,	al Clouds Amazon, Az	ure, Google	Bare Metal		
RUTGERS Data Stack (ABDS) with HPC Integration/Enhancement										

#### **Bringing High Performance to Data Analytics**

- On the systems side, we have two principles
  - The Apache Big Data Stack with ~120 projects has important broad functionality with a vital large support organization
  - HPC including MPI has striking success in delivering high performance with however a fragile sustainability model
- There are key systems abstractions which are levels in HPC-ABDS software stack where careful integration needed
  - -Resource management
  - Resource Fabric: Storage and Compute
  - Programming model -- horizontal scaling parallelism
  - Collective and Point to Point communication
  - -Support of iteration





HPBDS

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# Integrating Hadoop/Yarn with HPC





# **4 Forms of MapReduce**



MPI is Map followed by Point to Point or Collective Communication – as in style c) plus d) [slide courtesy Geoffrey Fox]


Increasing Communication

**Identical Computation** 

# RADICAL-Cybertools: Usage, Usage Modes and Applications

http://radical-cybertools.github.io/



#### **Pilot Abstractions**

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Working definition: A system that generalizes a placeholder job to provide multi-level scheduling to allow application-level control over the system scheduler via a scheduling overlay.



# Introduction to Pilot-Abstraction (2)

#### • Working definitions:

- A system that generalizes a placeholder job to provide multi-level scheduling to allow application-level control over the system scheduler via a scheduling overlay
- ".. defined as an abstraction that generalizes the reoccurring concept of utilizing a placeholder job as a container for a set of compute tasks; an instance of that placeholder job is referred to as Pilot-Job or pilot."
- Advantages of Pilot-Abstractions:
  - The Perfect Pilot: Decouples workload from resource management
  - Flexible Resource Management
    - Enables the fine-grained (ie "slicing and dicing") of resources
    - Tighter temporal control and other advantages of application-level Scheduling (avoid limitations of system-level only scheduling)
  - Move control, extensibility and flexibility "upwards"
    - Build higher-level capabilities without explicit resource management

#### Landscape of Pilot-Job Systems

- There are many PJS offerings, often semantically distinct
  - PanDA, DIANE, DIRAC, Condor Glide-In, SWIFT, ToPoS Falkon, BigJob...
    - Why do you think there has been a proliferation of PJs?
- Conceptual & practical barriers to extensibility (& interoperability)
  - The landscape of PJS reflects, in addition to PJS specifics, the broader ecosystem of distributed middleware & infrastructure
  - Software Engineering issues, interfaces, standardization
- Difference in the execution models of the PJ
  - We know "what" pilot-jobs do, but the "how" remains less clear
    - How to map tasks to pilot-jobs? How to choose/map optimal resource?
    - How to "slice and dice" resources?
- Data remains a dependent variable, not a primary variable

### P\* Model: Elements, Characteristics and API

- Elements:
  - Pilot-Compute (PC).
  - Pilot-Data (PD).
  - Compute Unit (CU).
  - Data Unit (DU).
  - Scheduling Unit (SU).
  - Pilot-Manager (PM).
- Characteristics:
  - Coordination.
  - Communication.
  - Scheduling.
- Pilot-API.



"P\*: A Model of Pilot-Abstractions", 8th IEEE International Conference on e-Science 2012, 2012

#### RADICAL-Pilot (BigJob): Architecture



# "Coarse-Grained" RADICAL-Pilot Performance

- Number of zero-payload tasks that BJ can dispatch per second:
  - Distributed: O(1)
  - Locally: > O(10)
- Number of Pilots (Pilot-Agents) that can be marshaled
  - Locally/Distributed: O(100)
- Typical number of tasks per Pilot-Agent:
  - Locally/distributed: O(1000)
- Number of tasks concurrently managed = Number of Pilot-Agents x tasks per each agent :
  - O(100) x O(1000)
- (Obviously) The above depends upon data per task:
  - BigJob has been used over O(1)--O(10<sup>9</sup>) bytes/task, for tasks of duration O(1) second to O(10<sup>5</sup>) seconds

#### RADICAL-Pilot http://radical-cybertools.github.io/radical-pilot



# **RADICAL-Pilot**

http://radical-cybertools.github.io/radical-pilot

- Lightweight, portable, fast, scalable pilot framework
- Scalability (up and out)
  - Lightweight data model
  - Bulk operations
  - Notifications / support for async programming
- Portability
  - Pure Python
  - Modular pilot agent
  - SAGA-Python as plumbing layer
- Supports Research
  - Pluggable schedulers
  - High degree of introspection, provenance
  - Consistent and verifiable performance



#### SAGA: A Standardized Interoperability Layer

- SAGA Simple API for Distributed ("Grid") Applications:
  - Allows access to different middleware / services through Python implementation of Open Grid Forum GFD.90.
  - Also unified semantics across middleware, backend plug-ins ("adaptors").
- HOW SAGA is Used?
  - Uniform Access-layer to DCI, e.g, XSEDE,
  - Build tools, middleware services and capabilities
    - Pilot-Jobs, workflow systems, science gateways and web portals
  - Domain-specific (distributed) applications, libraries and frameworks
- Functional component as well as a specific component XSEDE Architecture



### SAGA: Interoperability Layer for RP

- SAGA Simple API for Distributed ("Grid") Applications:
  - Application level standardized (Open Grid Forum GFD.90) API.
  - Application is a broad term: "one person's application is another person's tool (building block)".
- SAGA-Python:
  - Native Python implementation of Open Grid Forum GFD.90.
  - Allows access to different middleware / services through a unified interface
  - Provides access via different backend plug-ins ("adaptors").
  - SAGA-Python provides both a common API, but also unified semantics across heterogeneous middleware:
    - Transparent Remote operations (SSH / GSISSH tunneling).
    - Asynchronous operations.
    - Callbacks.
    - Error Handling.





### Conclusion

- A fundamental need for abstractions to support diverse set of dataintensive applications
  - Need for a balanced, interoperable and federated data CI
- Towards High-performance Data-Intensive Computing
  - Best of both: Hadoop/Apache Big Data stack meets HPC
- Set against these objectives: "Pilot Abstraction Works!"
  - Better integration into HPC
    - Platform independent libraries: different application types, execution modes, coupling schemes
  - Similar "abstractions" emerging in the Hadoop BDS



#### References

- RADICAL-Cybetools:
  - http://radical-cybertools.github.com/
- RADICAL-SAGA:
  - http://saga-project.github.io/radical-saga
- RADICAL-Pilot: An implementation of P\*
  - http://saga-project.github.io/radical-pilot/
- RADICAL:
  - http://radical.rutgers.edu/
- Publications:
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