Workflows as an Operational Tool for Scientific Computing using Data Science

İlkyay ALTINTAŞ, Ph.D.
Chief Data Science Officer, San Diego Supercomputer Center
Founder and Director, Workflows for Data Science Center of Excellence
SDSC is 31 Years Young!
Providing Cyberinfrastructure for Research and Education

Established as a national supercomputer resource center in 1985 by NSF
A world leader in HPC, data-intensive computing, and scientific data management
Current strategic focus on “Big Data” and “HPC Cloud” : versatile computing

Two discoveries in drug design from 1987 and 1991.
Ross Walker Group

SDSC continues to focus on versatile computing and big data!

Gordon: First Flash-based Supercomputer for Data-intensive Apps

Comet: Serving the Long Tail of Science

- 36 GPU nodes
- 4 Large Memory nodes
- 7 PB Lustre storage
- High performance virtualization

Standard racks

= 1944 nodes
= 46,656 cores
= 249 TB DRAM
= 622 TB SSD
= 2 Pflop/s
SDSC Data Science Office
-- Expertise, Systems and Training
for Data Science Applications --

SDSC DSO is a collaborative virtual organization at SDSC for collective
lasting innovation in data science research, development and education.

SDSC Expertise and Strengths

Big Data Platforms
Training
Industry
Applications

SDSC Data Science Office (DSO)
Computing Today has Many Shapes and Sizes

Enables dynamic data-driven applications

- Computer-Aided Drug Discovery
- Smart Cities
- Disaster Resilience and Response

- Smart Grid and Energy Management
- Personalized Precision Medicine
- Manufacturing

BIG DATA

Requires:
- Data management
- Data-driven methods
- Scalable tools for dynamic coordination and stateful resource optimization
- Skilled interdisciplinary workforce

New era of data science!
Needs and Trends for Scientific Computing under the Influence of Big Data and Cloud Systems

- More data-driven
- More dynamic
- More process-driven
- More collaborative
- More accountable
- More reproducible
- More interactive
- More heterogeneous

New era of data science!
BIG DATA

Volume

Size

Application-Specific Value

Complexity

Variety

Velocity

Valence

Connected

Quality

Speed

Veracity
Data Management and Processing in the Big Data Era has Unique Challenges!

- **Volume** → Scalable batch processing
- **Velocity** → Stream processing
- **Variety** → Extensible data storage, access and integration
These challenges come with new tools to tackle them.
How do we use these new tools and combine them with existing solutions in scientific computing and data science?
Example Big Data Processing Pipelines

Source: http://www.slideshare.net/BigDataCloud/big-data-analytics-with-google-cloud-platform

Source: https://www.mapr.com/blog/distributed-stream-and-graph-processing-apache-flink

Source: https://www.computer.org/csdl/mags/so/2016/02/mso2016020060.html

Source: http://www.slideshare.net/ThoughtWorks/big-data-pipeline-with-scala
COORDINATION AND WORKFLOW MANAGEMENT

ACQUIRE

PREPARE

ANALYZE

REPORT

ACQUIRE

PREPARE

ANALYZE

Kepler

http://kepler-project.org

Apache Zookeeper
Research Challenges

• How to easily program a workflow using the Big Data Patterns?
• How to parallelize legacy tools for Big Data?
• Which pattern(s) to use under which Big Data engine to use, e.g., as Hadoop, Flink or Spark?

End-to-end performance prediction for Big Data applications/workflows (how long to run)

Knowledge based: Analyze performance using profiling techniques and dependency analysis
Data driven: Predict performance based on execution history (provenance) using machine learning techniques

• On demand resource provisioning and scheduling for Big Data applications (where and how to run)

Find the best resource allocation based on execution objectives and performance predictions
Find the best workflow and task configuration on the allocated resources
Using Big Data Patterns in Kepler Workflows

- Define a separate DDP (Distributed Data-Parallel) task/actor for each pattern.
- These DDP actors partition input data and process each partition separately.
- User-defined functions are described as sub-workflows of DDP actors.
- DDP director: executes DDP workflows on top of Big Data engines.
- Visual programming
- Parallel execution of the DDP sub-workflows
- Existing actors can easily be reused for new tools.
A workflow is a combination of modules running in places and interacting with each other via data or message passing via a connection.

Workflow Performance == Composed Module Performance on an Infrastructure Instance
Optimization of Heterogeneous Resource Utilization using bioKepler
more traditional HPC and HTC workloads to the

Dynamic data-driven coordination & resource optimization

Requires: Ability to explore and scale on multiple platforms

Are workflows increasingly becoming the dynamic operations research tool for science?
Challenge: Make workflows more aware of distributed system and application state!
Some steps to get there...

1. Analyze each task in a workflow as an individual module based on all past executions of that executable task.
2. Model workflow performance as an aggregate of predictions of individual tasks to form prediction for entire workflow.
3. Include system level analytics at the workflow level to make sure scheduling can use system level information to account in a dynamic data-driven way.
Uses existing tools and computing systems!

Computing is just one part of big data workflows…

… new methods needed!
Goal: Methodology and tool development to build automated operational workflow-driven solution architectures on big data and HPC platforms.

Focus on the question, not the technology!

- Access and query data
- Support exploratory design
- Scale computational analysis
- Increase reuse
- Save time, energy and money
- Formalize and standardize

WorDS Center

Real-Time Hazards Management
wifire.ucsd.edu

Data-Parallel Bioinformatics
bioKepler.org

Scalable Automated Molecular Dynamics and Drug Discovery
nbcr.ucsd.edu
Examples: Use of Workflows as an Application Integration Tool for “Big” Data and Computational Science
Towards an Integrated Cyberinfrastructure for Scalable Data-Driven Monitoring, Dynamic Prediction and Resilience of Wildfires

Ilkay Altintas\textsuperscript{1}, Jessica Block\textsuperscript{2}, Raymond de Callafon\textsuperscript{3}, Daniel Crawl\textsuperscript{1}, Charles Cowart\textsuperscript{1}, Amarnath Gupta\textsuperscript{1}, Mai Nguyen\textsuperscript{1}, Hans-Werner Braun\textsuperscript{1}, Jurgen Schulze\textsuperscript{2}, Michael Gollner\textsuperscript{4}, Arnaud Trouve\textsuperscript{4} and Larry Smarr\textsuperscript{2}

\textsuperscript{1}San Diego Supercomputer Center, University of California San Diego, U.S.A.
\textsuperscript{2}Qualcomm Institute, University of California San Diego, U.S.A.
\textsuperscript{3}Dept. of Mechanical and Aerospace Engineering, University of California San Diego, U.S.A.
\textsuperscript{4}Fire Protection Engineering Dept., University of Maryland, U.S.A.

This work was supported mainly by NSF-1331615 under CI, Information Technology Research and SEES Hazards programs, and in part by NSF-112661, NSF-1062565 and NSF-0941692.

wifire.ucsd.edu
WIFIRE: A Scalable Data-Driven Monitoring, Dynamic Prediction and Resilience Cyberinfrastructure for Wildfires

Monitoring
Visualization
Fire Modeling

Big Data
Hybrid Data Processing Architecture

SPEED LAYER
- Stream processing
- Real-time data interfaces

BATCH LAYER
- Batch processing on all data
- Batch data collection generation

SERVING LAYER
- Querying

Data sources formally described
- Data merged from multiple sources into a single, unified model
- Measurements from weather stations and cameras
- Fire perimeters, e.g., InciWeb, GeoMac, SANDAG
- Model output, e.g., FARSITE, Firefly, etc.

Unified REST interface to access data multiple formats
Modeling Workflows in WIFIRE

- Real-time sensors
- Weather forecast
- Landscape data
- Monitoring & fire mapping
- Fire perimeter
Closing the Loop using Big Data
-- Wildfire Behavior Modeling and Data Assimilation --

- Computational costs for existing models too high for real-time analysis
- \textit{a priori} -> \textit{a posteriori}
  - Parameter estimation to make adjustments to the (input) parameters
  - State estimation to adjust the simulated fire front location with an \textit{a posteriori} update/measurement of the actual fire front location

\textit{Conceptual Data Assimilation Workflow with Prediction and Update Steps using Sensor Data}
Summary: Three questions about converged workflow applications!

1. How can we scale the products of exploratory steps in production mode?
2. Needs to run different parts of the workflow on changing distributed platforms:
   - Is workflow scheduling a closed control loop problem?
3. Accountability and reporting needed at each step:
   - What does provenance and reproducibility mean in dynamic applications?
Work funded by NSF, DOE, NIH, UC San Diego and industry partners.