Workflow Management System Simulation Workbench

- Accurate, scalable, and reproducible simulations

http://wrench-project.org
Scientific Workflows are key to advances in science and engineering

Their executions are complex:

Workflow structures are large and can be configured in various ways

Workflow Management Systems (WMS) are large multi-component software systems that employ ranges of decision making algorithms

Workflow execution platforms are heterogeneous and diverse

We need a strong “experimental science” approach to study these complex systems in a view to optimizing workflow executions

Yet real-world experiments are inherently limited

Time- and resource-intensive
Limited to existing configurations
Require full-fledged implementations
...
Objectives

Realize a workflow execution simulation methodology that has high simulation accuracy, low execution time, and low memory footprint.

This framework is to be used:

- By workflow users to study workflow executions
- By WMS developers to inform system and algorithm design decisions
- By educators to teach distributed computing in the context of workflows
What is WRENCH?

WRENCH enables novel avenues for scientific workflow use, research, development, and education in the context of large-scale scientific computations and data analyses.

WRENCH is an open-source library for developing simulators.

WRENCH exposes several high-level simulation abstractions to provide high-level building blocks for developing custom simulators.
Why SimGrid?

SimGrid is a **research project**

Development of **simulation models** of hardware/software stacks
Models are **accurate** (validated/invalidated) and **scalable** (low computational complexity, low memory footprint)

SimGrid is **open source usable software**

Provides different APIs for a range of simulation needs, e.g.:

- **S4U**: General simulation of Concurrent Sequential Processes
- **SMPI**: Fine-grained simulation of MPI applications

SimGrid is **versatile scientific instrument**

Used for (combinations of) **Grid, HPC, Peer-to-Peer, Cloud, Fog** simulation projects

First developed in 2000, latest release: v3.21 (September 2018)
System to Simulate

**Compute Services**
- Bare-metal servers
- Cloud platforms
- Virtualized Cluster platforms
- Batch-scheduled clusters

**Storage Services**
- Including scratch spaces

**File Registry Services**
- Replica catalog (key-value pairs)

**Network Proximity Services**
- Database of host-to-host network distances (Vivaldi)

**Workflow Management Systems**
- Decision-making for optimizing various objectives (static and dynamic)
- Pilot Jobs
Building a Simulator

Blueprint for a WRENCH-based simulator

- Create and initialize a simulation
- Instantiate a simulated platform
- Instantiate services on the platform
- Create at least one workflow
- Instantiate at least one WMS per workflow
- Launch the simulation
- Process simulation output

WRENCH + SimGrid internals

**Agent**: some code, some private data, running on a given host

**Task**: amount of work to do and of data to exchange

**Host**: location on which agents execute

**Mailbox**: Rendez-vous points between agents

You can send ‘data’ to a mailbox; you receive ‘data’ from a mailbox

Communication time between sender/receiver is accounted (**payload**) and depends on the network traffic
1000 Genome Sequencing Analysis Workflow

Identifies mutational overlaps using data from the 1000 genomes project

22 Individual tasks, 7 Population tasks, 22 Sifting tasks, 154 Pair Overlap Mutations tasks, and 154 Frequency Overlap Mutations tasks (Total 359 tasks)
Preliminary Results

Experiment Configuration

Simulation based on a real Computing Infrastructure

**ExoGENI testbed**

Network IaaS national testbed powered by the ORCA (Open Resource Control Architecture) control software used for GENI

ORCA allows users to create mutually isolated slices of interconnected infrastructure from multiple independent providers (compute, network, and storage) and commodity infrastructure.
Preliminary Results

Simulated Platform

![Diagram of a simulated platform with a data node, master server (submit host), and worker nodes. The worker nodes are modeled as 4 cores each and the master server is a submit host.]

SimGrid Platform description file

```xml
<?xml version='1.0'?>
<!DOCTYPE platform SYSTEM "http://simgrid.gforge.inria.fr/simgrid/simgrid.dtd">
<platform version="4.1">
    <zone id="AS0" routing="Full">
        <host id="master" speed="1f" core="4"/>
        <host id="data" speed="1f" core="1"/>
        <host id="workers1-0" speed="1f" core="4"/>
        <host id="workers1-1" speed="1f" core="4"/>
        <host id="workers1-2" speed="1f" core="4"/>
        <host id="workers1-3" speed="1f" core="4"/>
        <host id="workers1-4" speed="1f" core="4"/>
        <link id="1" bandwidth="125MBps" latency="100us"/>
        <link id="2" bandwidth="55MBps" latency="100us"/>
        <route src="master" dst="workers1-2">
            <link_ctn id="1"/>
        </route>
        <route src="master" dst="workers1-0">
            <link_ctn id="1"/>
        </route>
        <route src="master" dst="workers1-3">
            <link_ctn id="1"/>
        </route>
        <route src="master" dst="workers1-1">
            <link_ctn id="1"/>
        </route>
        <route src="master" dst="workers1-4">
            <link_ctn id="1"/>
        </route>
        <route src="data" dst="master">
            <link_ctn id="2"/>
        </route>
    </zone>
</platform>
```
Preliminary Results

Simulated Workflow Management System

https://github.com/wrench-project/pegasus
**Preliminary Results**

*Simulation Results and Accuracy*

> 98% workflow makespan accuracy

Simulated **compute** and **data transfer** tasks includes simulation of auxiliary tasks (e.g., create_dir, cleanup, and registration), and PRE and POST script jobs

Simulates delays on both DAGMan and HTCondor daemons
# Software Availability

## Code Repository, Releases, Software Engineering Process

### Open-source repository

[https://github.com/wrench-project/wrench](https://github.com/wrench-project/wrench)

### Releases

<table>
<thead>
<tr>
<th>Version</th>
<th>Date</th>
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<tbody>
<tr>
<td>1.0</td>
<td>(June 16, 2018)</td>
</tr>
<tr>
<td>1.0-beta</td>
<td>(April 15, 2018)</td>
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<tr>
<td>1.0-alpha</td>
<td>(December 1, 2017)</td>
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### Upcoming releases (estimated)

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<th>Version</th>
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<tr>
<td>1.0.1</td>
<td>(August 2018)</td>
</tr>
<tr>
<td>1.1</td>
<td>(September 2018)</td>
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### Continuous Integration

[https://travis-ci.org/wrench-project/wrench](https://travis-ci.org/wrench-project/wrench)

### Tests Coverage

[https://coveralls.io/github/wrench-project/wrench](https://coveralls.io/github/wrench-project/wrench)

### Code Review

[https://sonarcloud.io/dashboard?id=wrench](https://sonarcloud.io/dashboard?id=wrench)
It is crucial to teach undergraduate students parallel and distributed computing. But it is not easy giving students access to sufficiently diverse and realistic software/hardware platforms dealing with platform down-times and instabilities dealing with time-consuming and possible costly executions.

Simulation resolves these difficulties and WRENCH provides the foundation for pedagogic modules on parallel and distributed computing that use workflows as a motivating context.
Simulation Building Blocks
Prototype implementations of Workflow Management System (WMS) components and underlying algorithms

Simulation Accuracy
Captures the behavior of a real-world system with as little bias as possible via validated simulation models

Scalability
Low ratio of simulation time to simulated time, ability to run large simulations on a single computer with low compute, memory, and energy footprints

Reproducible Results
Enable the reproduction or repetition of published results by a party working independently using the same or different simulation models
Our Team

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