Flash-X, An Open-Source Simulation Software Instrument

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Mathematics and Computer Science,
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Lemont, IL

GitHub Open-Source Fridays
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FUNDING ACKNOWLEDGMENT

LAND ACKNOWLEDGMENT

The City of Chicago is located on land that is and has long been a center for Native peoples. The area is the traditional homelands of the Anishinaabe, or the Council of the Three Fires: the Ojibwe, Odawa, and Potawatomi Nations. Many other Nations consider this area their traditional homeland, including the Myaamia, Ho-Chunk, Menominee, Sac and Fox, Peoria, Kaskaskia, Wea, Kickapoo, and Mascouten

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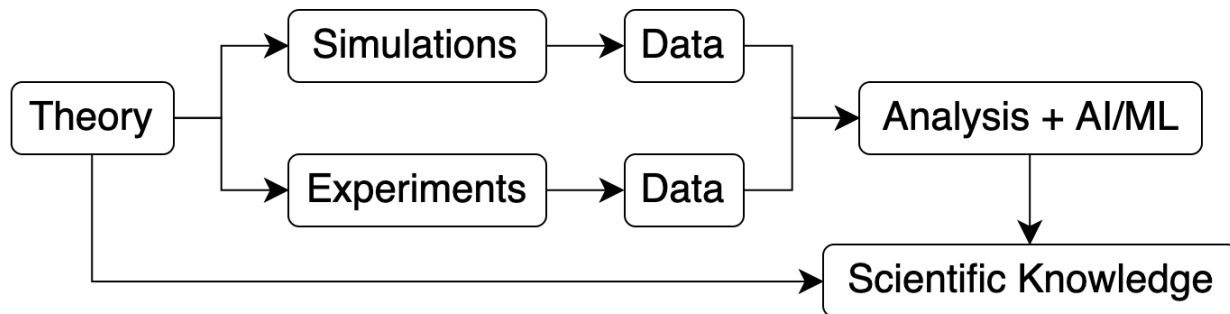- Elias Balaras

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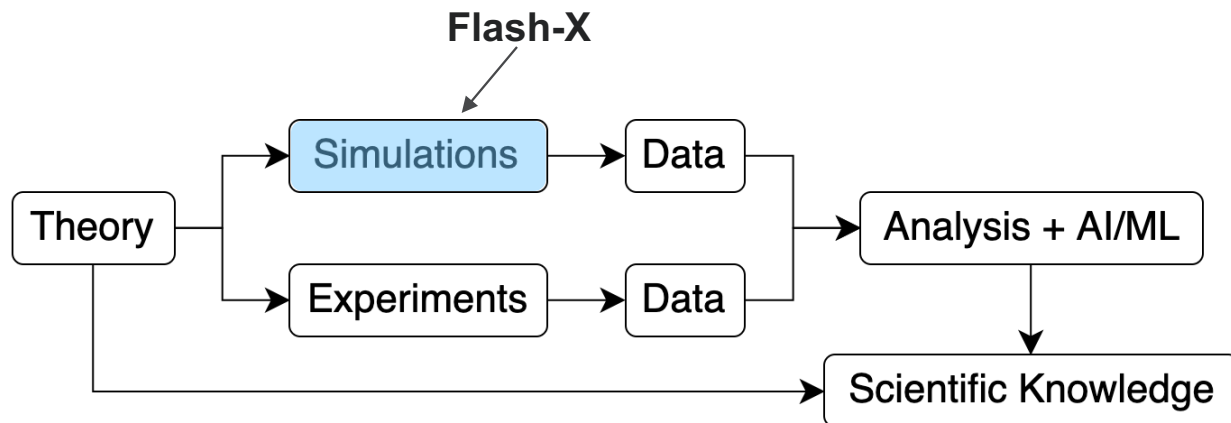- Rajeev Jain
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SCIENTIFIC WORKFLOW

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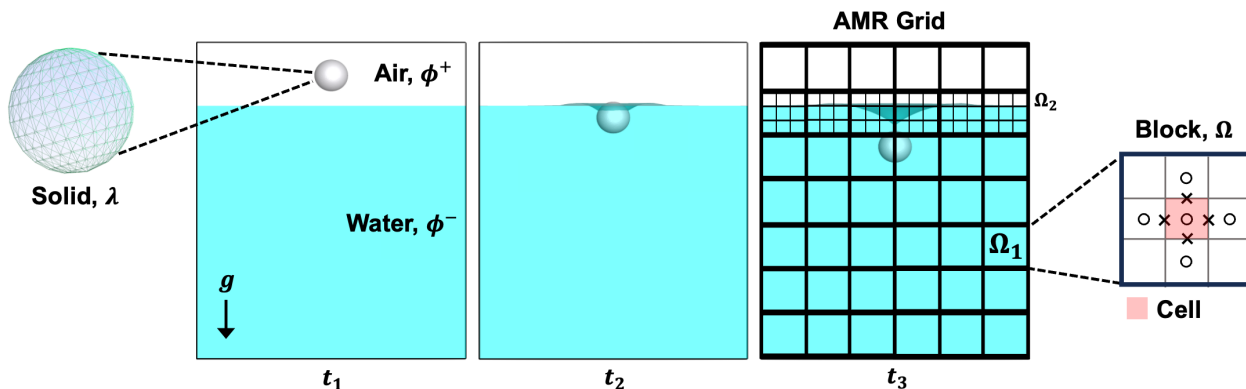
SCIENTIFIC WORKFLOW

Simulations solve physics-based partial differential equations in space and time

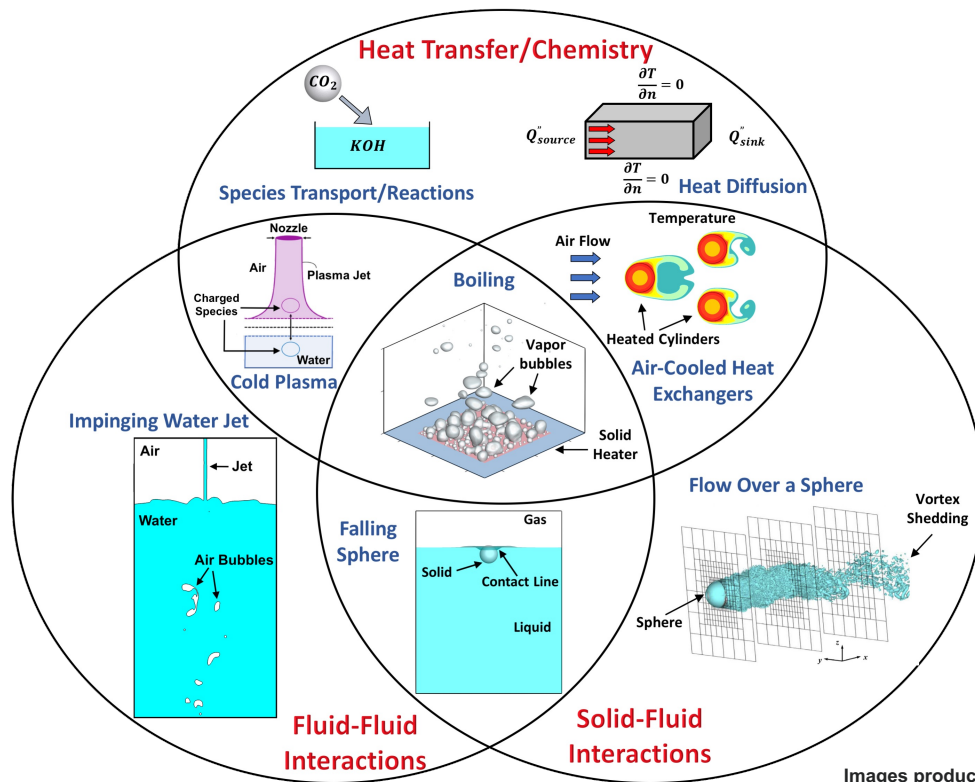$$\frac{\partial Q}{\partial t} - \vec{u} \cdot \nabla Q = K\nabla^2 Q + f$$

Temporal Evolution — $\frac{\partial Q}{\partial t}$

Advection — $\vec{u} \cdot \nabla Q$

Diffusion — $K\nabla^2 Q$

Source Terms — f

- *Solid-Fluid and Liquid-Gas interfaces are presented with level-set functions, λ (+ in solid, - in fluids) and ϕ (+ in gas, - in liquid) respectively.*

- *AMR – Adaptive Mesh Refinement*

Venn diagram of Multiphysics interactions and applications that can be modeled using Flash-X
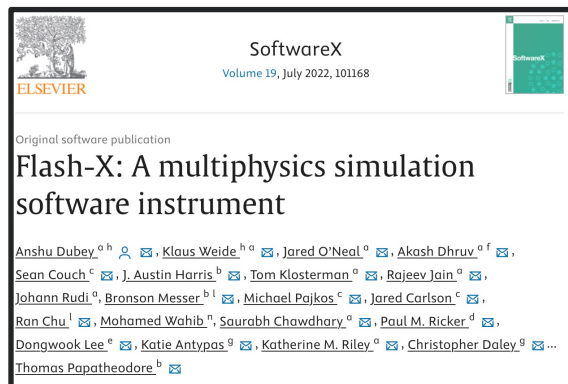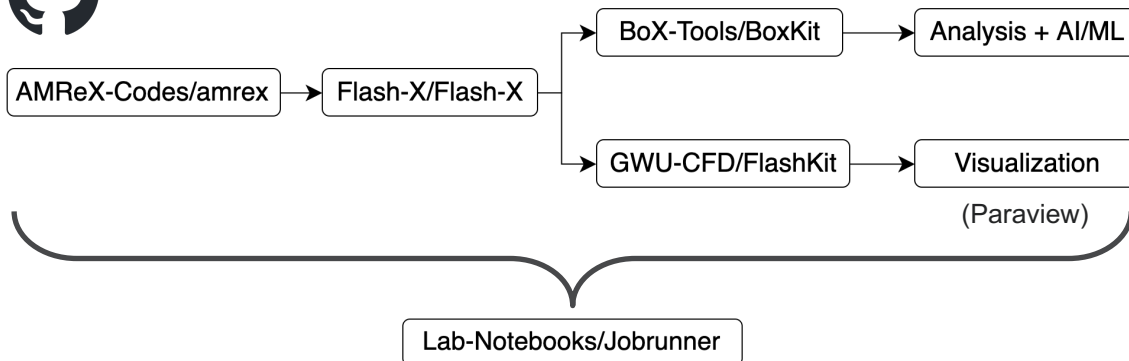

Images produced by:
- Akash Dhruv, GWU, 2015-2019
- Luis Martinez, GWU, 2016-2019
- Marcos Vanella, GWU, 2009-2010

FLASH-X WORKFLOW

Open-source with Apache 2.0 license (**https://flash-x.org**), designed for exascale platforms. Recipient of 2022 R&D 100 award.

LABORATORY NOTEBOOKS

- **Laboratory notebooks are a common practice in experimental science to record and reproduce scientific observations.**

- **Computational science lacks this rigor.**

- **In-depth analysis by Jared O'Neal (https://www.youtube.com/watch?v=OpzofH8U0Bs).**

LABORATORY NOTEBOOKS

```
# Setting up software and dependencies
jobrunner setup software/amrex
jobrunner setup software/flashx

# Setting up and running experiments
jobrunner setup simulation/FlowBoiling
jobrunner submit simulation/FlowBoiling

# Archiving results to jobnode.archive
jobrunner archive \
          simulation/FlowBoiling

# Running Flash-X test suite
jobrunner submit tests
```

FIGURE ⬜ Jobrunner commands for setting up dependencies, running tests and experiments, and archive data. These commands are executed from the root of the directory-tree
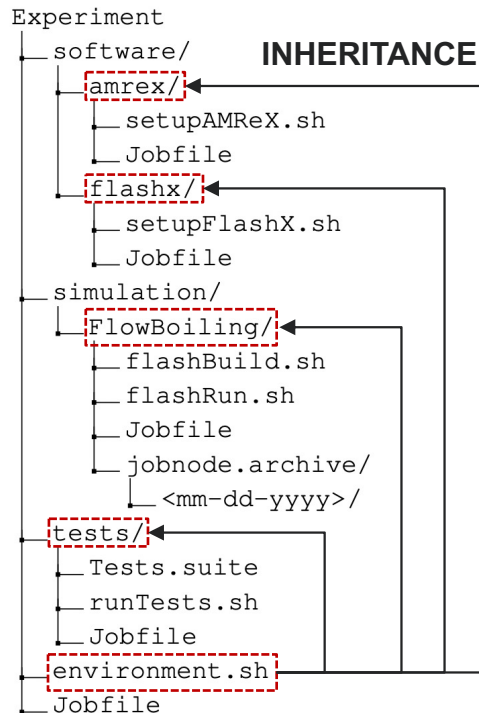
Lab-Notebooks / **Jobrunner**

```
Experiment
 ├─ software/                    INHERITANCE
 │   ├─ amrex/
 │   │   ├─ setupAMReX.sh
 │   │   └─ Jobfile
 │   ├─ flashx/
 │   │   ├─ setupFlashX.sh
 │   │   └─ Jobfile
 ├─ simulation/
 │   ├─ FlowBoiling/
 │   │   ├─ flashBuild.sh
 │   │   ├─ flashRun.sh
 │   │   ├─ Jobfile
 │   │   └─ jobnode.archive/
 │   │       └─ <mm-dd-yyyy>/
 ├─ tests/
 │   ├─ Tests.suite
 │   ├─ runTests.sh
 │   └─ Jobfile
 ├─ environment.sh
 └─ Jobfile
```

FIGURE ⬜ Directory tree for a Flash-X experiment.

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LABORATORY NOTEBOOKS

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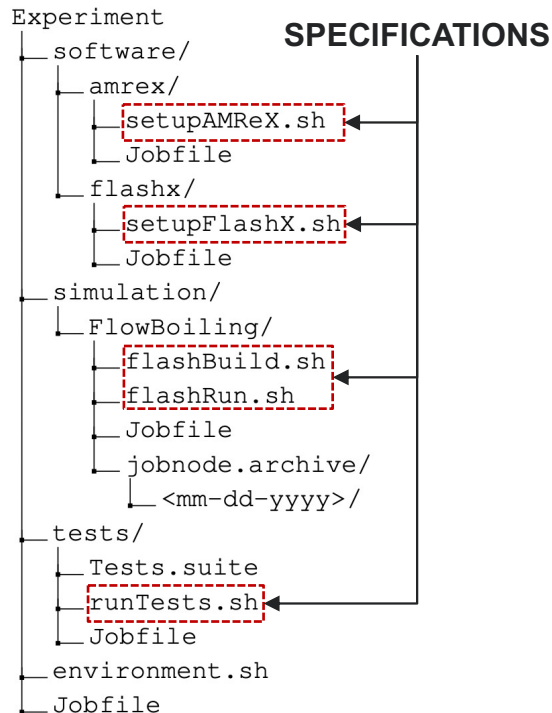
Lab-Notebooks / **Jobrunner**

SPECIFICATIONS

```
Experiment
└── software/
    └── amrex/
        ├── setupAMReX.sh
        └── Jobfile
    └── flashx/
        ├── setupFlashX.sh
        └── Jobfile
└── simulation/
    └── FlowBoiling/
        ├── flashBuild.sh
        ├── flashRun.sh
        ├── Jobfile
        └── jobnode.archive/
            └── <mm-dd-yyyy>/
└── tests/
    ├── Tests.suite
    ├── runTests.sh
    └── Jobfile
└── environment.sh
└── Jobfile
```

FIGURE ☐ Directory tree for a Flash-X experiment.

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LABORATORY NOTEBOOKS

EDITORS: Lorena A. Barba, labarba@gwu.edu
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DEPARTMENT: REPRODUCIBLE RESEARCH

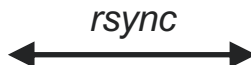## Managing Software Provenance to Enhance Reproducibility in Computational Research

Akash Dhruv and Anshu Dubey, *Argonne National Laboratory, Lemont, IL, 60439, USA*

Lab-Notebooks

Execution Environment

rsync

Data Clone

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