Flash-X, An Open-Source Simulation Software Instrument

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Argonne National Laboratory,
Lemont, IL

GitHub Open-Source Fridays
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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

COLLABORATIONS

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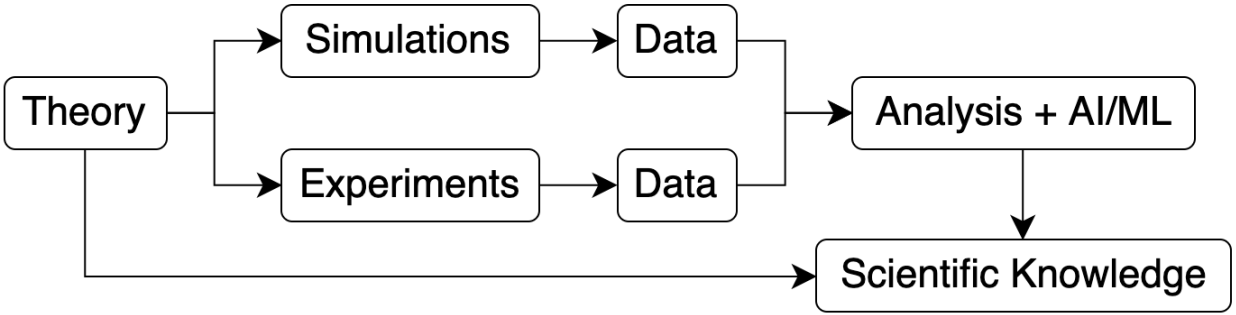
- Youngjun Lee
- Klaus Weide
- Tom Klosterman
- Rajeev Jain
- Wesley Kwiecinski

SCIENTIFIC WORKFLOW



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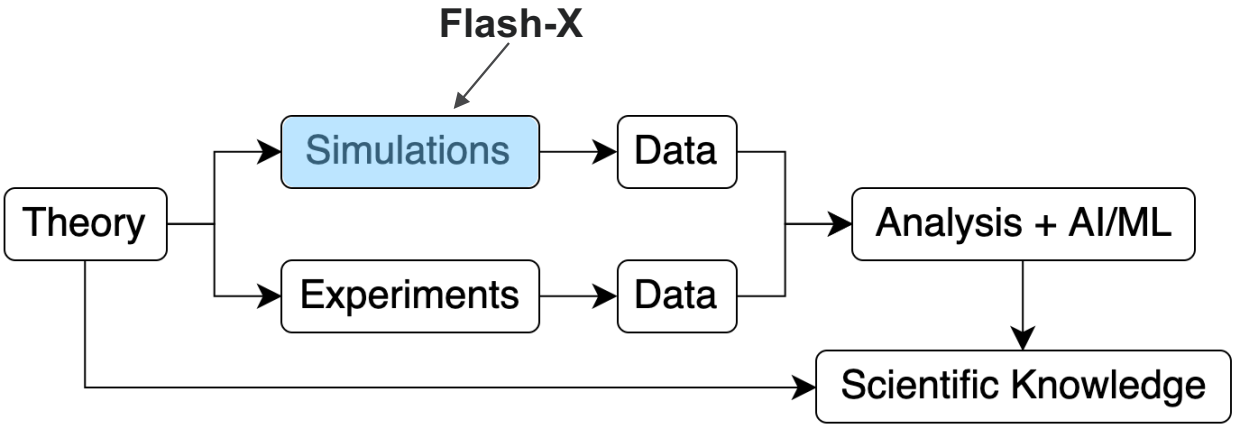
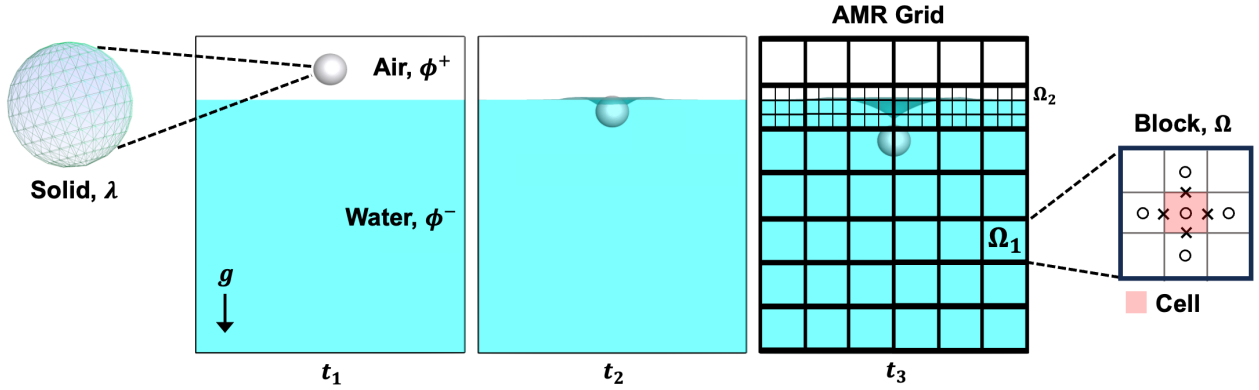
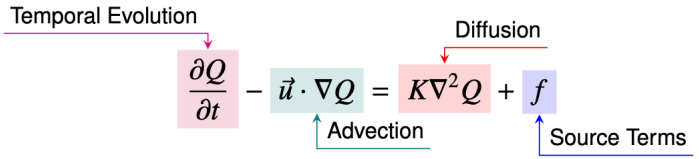


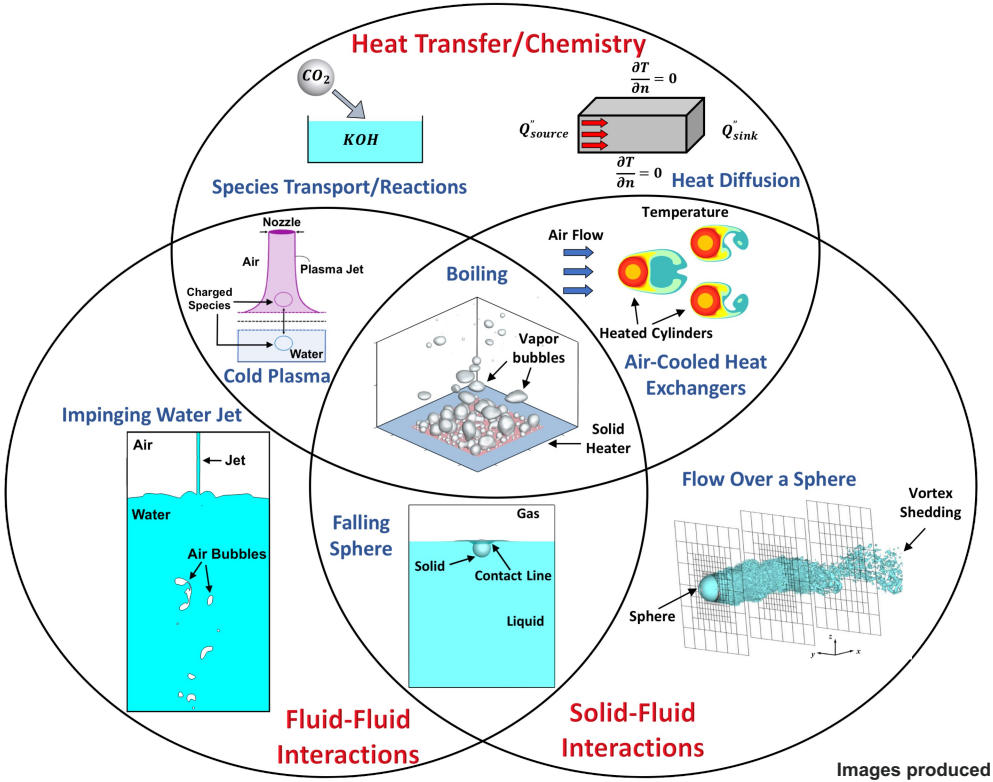
Simulations solve physics-based partial differential equations in space and time





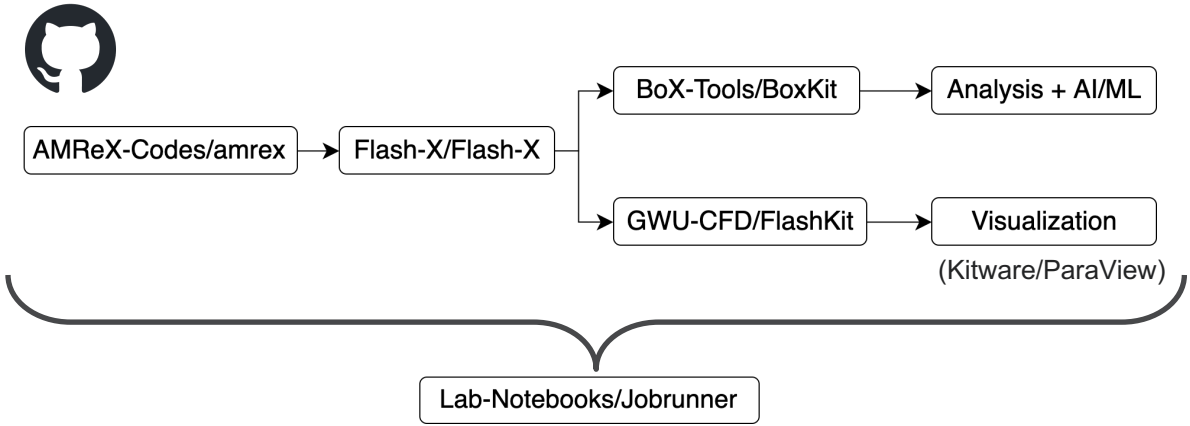
- ***Solid-Fluid and Liquid-Gas interfaces are presented with level-set functions, λ (+ in solid, - in fluids) and ϕ (+ in gas, - in liquid) respectively.***
- ***AMR – Adaptive Mesh Refinement***

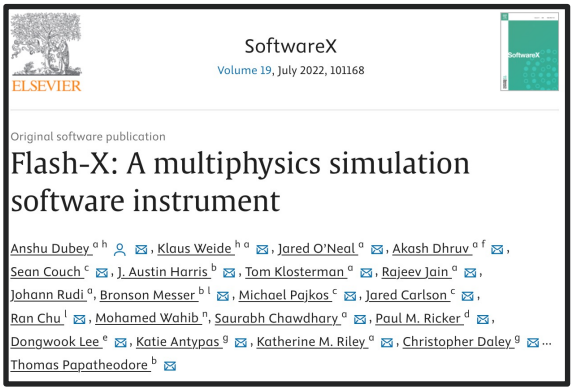
Venn diagram of Multiphysics interactions and applications that can be modeled using Flash-X



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

FLASH-X WORKFLOW





SoftwareX
Volume 19, July 2022, 101168

Original software publication

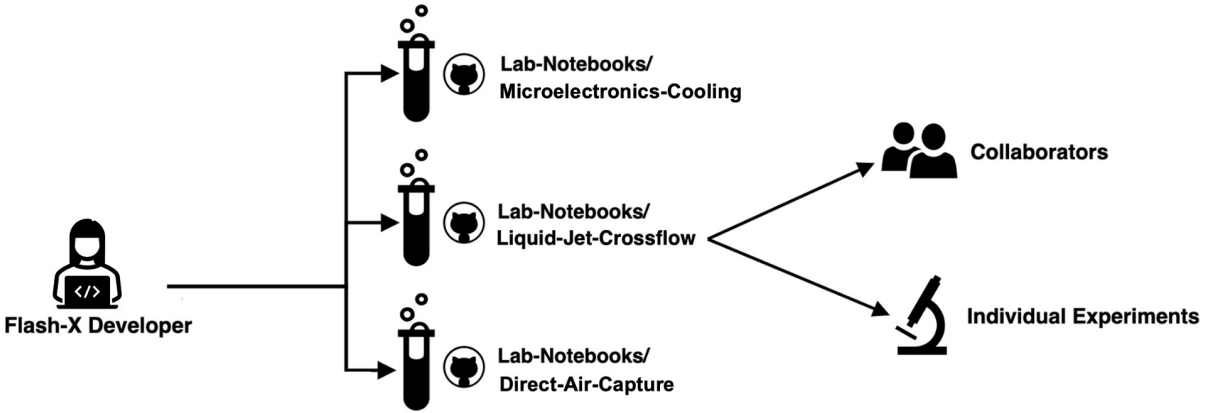
Flash-X: A multiphysics simulation software instrument

Anshu Dubey [a h], Klaus Weide [h a], Jared O'Neal [a], Akash Dhruv [a f], Sean Couch [c], J. Austin Harris [b], Tom Klosterman [a], Rajeev Jain [a], Johann Rudi [a], Bronson Messer [b l], Michael Pajkos [c], Jared Carlson [c], Ran Chu [l], Mohamed Wahib [n], Saurabh Chawdhary [a], Paul M. Ricker [d], Dongwook Lee [e], Katie Antypas [g], Katherine M. Riley [a], Christopher Daley [g] ... Thomas Papatheodore [b]

- Open-source with Apache 2.0 license (**https://flash-x.org**), designed for exascale platforms. Recipient of 2022 R&D 100 award.
- Interoperability between FORTRAN, C++, and Python.
- Multinode parallelization on supercomputers using Message Passing Interface (MPI) and OpenMP.
- Hybrid CPU-GPU computations.

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**

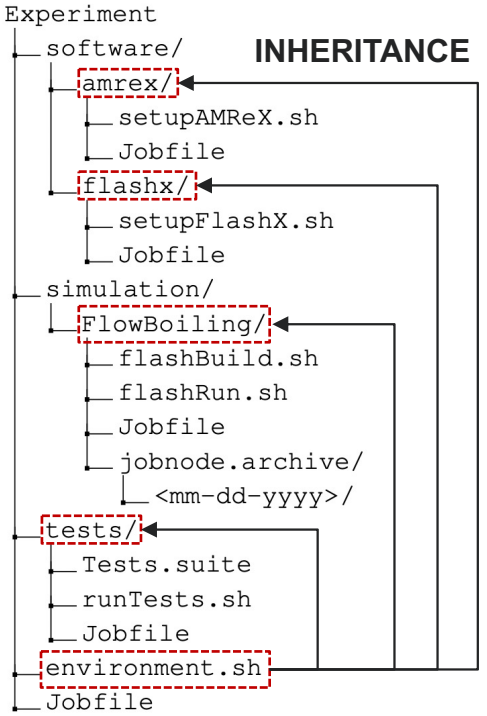


FIGURE Directory tree for a Flash-X experiment.

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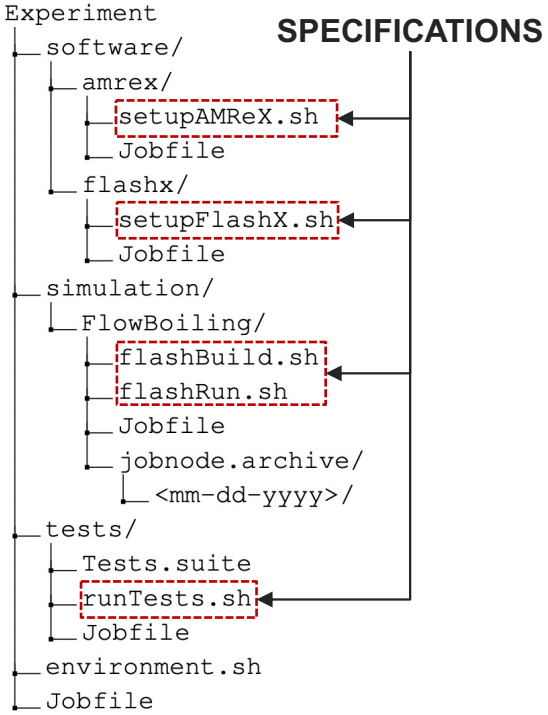

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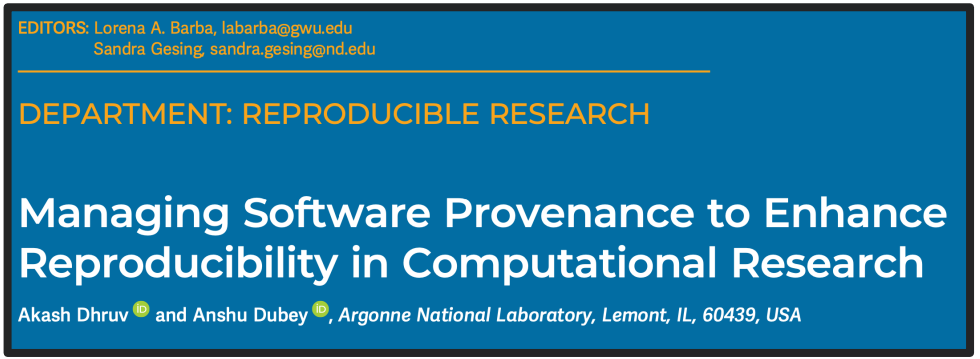
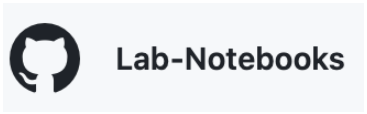
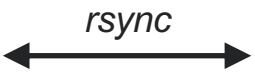




Execution Environment



Data Clone