Using Occam for accelerating Material Science Research

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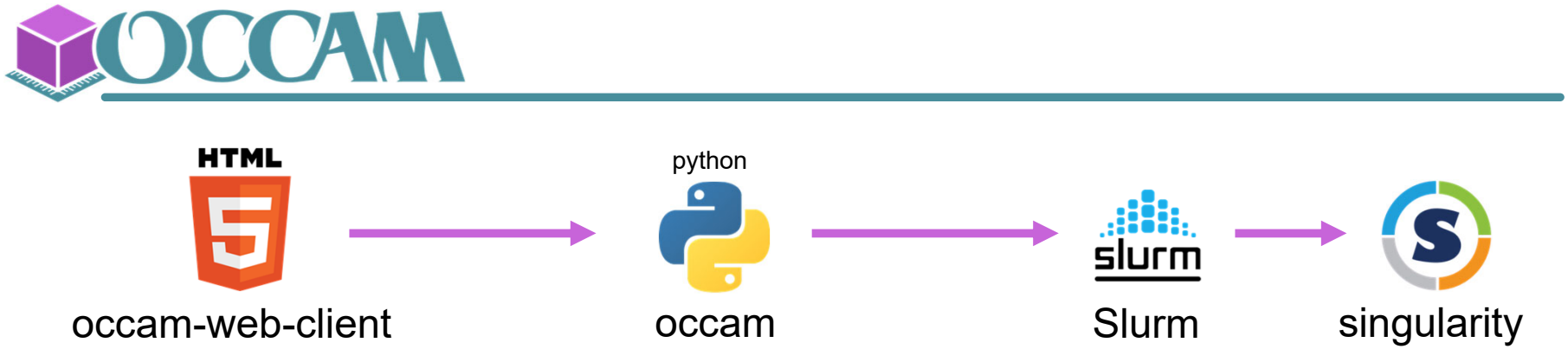
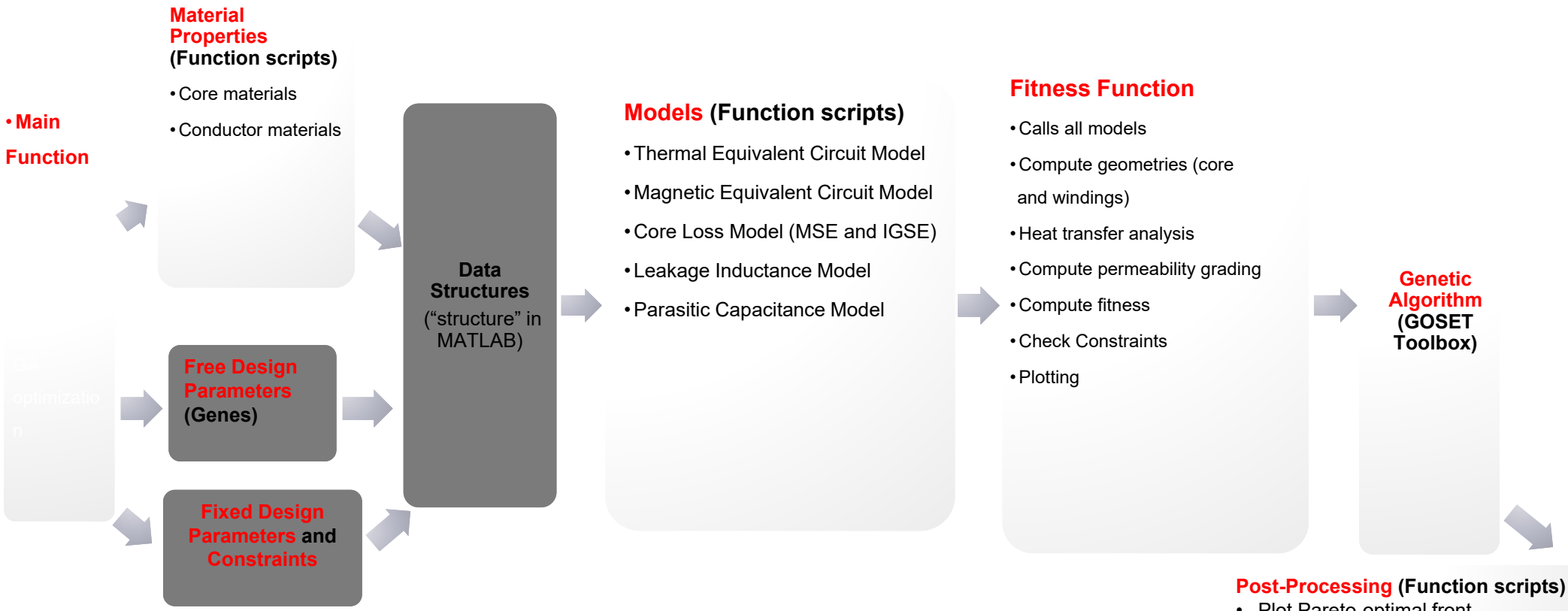
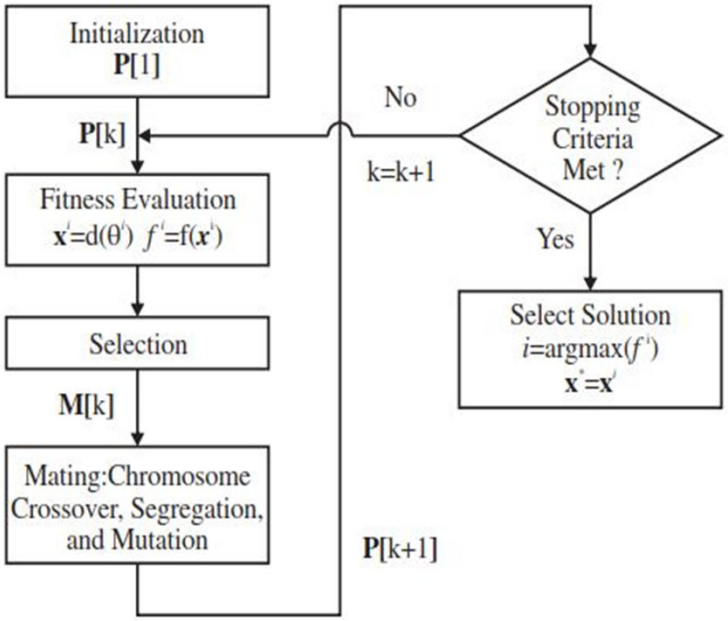
- Occam is a distributed workflow engine and software preservation system.
  - Primarily an object storage system with a web-based client.
  - Each Occam object is executed in a cluster node using containers services
  - Open source (gitlab) using existing free and open-source technology. Docker and Singularity and queuing systems such as Slurm.



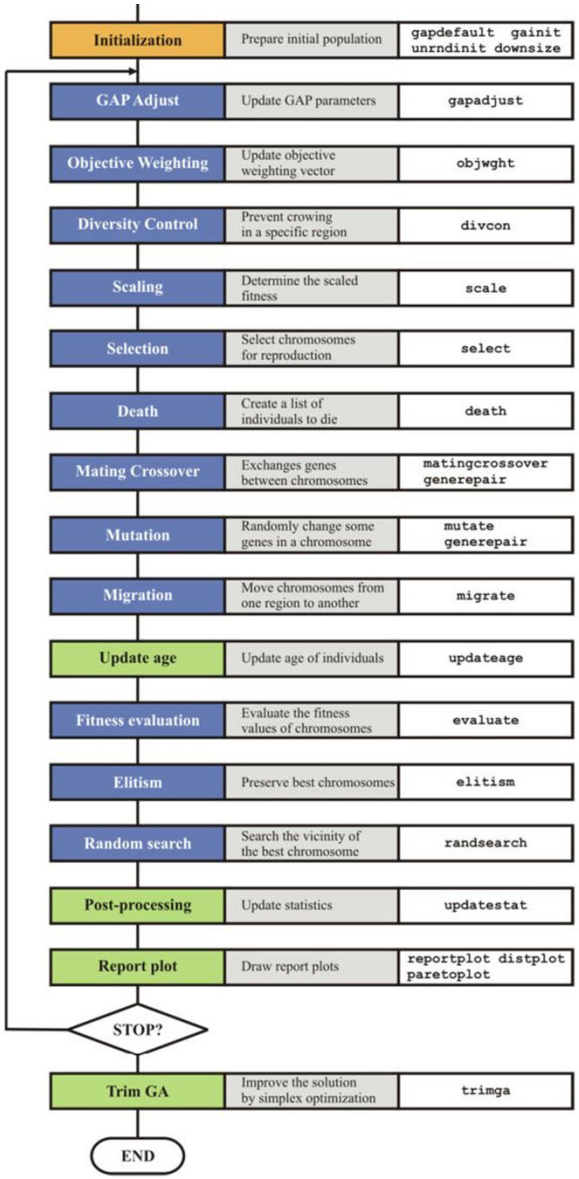
GOSET: Genetic Algorithm-based Tool for Magnetic Materials Optimization (Execution Flow)



GOSET Toolbox (GA) Execution Flow



General Genetic Algorithm



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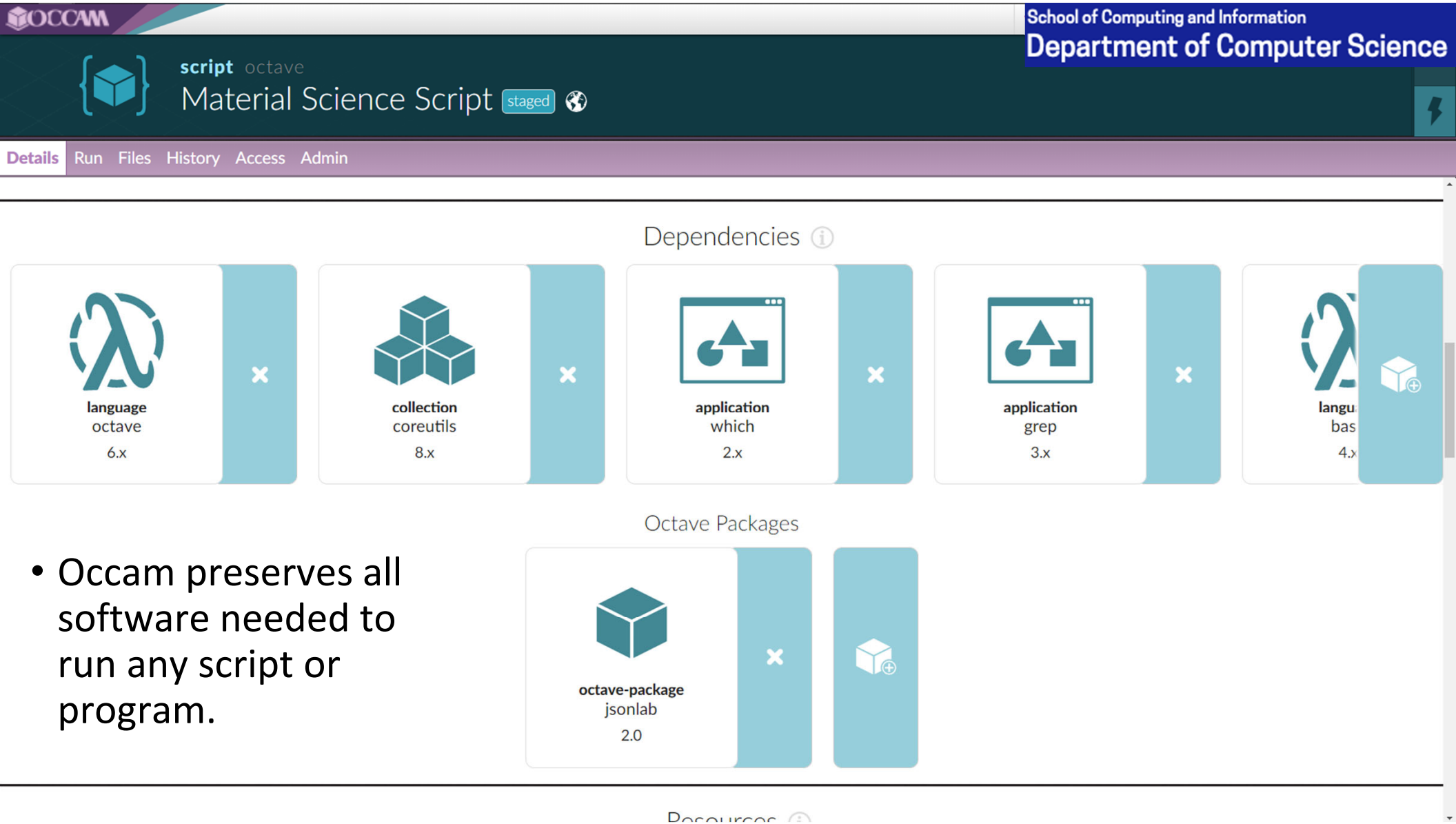
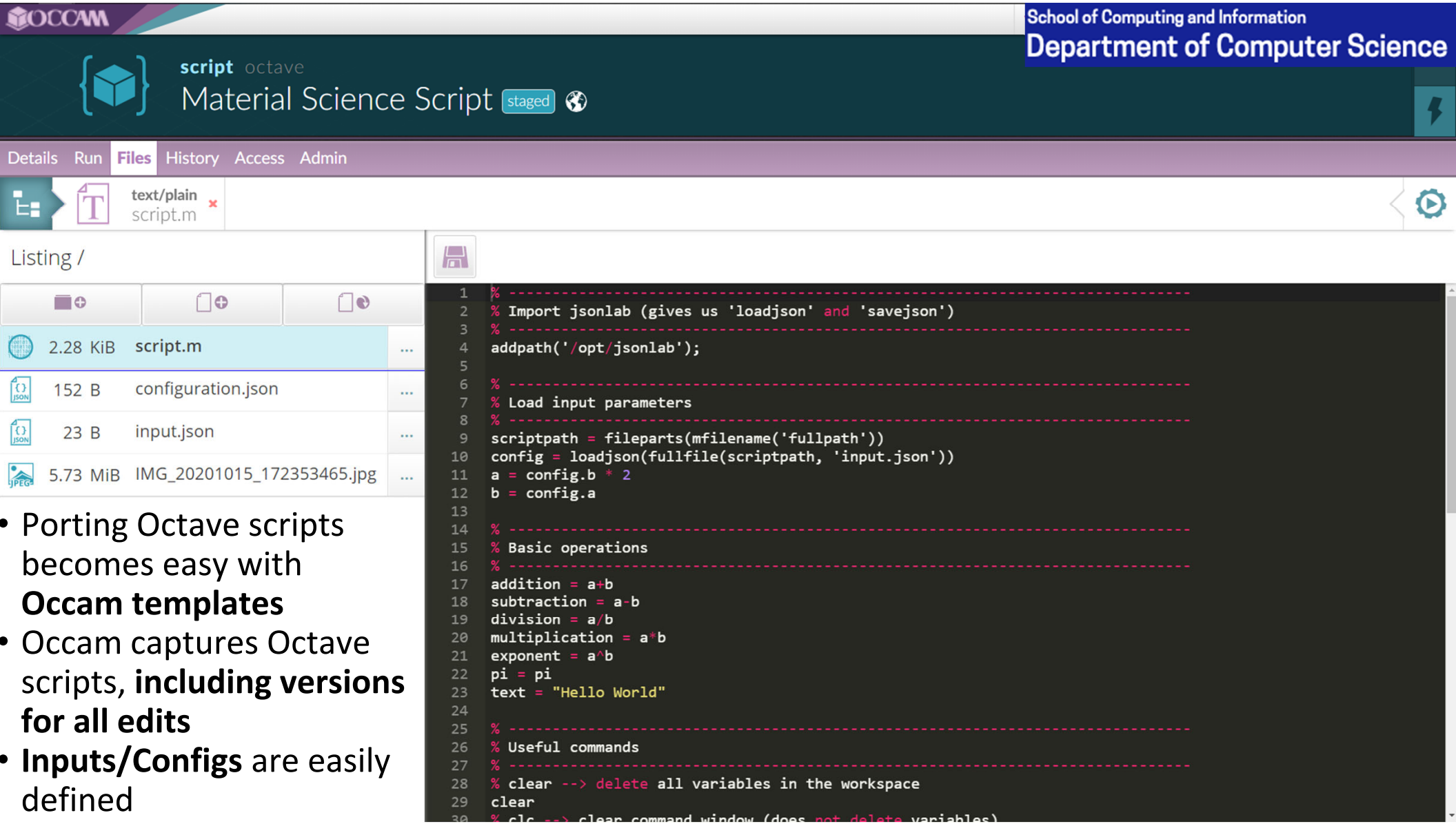
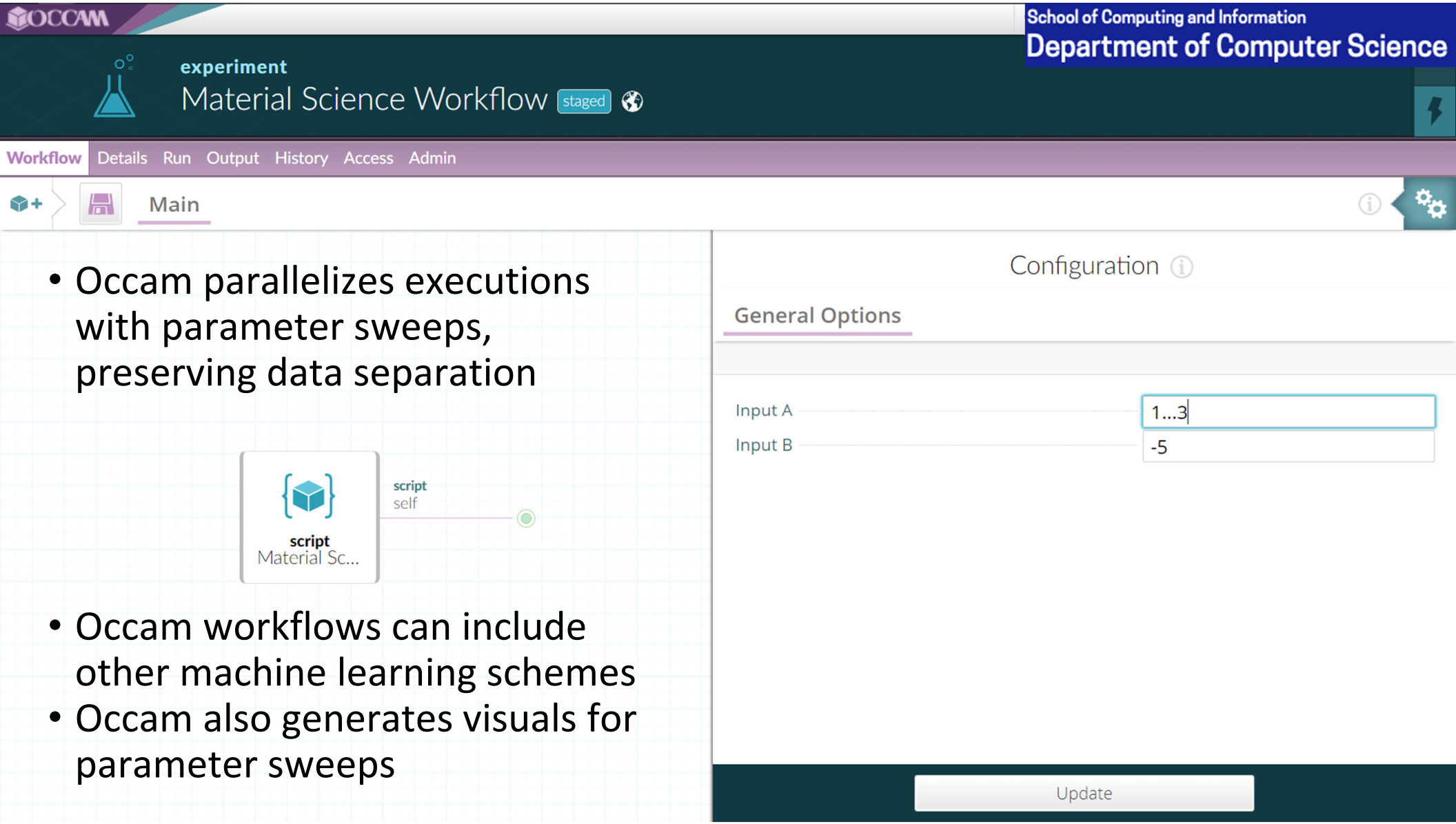
Actual GA Execution in GOSET



- Occam preserves all software needed to run any script or program.



- Porting Octave scripts becomes easy with **Occam templates**
- Occam captures Octave scripts, **including versions for all edits**
- **Inputs/Configs** are easily defined



- Occam parallelizes executions with parameter sweeps, preserving data separation

- Occam workflows can include other machine learning schemes
- Occam also generates visuals for parameter sweeps