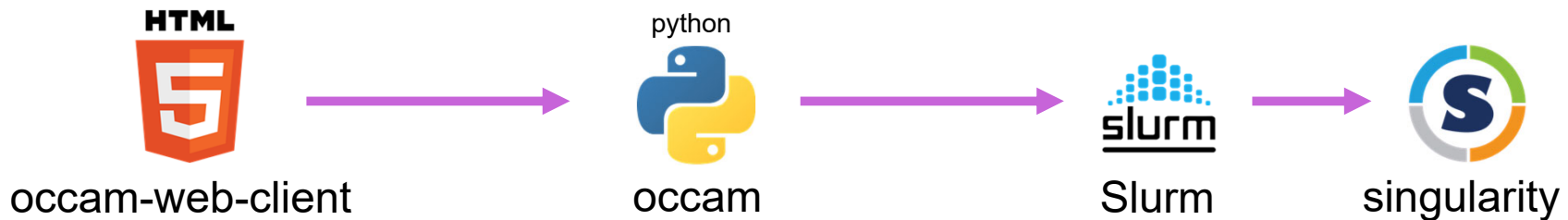


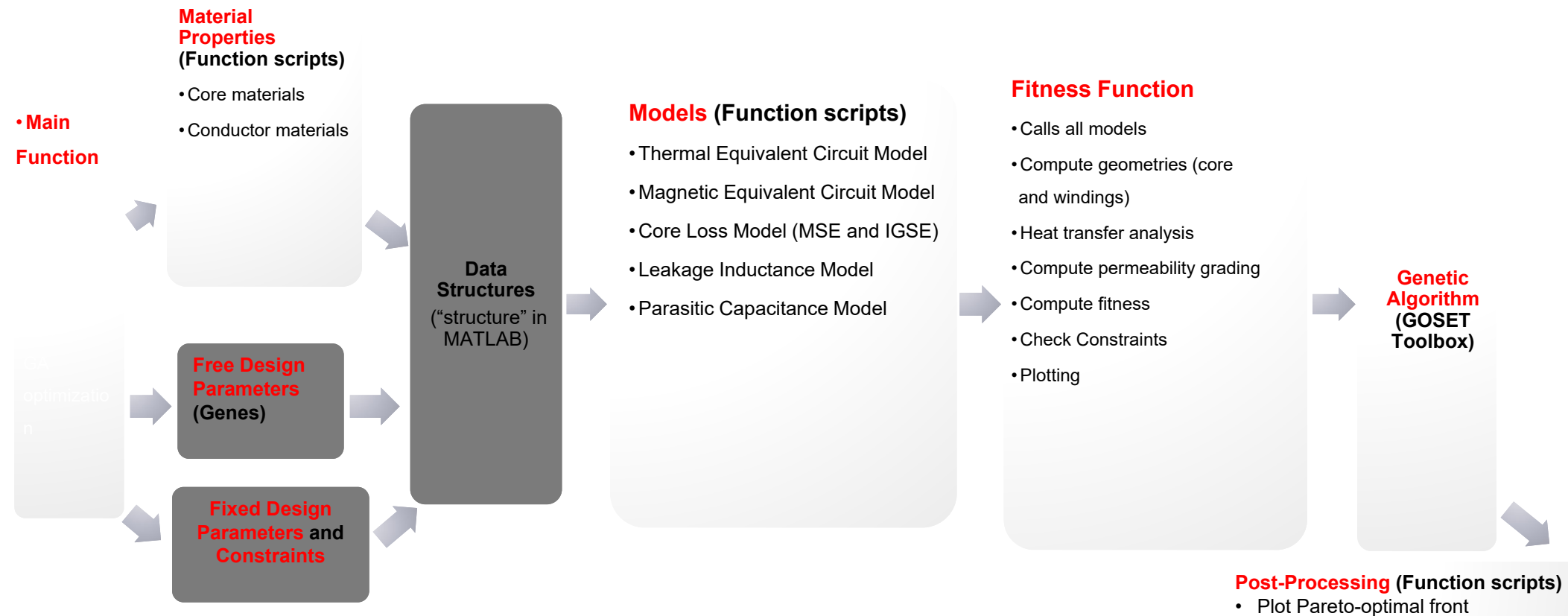
# Using Occam for accelerating Material Science Research

Bruce Childers, Daniel Mosse, and David Wilkinson  
Computer Science Dept, University of Pittsburgh

- 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.



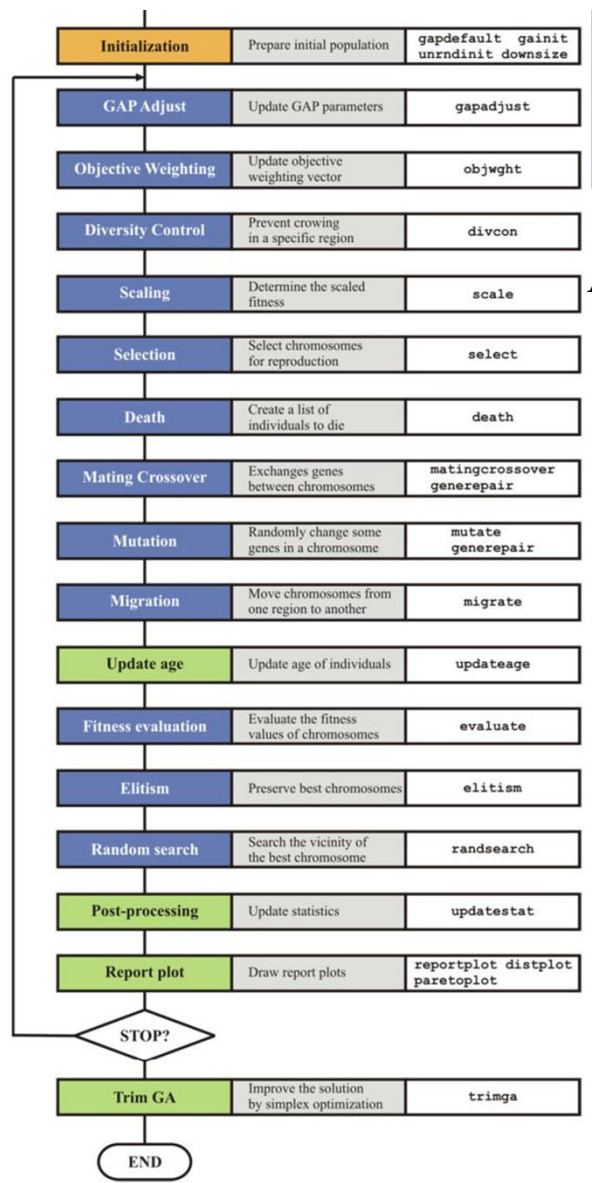
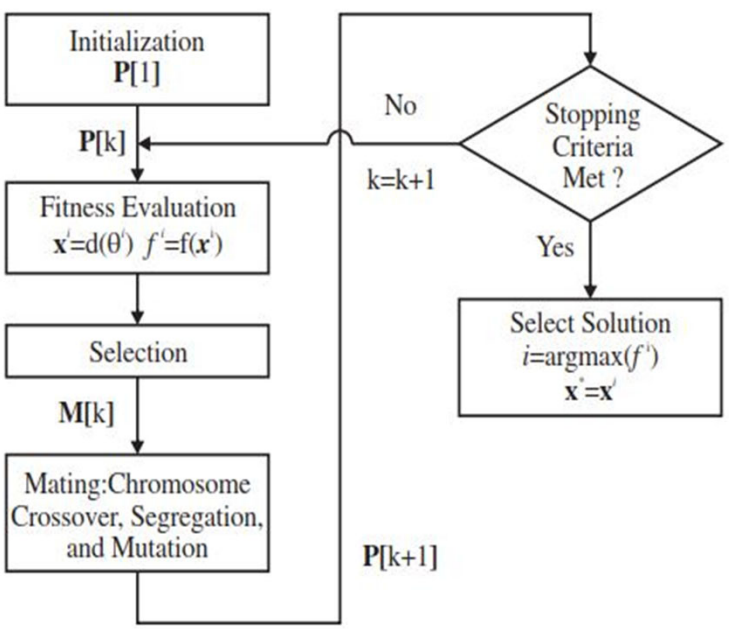
# GOSET: Genetic Algorithm-based Tool for Magnetic Materials Optimization (Execution Flow)



# GOSET Toolbox (GA) Execution Flow



Actual GA Execution  
in GOSET



General Genetic Algorithm



script octave

Material Science Script staged [Details](#) [Run](#) [Files](#) [History](#) [Access](#) [Admin](#)

## Dependencies

language  
octave  
6.xcollection  
coreutils  
8.xapplication  
which  
2.xapplication  
grep  
3.xlanguage  
basic  
4.x

## Octave Packages

octave-package  
jsonlab  
2.0

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

## Resources



script octave

Material Science Script staged Details Run **Files** History Access Admintext/plain  
script.m

Listing /

Size	Name	...
2.28 KiB	script.m	...
152 B	configuration.json	...
23 B	input.json	...
5.73 MiB	IMG_20201015_172353465.jpg	...

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

```
1 % -----
2 % Import jsonlab (gives us 'loadjson' and 'savejson')
3 % -----
4 addpath('/opt/jsonlab');
5
6 % -----
7 % Load input parameters
8 % -----
9 scriptpath = fileparts(mfilename('fullpath'))
10 config = loadjson(fullfile(scriptpath, 'input.json'))
11 a = config.b * 2
12 b = config.a
13
14 % -----
15 % Basic operations
16 % -----
17 addition = a+b
18 subtraction = a-b
19 division = a/b
20 multiplication = a*b
21 exponent = a^b
22 pi = pi
23 text = "Hello World"
24
25 % -----
26 % Useful commands
27 % -----
28 % clear --> delete all variables in the workspace
29 clear
30 % clc --> clear command window (does not delete variables)
```



experiment

Material Science Workflow staged 

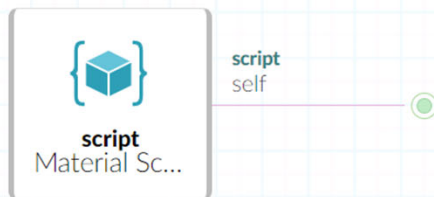
Workflow Details Run Output History Access Admin



Main



- Occam parallelizes executions with parameter sweeps, preserving data separation



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

Configuration General Options

Input A

Input B