Semantically-Organized Containers for Reproducible Research

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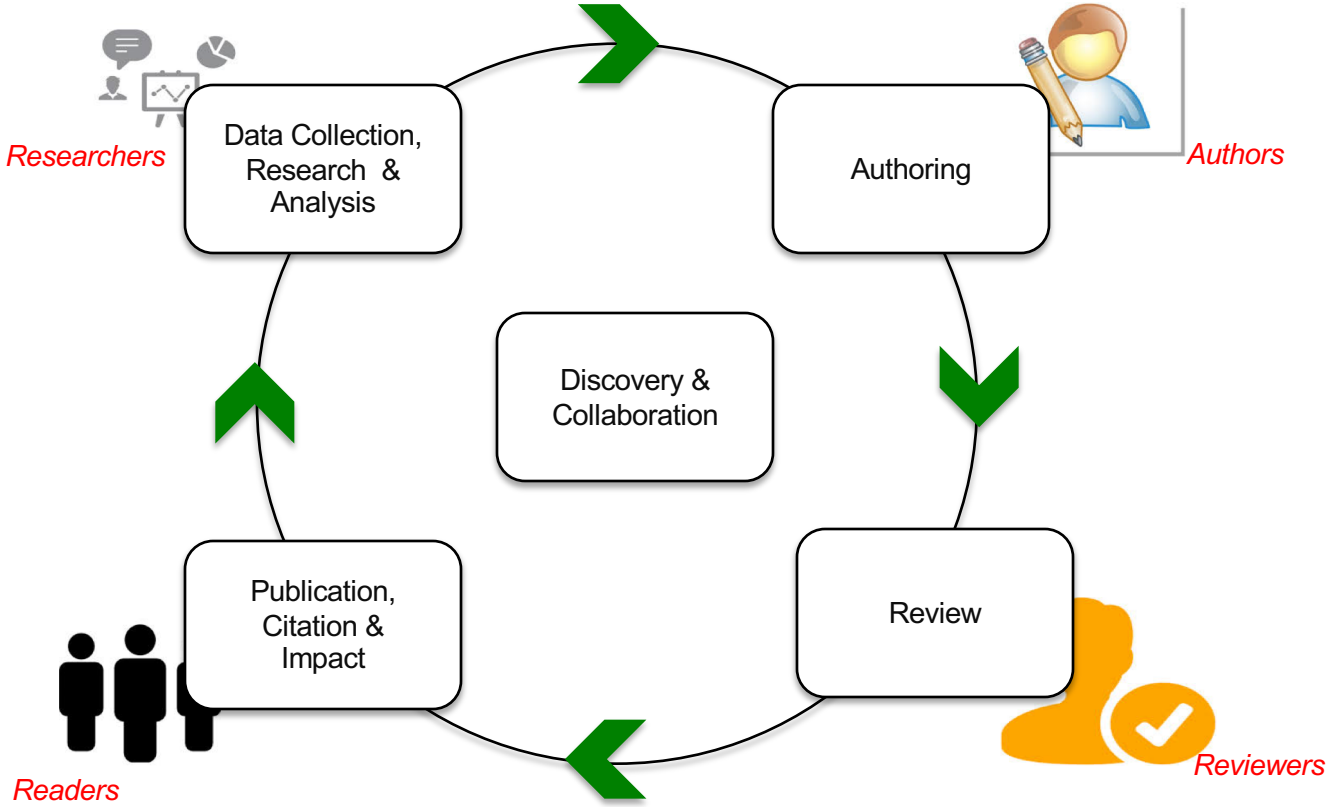
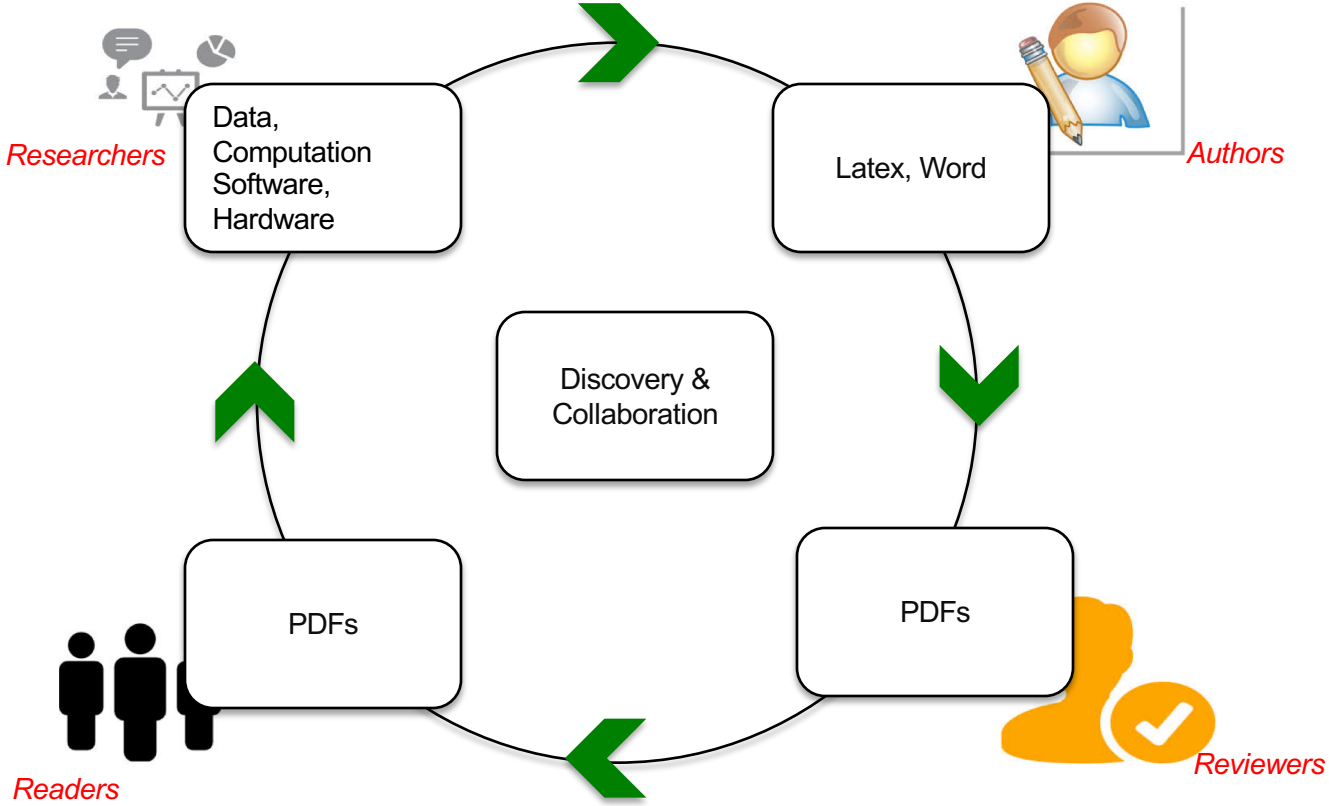
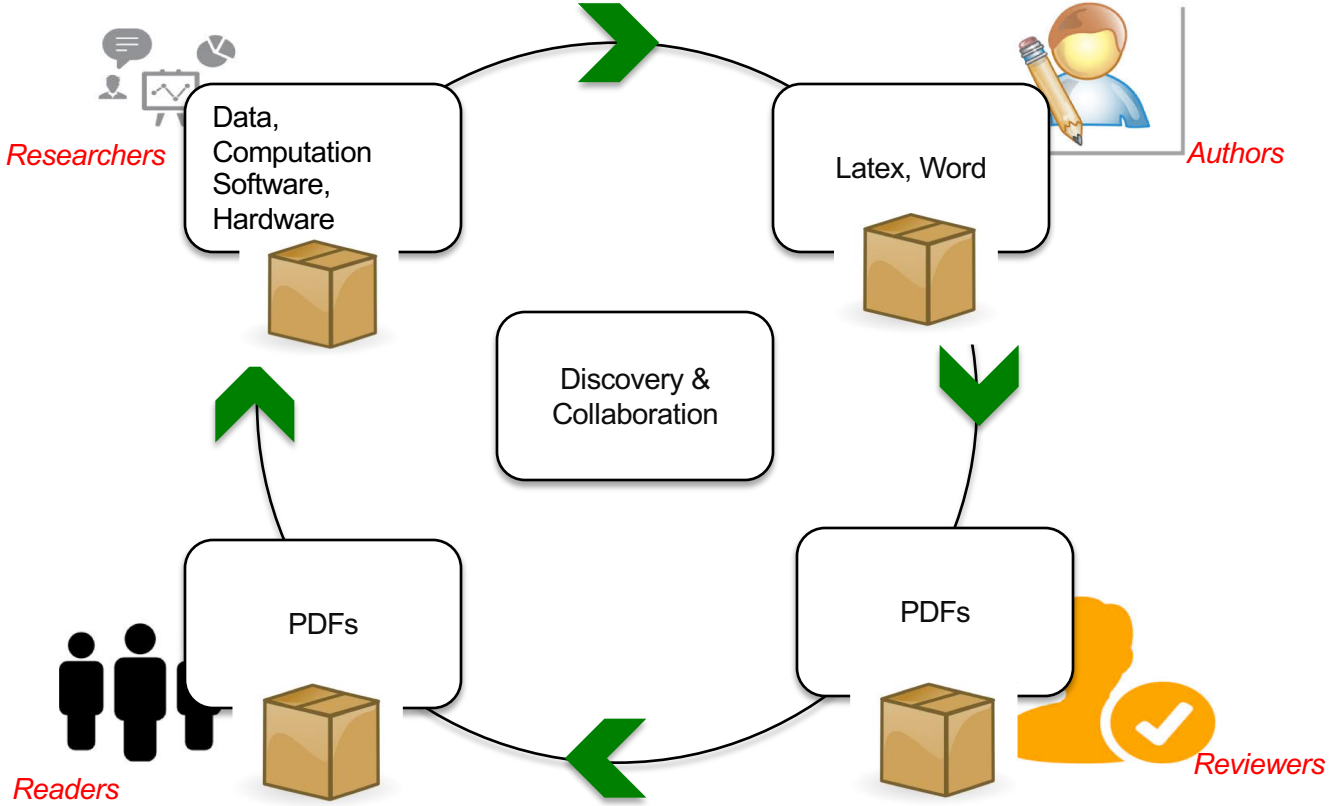
Scientific Publication Cycle



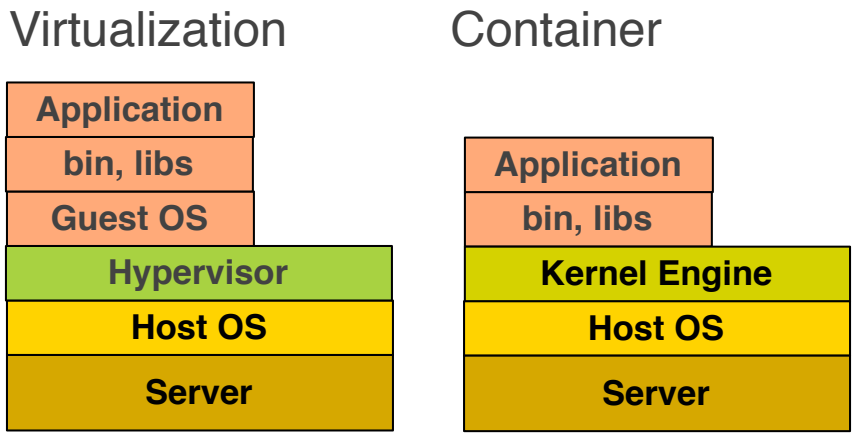
Scientific Publication Handoffs



Scientific Publication with Computational Handoffs



Containers



- Containers are lightweight alternative to virtualization.

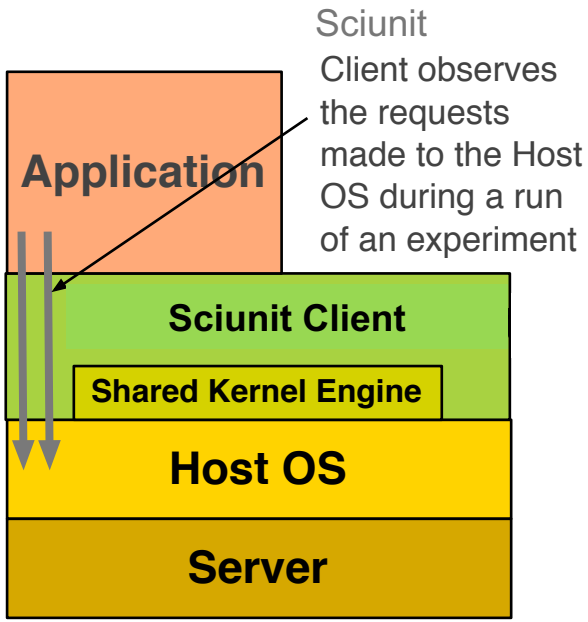
Containers for Reproducible Research

- Programmatic capture
  - Contain items that are irrelevant to the applications
  - E.g. various shell utilities and library versions unknown to user
- Rigid composition
  - No automatic way to distinguish input files from outputs to OS files or have any organization
- Large image sizes
  - Duplicate user software, environment and datasets arising from multiple runs
- Inefficient execution
  - Use layered file systems which can take a performance hit

Sciunit: Reusable Research Objects. In IEEE eScience '17

Sciunit: Automatic Containerization of Executions

http://sciunit.run



Sciunit

1. Create

2. Share

3. Run

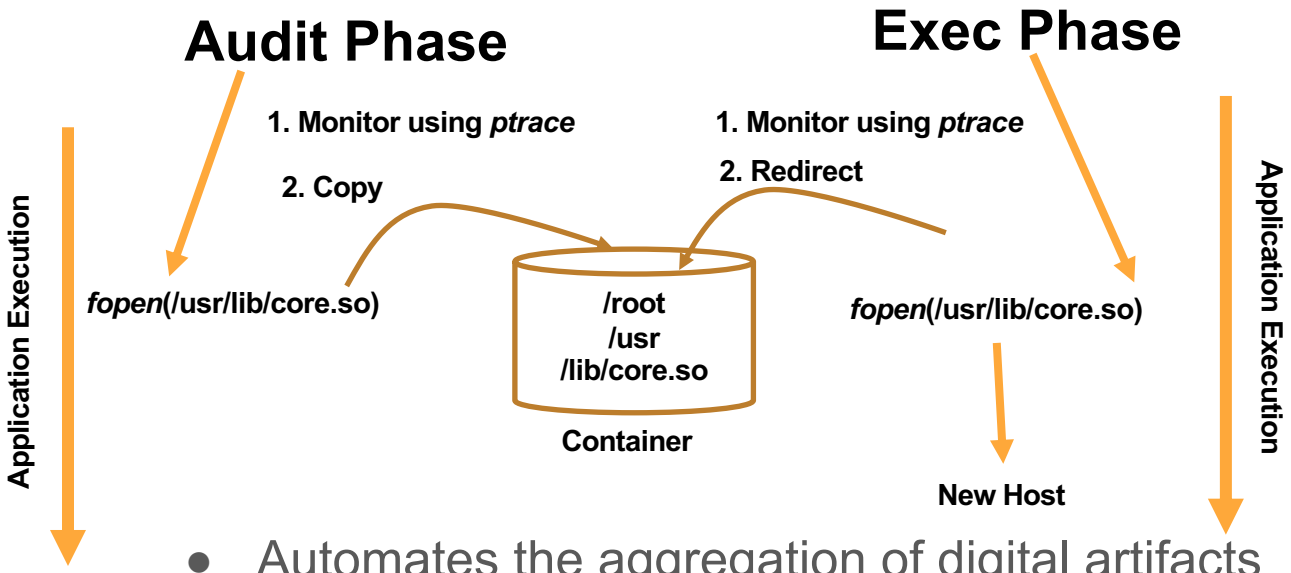




Globus RDP

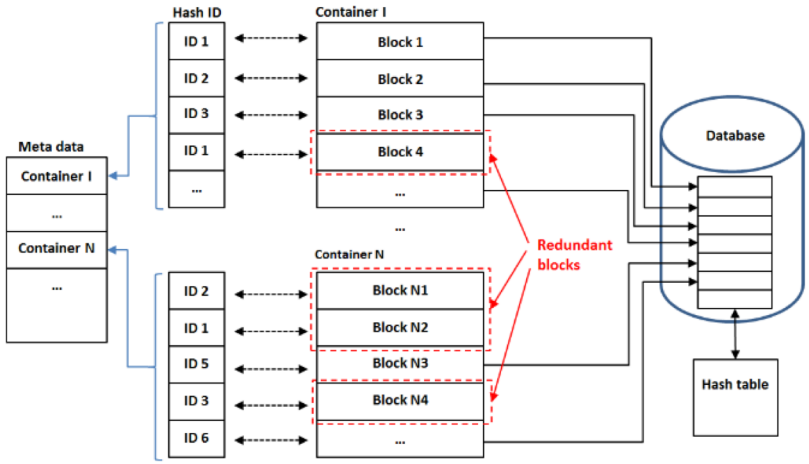


Application Virtualization



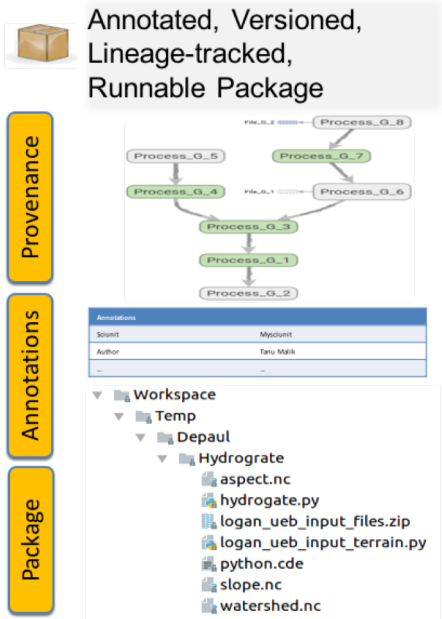
- Automates the aggregation of digital artifacts
  - Makes the computation portable and verifiable across environments.

Sciunit Storage



Deduplicated Container Storage

Sciunit


Annotated, Versioned,
Lineage-tracked,
Runnable Package
Provenance
Annotations
Package
Process_G_8
Process_G_5
Process_G_7
Process_G_4
Process_G_6
Process_G_3
Process_G_1
Process_G_2
Annotations
Sciunit
Mysciunit
Author
Tanu Malik
Workspace
Temp
Depaul
Hydrograte
aspect.nc
hydrogate.py
logan_ueb_input_files.zip
logan_ueb_input_terrain.py
python.cde
slope.nc
watershed.nc

Sample Interaction

```
1. > sciunit create FIE
2. > sciunit exec ./FIE.sh ./DATA/weather_201710.Rds
     0. Download…
     1. Calculate violation matrix…
     2. Calculate heat map…
     3. Generate model data with ./DATA/weather_201710.Rds…
     4. Apply random forest model…
     5. Evaluation…
3. > sciunit list
     e1 Dec 4 12:44 ./FIE.sh ./DATA/weather_201710.Rds
4. > sciunit show
     id: e1
     sciunit: FIE
     command: ./FIE.sh ./DATA/weather_201710.Rds
     size: 306.6 MB
     started: 2017-12-04 12:44
5. > sciunit push
     …
     Title for the new article: FIE
     new: 306.6 MB [01:05, 4.72MB/s]
6. > sciunit copy
     mSLLTj#
```

Host Computer

```
1. > sciunit repeat e1
     …
     0. Download…
     1. Calculate violation matrix…
     2. Calculate heat map…
     3. Generate model data with ./DATA/weather_201710.Rds…
     4. Apply random forest model…
     5. Evaluation…
     …
2. > sciunit repeat e1 <27050>
     …
     3. Generate model data with ./DATA/weather_201710.Rds…
     …
3. > sciunit given '/tmp/weather_201801.Rds' e1 %
     …
     0. Download…
     1. Calculate violation matrix…
     2. Calculate heat map…
     3. Generate model data with /tmp/weather_201801.Rds…
     4. Apply random forest model…
     5. Evaluation…
     …
```

Target Computer

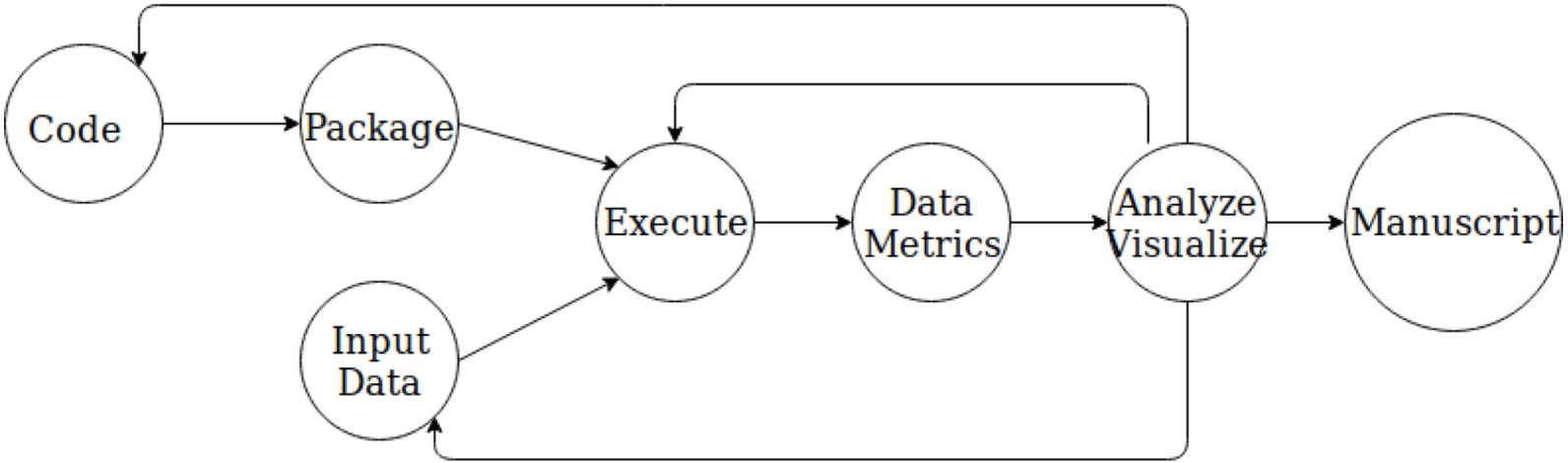
Containers for Reproducible Research

- ~~Programmatic capture~~
  - Captures necessary and sufficient program dependencies using *ptrace*
- Rigid composition
  - No automatic way to organize the container content in meaningful ways
- ~~Large image sizes~~
  - Uses content de-duplication to disambiguate at block level
- ~~Inefficient execution~~
  - Use *ptrace* for re-execution and native file systems for re-execution.

Popper: Incentivizing organization

- Convention to provide versioning, structure, clarity, and repeatability to a workflow
- Build *pipelines* which utilize common DevOps tools (Docker, CI, and validation tools) to conduct computational experiments
- Pipeline initialized as a git repository with metadata and scripts which produce the entirety of a research work

Steps covered by Popper flow

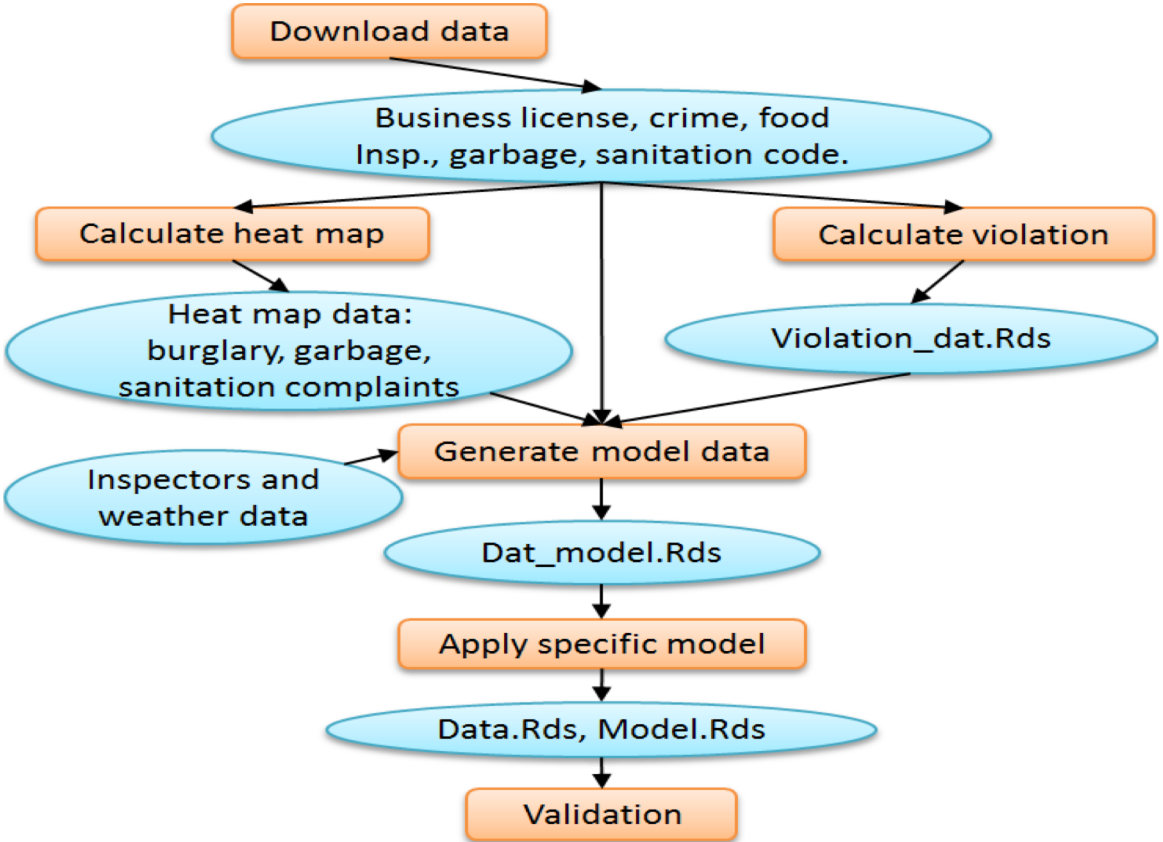


Adapted from Ivo Jimenez, Michael Sevilla, Noah Watkins, Carlos Maltzahn, Jay Lofstead, Kathryn Mohror, Andrea Arpaci-Dusseau and Remzi Arpaci-Dusseau. *The Popper Convention: Making Reproducible Systems Evaluation Practical*. In 2017 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), 1561–70, 2017.

Sciunit-Popper integration

- Should the convention be followed within a container or should the containers be part of a convention

Food Inspection Evaluation -- An example workflow

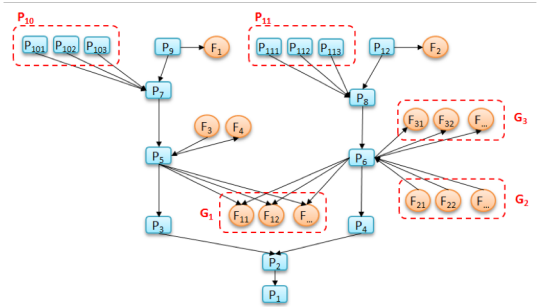


Provenance

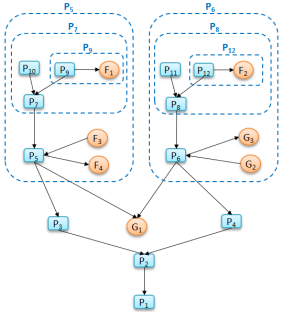
```
1507596280 10770 CLOSE /usr/lib/python2.7/site-packages/chardet-3.0.4-py2.7.egg
1507596280 10770 READ /usr/lib/python2.7/site-packages/ipaddress-1.0.18-py2.7.egg
1507596280 10770 CLOSE /usr/lib/python2.7/site-packages/ipaddress-1.0.18-py2.7.egg
1507596280 10770 CLOSE /usr/lib64/python2.7/site.py
1507596280 10770 READ /usr/lib/locale/locale-archive
1507596280 10770 CLOSE /usr/lib/locale/locale-archive
1507596280 10770 READ /usr/lib64/python2.7/encodings/__init__.py
1507596280 10770 READ /usr/lib64/python2.7/encodings/__init__.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/__init__.pyc
1507596280 10770 READ /usr/lib64/python2.7/codecs.py
1507596280 10770 READ /usr/lib64/python2.7/codecs.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/codecs.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/codecs.py
1507596280 10770 READ /usr/lib64/python2.7/encodings/aliases.py
1507596280 10770 READ /usr/lib64/python2.7/encodings/aliases.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/aliases.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/aliases.py
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/__init__.py
1507596280 10770 READ /usr/lib64/python2.7/encodings/utf_8.py
1507596280 10770 READ /usr/lib64/python2.7/encodings/utf_8.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/utf_8.pyc
1507596280 10770 CLOSE /usr/lib64/python2.7/encodings/utf_8.py
1507596280 10770 READ /home/gfils/pydelty3.py
1507596280 10770 CLOSE /home/gfils/pydelty3.py
1507596280 10770 READ /home/gfils/pydelty3.py
1507596280 10770 CLOSE /home/gfils/pydelty3.py
1507596280 10770 SPAWN 10771
1507596280 10770 EXECVE 10771 /bin/sh /home/gfils ["sh", "-c", "rm tmp.*"]
1507596280 10771 EXECVE2 10770
1507596280 10770 MEM 136056832
1507596280 10770 MEM 136056832
1507596280 10771 MEM 1409024
1507596280 10771 READ /etc/ld.so.cache
1507596280 10771 CLOSE /etc/ld.so.cache
1507596280 10771 READ /lib64/libtinfo.so.6
```

Part Of A Normal (Verbose) Provenance Log

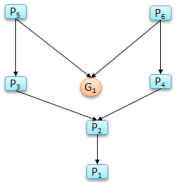
Small Section Of Graph Built From Normal Provenance Log



Full Graph

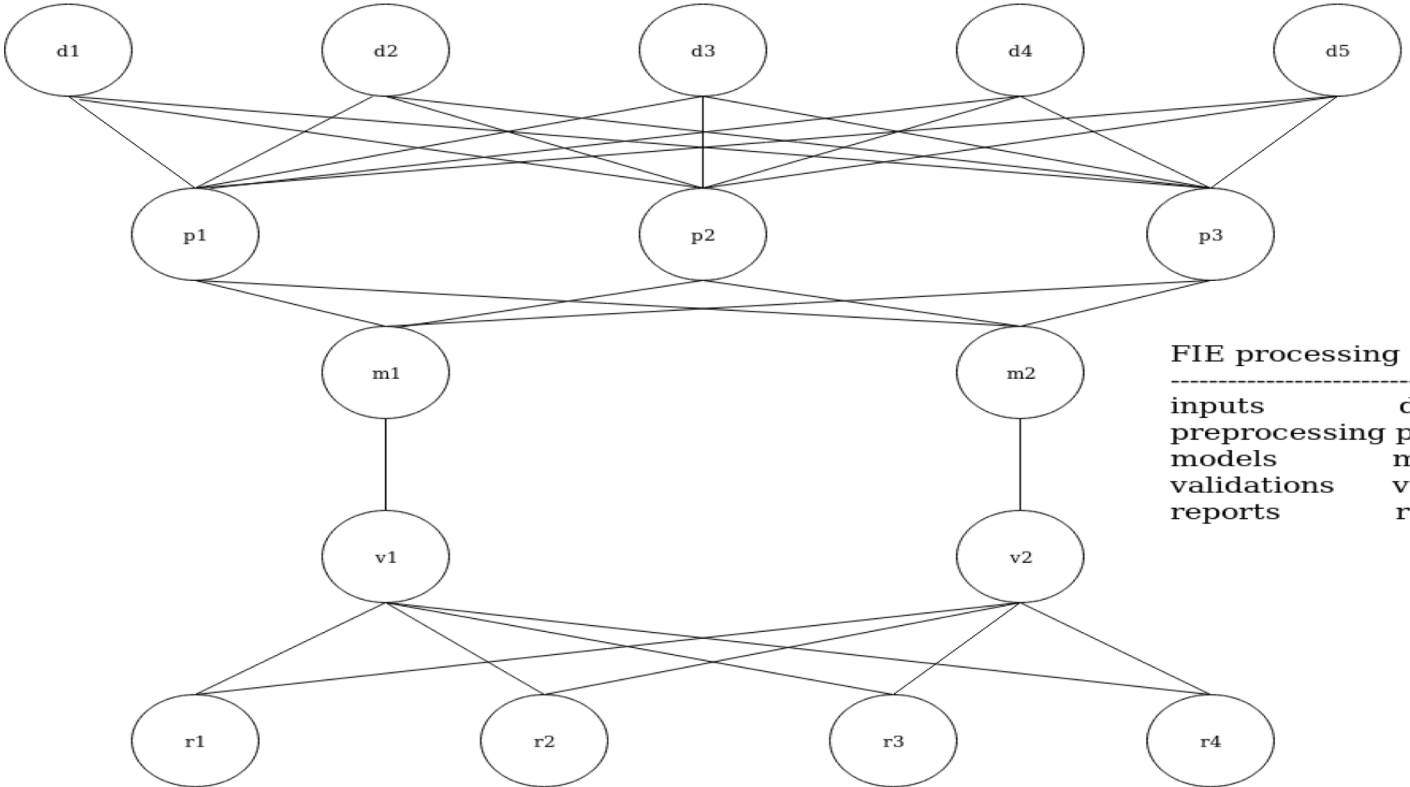


Similarity Applied



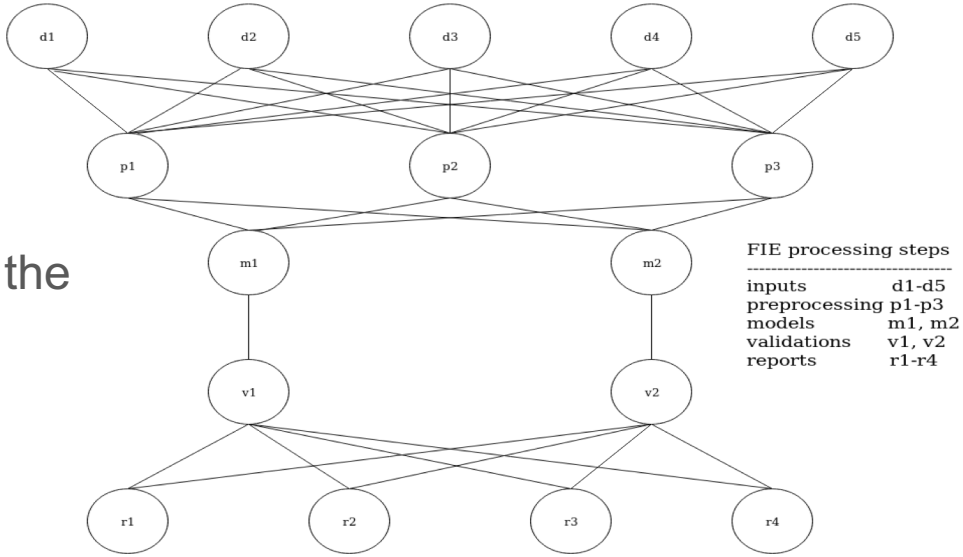
Packability Applied

Our workflow another way -- Each circle represents an input or processing step

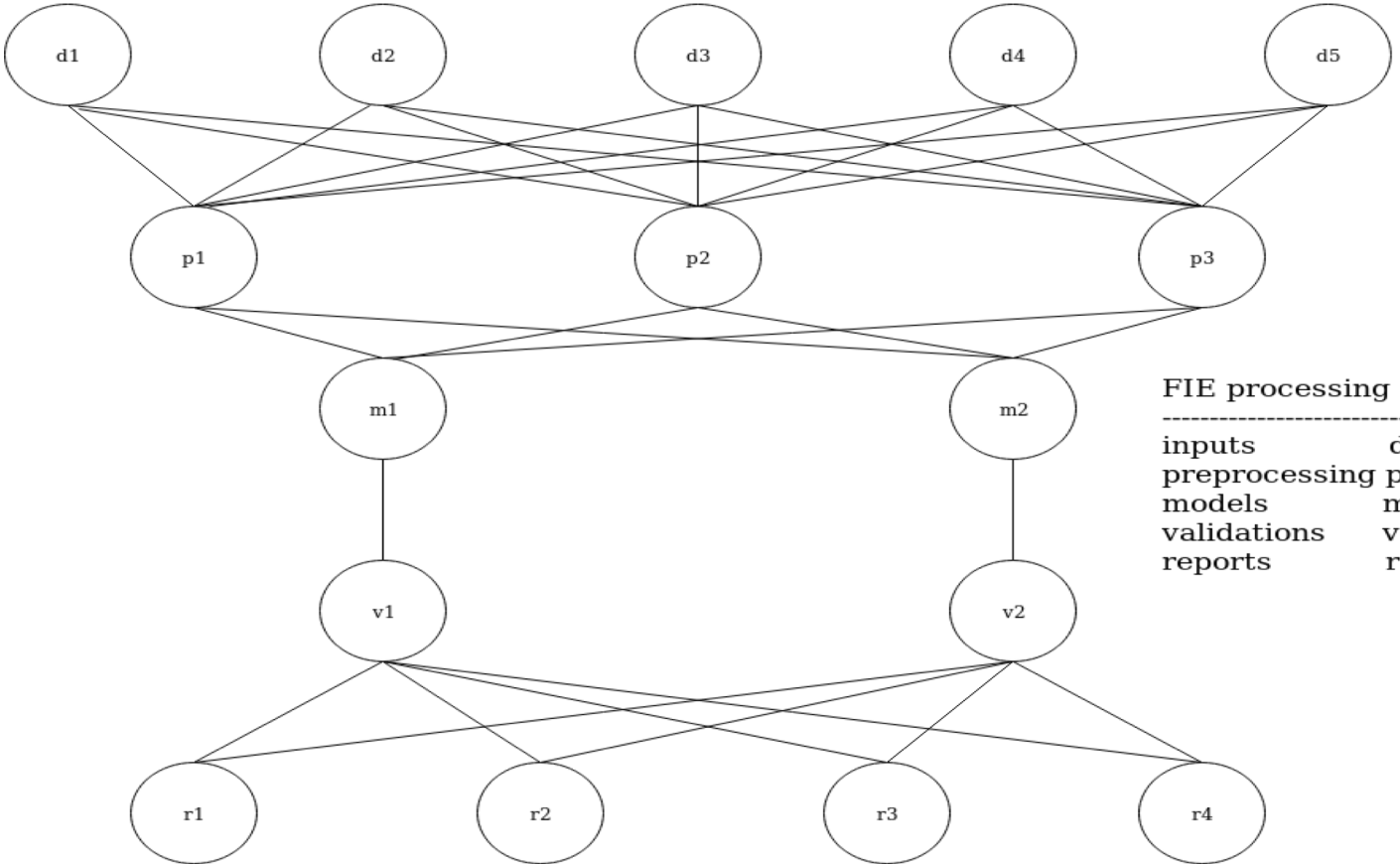


There are many possible combinations of groupings

- One container contains all
- A container for each step
- Or perhaps a container for the top two rows, a left branch container, a right branch container, and then a container to merge and produce results.



There are many possible combinations of groupings



FIE processing steps

inputs	d1-d5
preprocessing	p1-p3
models	m1, m2
validations	v1, v2
reports	r1-r4

Picking the “right” set of groupings

- We don’t know of any objective measure to evaluate grouping granularity.
- Given any particular set of groupings there will be a shortcoming -- less ability to reuse parts, increased risk of portability failure, etc.
- Grouping according to likelihood of reuse of the group seems a good rule of thumb. A tradeoff between transparency/reusability and portability.
- Could be a time consuming task for an author.

Sciunit and Popper

Browse: http://sciunit.run

Contribute: https://bitbucket.org/geotrust/sciunit-cli

Issues: pr@sciunit.run

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POPPER: http://falsifiable.us/

NSF: 1450488

Sciunit-Popper: https://github.com/popperized/sciPopper