Tools for Transparency and Replicability of Simulation in Archaeology

Mark E. Madsen and Carl P. Lipo

University of Washington, Seattle
California State University at Long Beach

Session: **Open methods in archaeology: how to encourage reproducible research as the default practice**

Why We Simulate

- Express models of social and evolutionary dynamics
- Understand model outcomes
- Predict archaeologically relevant patterns
- Compare archaeological data to the patterns

Why Simulation Is Hard

- Difficult to demonstrate correctness
- Hard to manage data, software, parameters
- Hard to separate exploration from rigorous experimentation

Our Toolset

Open Source Tools

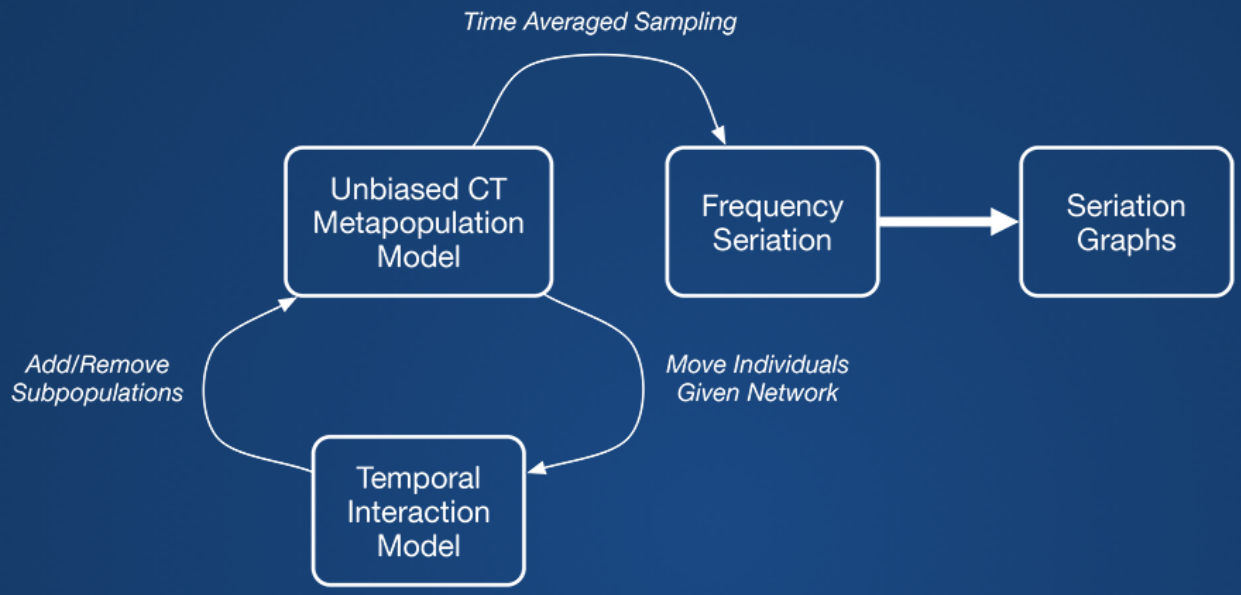
- Anaconda Scientific Python
- simuPOP
- MongoDB
- Github
- Graphviz
- R and R Studio

- http://continuum.io
- http://simupop.sourceforge.net
- http://www.mongodb.com
- https://github.com
- http://graphviz.org
- http://www.r-project.org

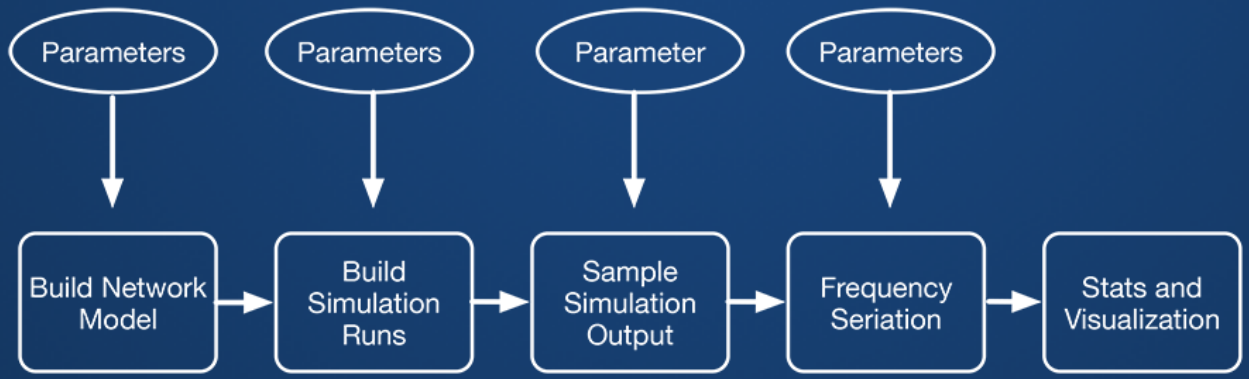
Commercial Resources

- Amazon EC2: compute cluster
- Amazon S3: long-term bulk storage

https://github.com/mmadsen/seriationct



https://github.com/mmadsen/experiment-seriationct (-2)



Best Practices

- Everything lives in a revision control system (Git/Github, Subversion, Mercurial)
- Experiments and data in separate repository from code.
- Production work is templated and scripted
- Every simulation run gets a Universally Unique Identifier (UUID)
- Random seeds are generated beforehand, and stored with all results
- All components take command line parameters for ease of scripting and scaling from laptop to cloud compute clusters.

Creating New Experiment

```
$ create-experiment-directory.sh \
seriationct-9

demo-experiment
├── README.md
├── bin
│   ├── annotate-seriation-output.sh
│   ├── build-networkmodel.sh
│   ├── build-simulations.sh
│   ├── run-seriations.sh
│   └── simulation-postprocess.sh
├── exported-data
│   └── README
├── jobs
│   └── README
├── networks
├── rawnetworkmodels
├── run-experiment-steps.sh
├── sampled-data
│   └── README
├── seriation-results
│   └── README
├── seriationct-priors.json
├── temporal
│   └── README
└── xyfiles
    └── README

9 directories, 14 files
```

Experiment in Progress...

```
├── README.md
├── bin
│   ├── annotate-seriation-output.sh
│   ├── build-networkmodel.sh
│   ├── build-simulations.sh
│   ├── run-seriations.sh
│   └── simulation-postprocess.sh
├── jobs
│   └── job-seriationct-9-simulations.sh
├── rawnetworkmodels
│   ├── seriationct-9-full-network.zip
│   └── seriationct-9-networkmodel
│       ├── build-networkmodel.sh
│       ├── seriationct-9-001.gml
│       ├── seriationct-9-002.gml
│       ├── seriationct-9-003.gml
│       ├── seriationct-9-004.gml
│       └── seriationct-9-005.gml
├── run-experiment-steps.sh
├── sampled-data
│   ├── 36acbc00-d441-11e4-b725-b8f6b1154c9b-0-sampl
│   ├── 6aa72822-d443-11e4-bed5-b8f6b1154c9b-0-sampl
├── seriation-results
│   ├── 36acbc00-d441-11e4-b725-b8f6b1154c9b-0-sampled-
│   ├── 6aa72822-d443-11e4-bed5-b8f6b1154c9b-0-sampl
│   └── README
├── seriationct-priors.json
```

Universally Unique Identifiers

Internet RFC 4122:
https://www.ietf.org/rfc/rfc4122.txt

```
import uuid

# uuid1 incorporates hardware address and time
unique_id = uuid.uuid1()

print unique_id

ba3a318a-d4cb-11e4-b4f9-b8f6b1154c9b
```

- Component of all file names
- Field in all database records
- Primary means of tying data elements together

Simulation Metadata


```
{
    "simulation_run_id" : "urn:uuid:eaf71706-ce8c-11e4-a9ac-b8f6b1154c9b",
    "random_seed" : 2127774500,
    "elapsed_time" : 257.4463579654694,
    "experiment_name" : "seriationct-1",
    "full_command_line" : "sim-seriationct-networkmodel.py -mf 0.0938
    --popsize 250 --nm hier-1.zip"
}
```


Simulation Output Data


```
{
    "_id" : ObjectId("5514e910544bd6744cae8aec"),
    "simulation_run_id" : "urn:uuid:36acbc00-d441-11e4-b725-b8f6b1154c9b",
    "random_seed" : 1601673696,
    "replication" : 0,
    "class_freq" : {
        "0-3-4" : 0.6857142857142857,
        "2-4-1" : 0.1428571428571428,
        "0-4-4" : 0.1714285714285714
    },
    "simulation_time" : 3000,
    "subpop" : "assemblage-33-6",
    "mutation_rate" : 0.00668494110834,
    "population_size" : 250,
    "class_richness" : 3
}
```

Issues with Large Projects

- Github repositories soft limited to 1G or less
- Github hard limit on file size 100MB
- Figshare limits files to 250MB with free plan

Workarounds

- Currently compressing some intermediate files after processing
- Moving some raw DB files to S3 buckets for long term storage after extracting analysis dataset
- "Continuation" repositories with additional analysis

https://github.com/mmadsen/experiment-seriationct-2

Other Tools

Sumatra

http://neuralensemble.org/sumatra/

Numerical analysis or simulation project tracking and replicability tool

Lancet

http://ioam.github.io/lancet/

Strong parameter management and experiment execution library

Where We're Headed

- Sumatra needs files as "data" capture, extend to handle database as data store, requires archival scheme
- Lancet replacing our simple execution scripts and parameter JSON files
- *Combination of Sumatra for object management and Lancet for simulation control, with UUIDs and random seeds scripted as in our current example*
- Raw data archiving is still a problem -- exploring Amazon Glacier for post-analysis storage

Thank You

For more information, templates, etc:

mark@madsenlab.org
http://notebook.madsenlab.org