



Opening the Black Box

Enabling Transparency in Scientific Computation

*Michael Barton, Marco Janssen, Dawn Parker,
Allen Lee, Sean Bergin, and Nathan Rollins*



Reproducibility in Science

- Reproducibility the *gold standard* of science as a knowledge system



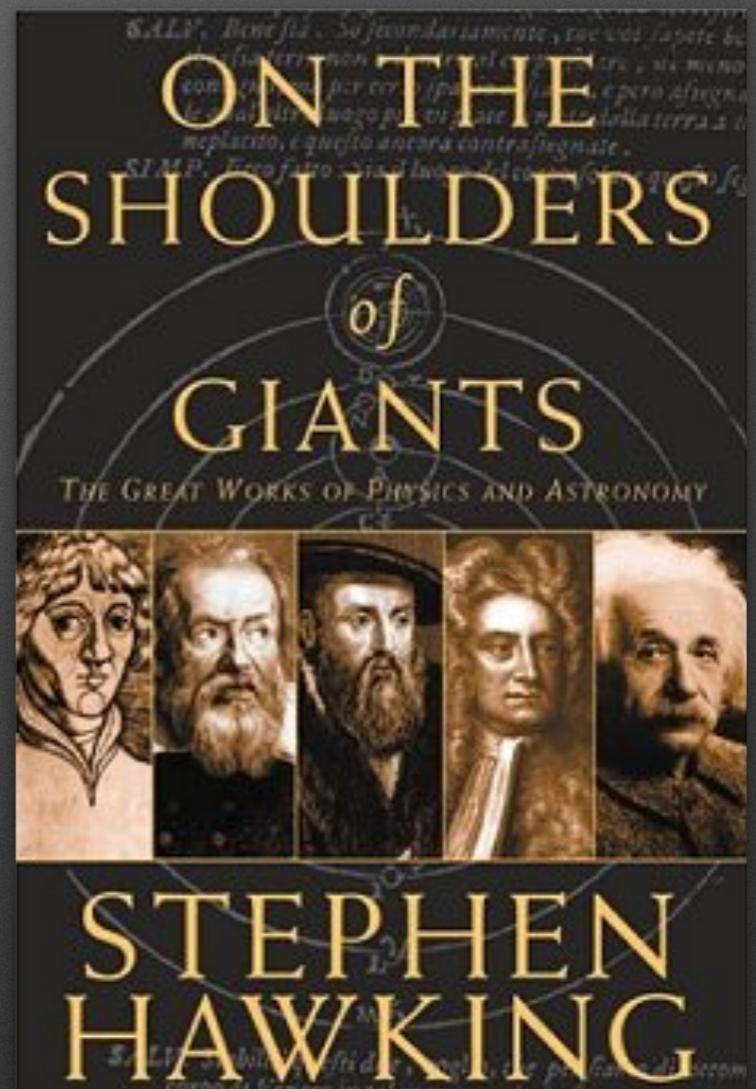
Reproducibility in Science

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- *Potential* to be reproduced, not repetition, enforces quality in research



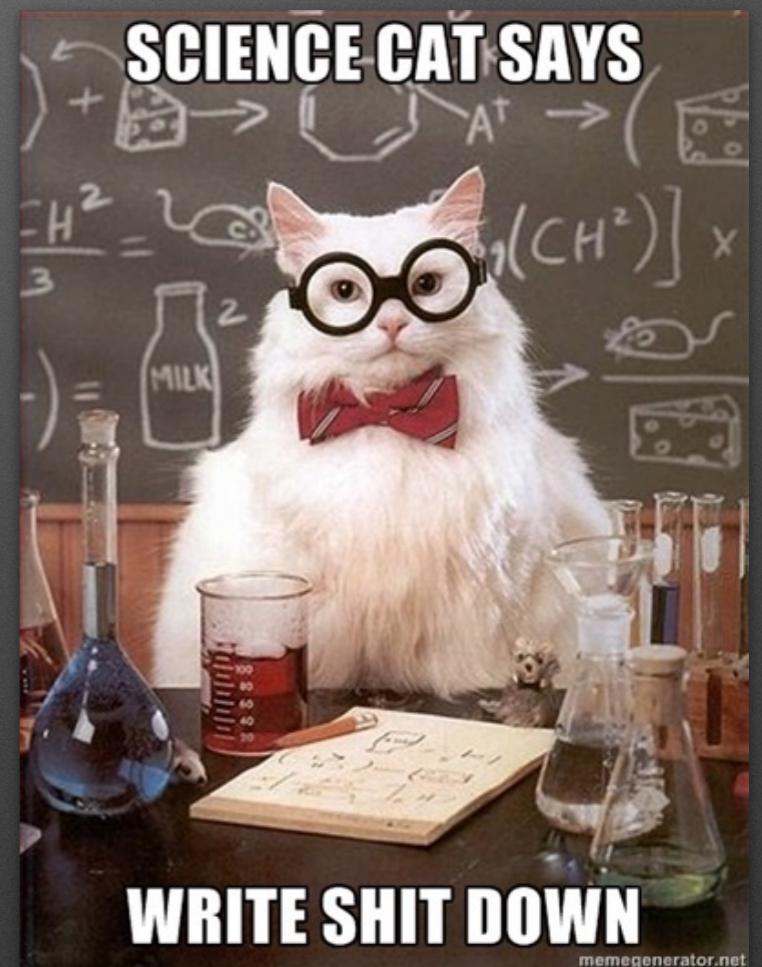
Reproducibility in Science

- Reproducibility the *gold standard* of science as a knowledge system
- *Potential* to be reproduced, not repetition, enforces quality in research
- Reproducibility creates knowledge scaffolding that drives scientific advance



Reproducibility in Science

- Requires sufficient information
 - About concepts
 - About methods
 - About data
- Information about *HOW* to replicate a study needs to be accessible to others
- Underscores importance of open science



Reproducibility in Archaeology

- Field work inherently non-reproducible
 - Recognized importance of careful recording of field observations and methods



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 - Curation of archaeological collections important because that is all that remains of unreproducible fieldwork



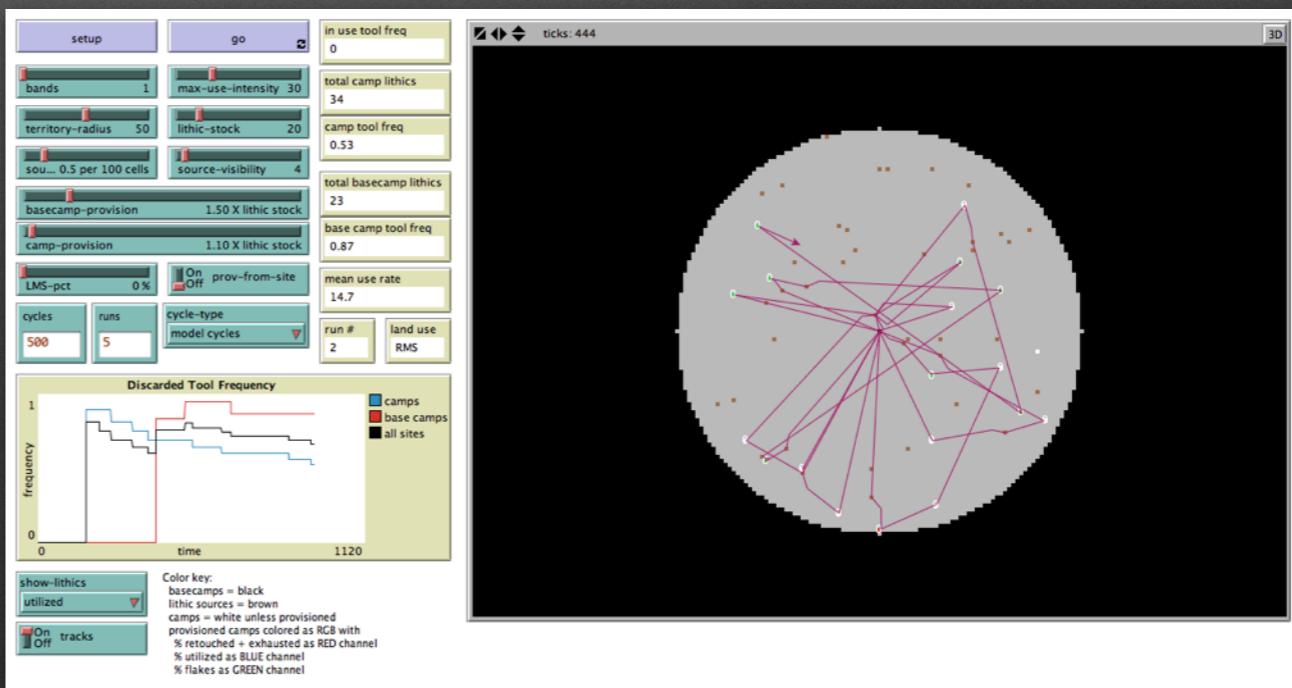
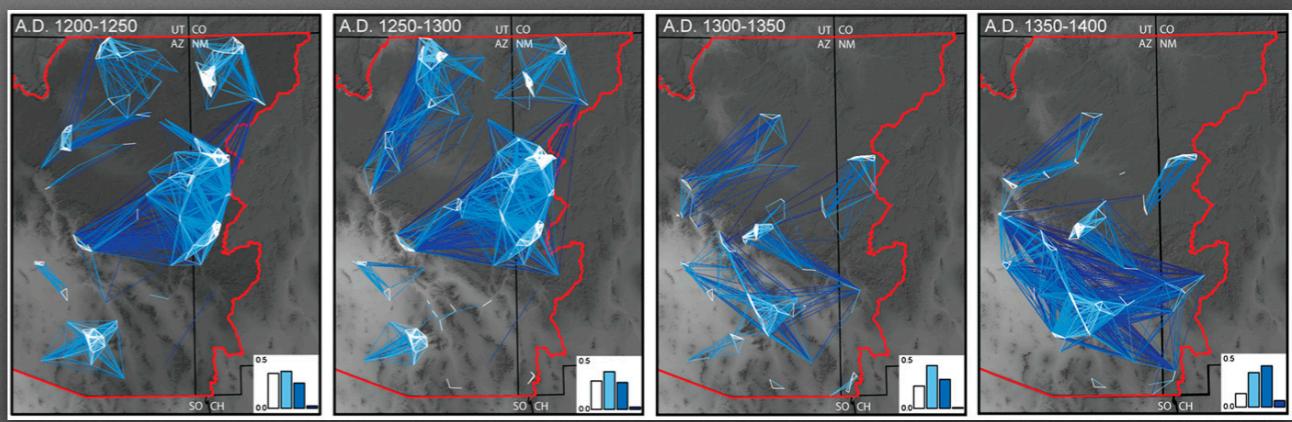
Reproducibility in Archaeology

- Field work inherently non-reproducible
 - Recognized importance of careful recording of field observations and methods
 - Curation of archaeological collections important because that is all that remains of unreproducible fieldwork
- More recent consideration of care of *DATA* (measurements made on archaeological materials)

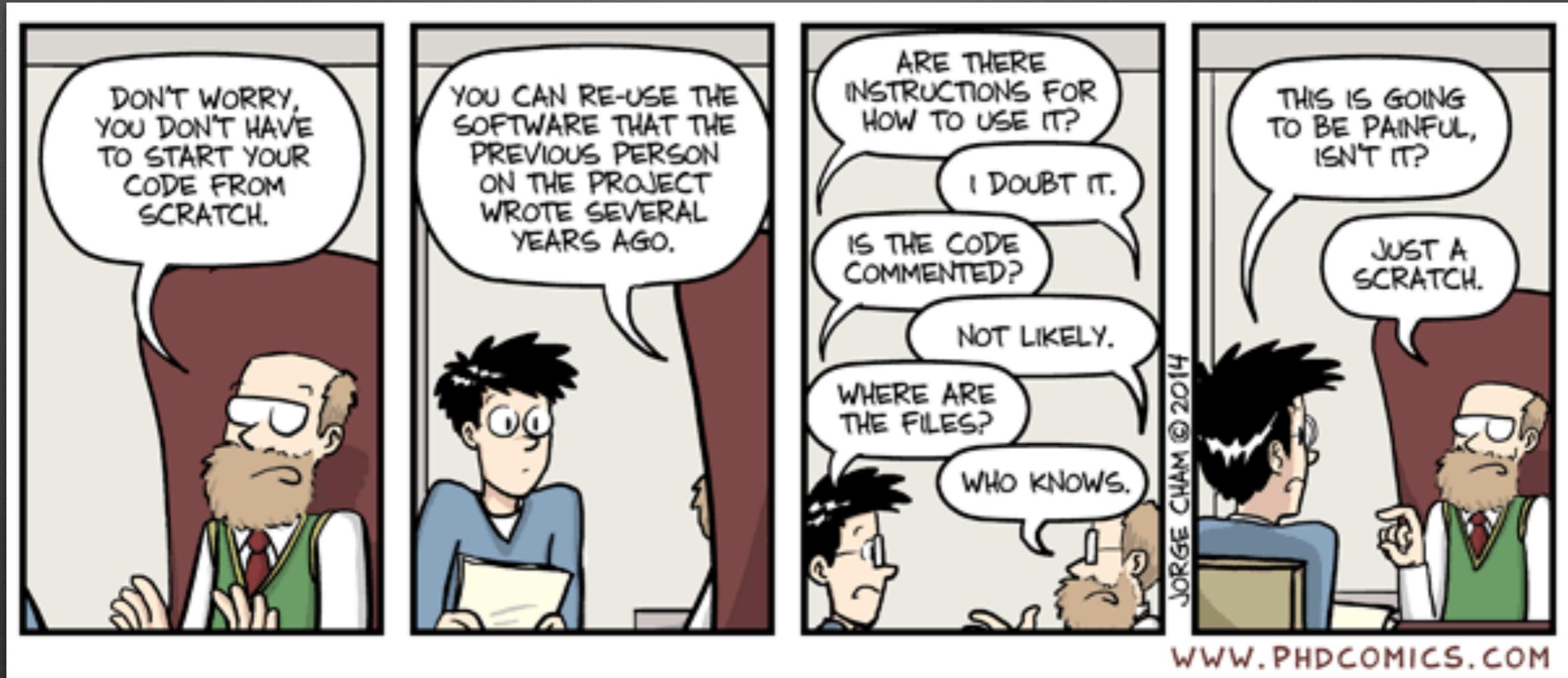


Computation in Archaeology

- Computation as digital experiment
- Recent significant expansion in archaeological practice (SAA sessions)
- But no consideration yet of how to achieve transparency and reproducibility in scientific computation



Transparency in Scientific Computation

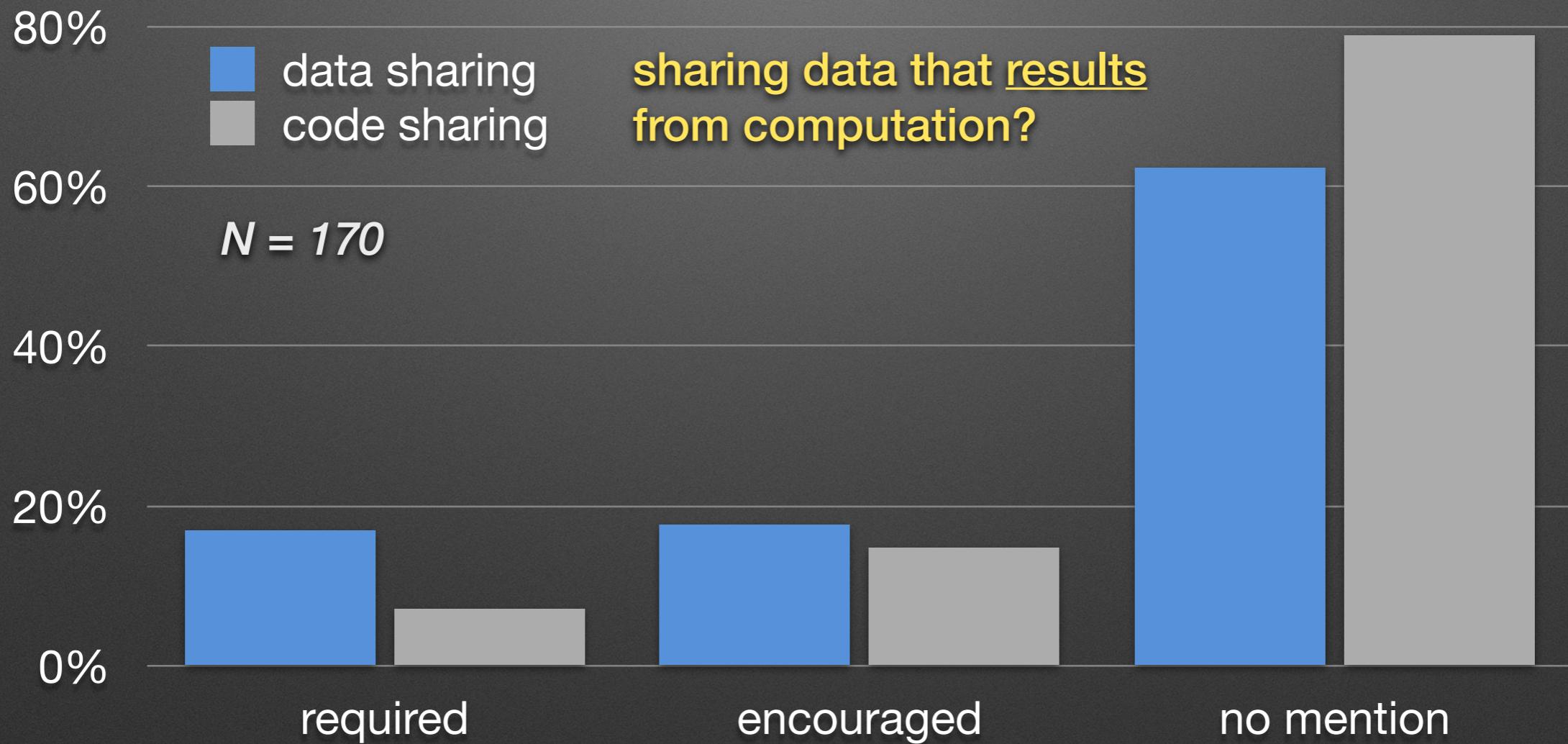


- Transparency in scientific computation increasingly important across all science

Transparency in Scientific Computation

- Computation becoming ubiquitous across science
- Programming code is laboratory for complex experiments
- Reproducibility requires making code accessible to other scientists
- Code also needs to be accompanied by detailed metadata to explain procedures
- Some computation—especially modeling—also produces new data
- Code, metadata, data from scientific computation cannot be published easily in current journal venues

Transparency in Scientific Computation



Journal Policies for Sharing Data and Code
in 2012 (Stodden et al 2013)

Transparency in Scientific Computation

- Computational modeling bibliographic analysis project
 - Goal is to analyze current practices sharing code and any benefits that come from this knowledge sharing
 - Plan to survey all papers using computational modeling in past 20 years (>3000)

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Transparency in Scientific Computation

- Computational modeling bibliographic analysis project
 - Goal is to analyze current practices sharing code and any benefits that come from this knowledge sharing
 - Plan to survey all papers using computational modeling in past 20 years (>3000)
- To date: 545 papers, from 209 different journals, between 1998 and 2014
- *85% do not provide any information about how to access code*

Transparency in Scientific Computation

140

Code Accessibility in Published Papers Using Computational Modeling (n = 545)

105

70

35

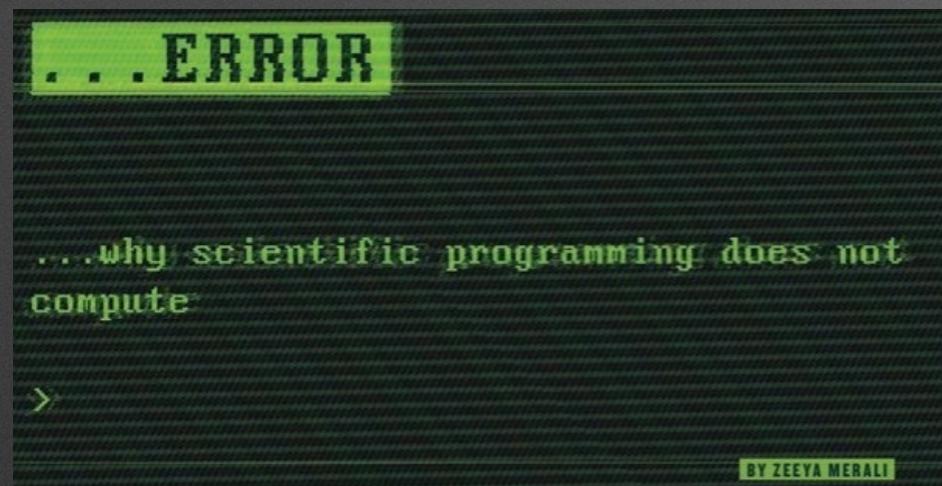
0

- code not available
- code in CoMSES CML
- code in other repository
- code archived with journal
- code on web site

<2004 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014

Transparency in Scientific Computation

- Calls to establish community repositories and standards for code and documentation



Nature. 467, 775–777 (2010).

Shining Light into Black Boxes

A. Morin,¹ J. Urban,² P. D. Adams,³ I. Foster,⁴ A. Sali,⁵ D. Baker,⁶ P. Sliz^{1*}

Science. 336, 159–160 (2012).

PERSPECTIVE
Reproducible Research in Computational Science
Roger D. Peng

Science. 334, 1226 –1227 (2011).



Publish your computer code: it is good enough

Freely provided working code — whatever its quality — improves programming and enables others to engage with your research, says Nick Barnes.

Nature. 467, 753 (2010).

Troubling Trends in Scientific Software Use

Lucas N. Joppa,^{1*} Greg McInerny,¹² Richard Harper,¹ Lara Salido,³ Kenji Takeda,¹ Kenton O'Hara,¹ David Gavaghan,² Stephen Emmott¹

Science. 340, 814–815 (2013).



The CoMSES Network

The screenshot shows the homepage of the CoMSES Network. At the top, there is a navigation bar with links to various categories like Bonjour, Google, Apple Stuff, ASU Stuff, classes, GRASS, NSF&NIH, Cloud, Clippers, and programming. Below the navigation bar is the CoMSES logo and the text "OpenABM NETWORK". To the right of the logo are links for Model Library, Event Calendar, Community, Resources, About, Search, Login, and Become a Member. The main content area features a large image of a simulation interface showing various plots and data tables related to an innovation diffusion model. To the right of this image is a "Featured Content" section with the title "9 Maturity levels in Empirical Validation - An innovation diffusion example". Below this title is a descriptive paragraph about the model and a "View Model" button. On the left side of the main content area, there is a sidebar with the text "The Computational Model Library is a library of downloadable agent-based models" and three buttons: "Find models", "When to use agent-based models?", and "Submit a model to the library". At the bottom of the page, there are two blue buttons: "Model Activity" and "Latest Jobs & Appointments". To the right of the main content area is a sidebar titled "Welcome to CoMSES Net" which provides a brief overview of the network's purpose and resources.

- Network NSF sponsored Research Coordination Network for Computational Modeling in Social & Ecological Sciences
- A collaborative community of practice for scientists using advanced modeling to study human and natural systems

<http://www.openabm.org>

CoMSES Net

- Founded 2006 as response to NSF challenges in modeling science
- Building framework for interaction and professional development
- Mitigating infrastructural challenges to knowledge dissemination and sharing

The screenshot shows two views of the OpenABM website. The top view displays the 'Jobs and Appointments' section, featuring a sidebar with links to Home, Model Library, Education, Resources, and Bibliographic Library. The main content area lists two job posts: 'Postdoctoral Fellowships: Disease Modelling, Health Economics' and 'Assistant Professorship in Computational Social Science'. The bottom view shows a calendar for June 2014, highlighting specific dates like the 'Modeling Conference 10/22/2014' and '10/14 to 10/31/2014 In Business Conference'.

open
abm ... a node in the CoMSES Network

Jobs and Appointments

Log in to post new content in the forum.

| Topic / Topic starter | Replies | Views | Last post |
|---|---------|-------|--------------------------------------|
| Postdoctoral Fellowships: Disease Modelling, Health Economics | 0 | 82 | by moghadas Sat, 10/11/2014 - 20:09 |
| Assistant Professorship in Computational Social Science | 0 | 116 | by marcojanssen , 10/06/2014 - 11:43 |

open
abm ... a node in the CoMSES Network

Newly certified models in the CoMSES model library and newly published models added to the model library.

Month Week Day Year

014 « Prev Next »

| Fri | Sat |
|-----|-----|
| 2 | 3 |
| 9 | 10 |
| 16 | 17 |
| 23 | 24 |
| 30 | 31 |

... a node in the CoMSES Network

CoMSES Digest: Summer 2014

Volume 2, No.2 March 15, 2014 – June 16, 2014

Welcome to the Summer 2014 issue of the CoMSES Digest! With this issue the CoMSES Digest approaches its first anniversary: this is the fourth issue of our now-quarterly publication. We hope the year has been good to all of you.

The model library at OpenABM continues to grow. In the most recent quarter ten new models have been published to the library. The range of topics covered by these models is as wide as we have seen before. There are models of opinion dynamics, political participation, and conformity and the spread of social norms; alongside these are models of urban expansion in China and water storage in Nepal. Supply chain marketing and college sorting are explored as well, and a model of a thermostat is a nice pedagogical addition.

Two models have undergone the certification process, and both deal with archaeology. One is a replication of a model of the procurement of raw material for stone tools; it's a nice example of a simple and abstract model that allows us to test basic hypotheses. The other is a more ambitious model that studies population interaction (demographics and genetics) and was originally applied to the Late Pleistocene across Western Eurasia. Certification means that the models have been demonstrated to execute properly and include documentation about what they do and how they can be used.

Computational Model Library

- Integrated strategy for knowledge dissemination

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open abm

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CoMSES Computational Model Library

Browse Search Add Help

Showing 1 - 15 of 240 models.

| Title | Submitter | Post date |
|---|---------------------|--------------|
| A Complex Model of Voter Turnout This is a complex "Data Integration Model", following a "KIDS" rather than a "KISS" methodology - guided by the available evidence. It looks at the complex mix of social processes that may determine why people vote or not. | B Edmonds | Oct 13, 2014 |
| Garbage can model Excel reconstruction Reconstruction of the original code M. Cohen, J. March, and J. Olsen garbage can model, realized by means of Microsoft Office Excel 2010 | S Ivan | Aug 19, 2014 |
| IDEAL IDEAL: Agent-Based Model of Residential Land Use Change where the choice of new residential development is based on the Ideal-point decision rule. | A Ligmann-Zielinska | Aug 06, 2014 |
| Thermostat II A thermostat is a device that allows to have the temperature in a room near a desire value. | M Pereda | Jun 12, 2014 |
| Thoughtless conformity and spread of norms in an artificial society (Grid Model) This model is a small extension (rectangular layout) of Joshua Epstein's (2001) model on development of thoughtless conformity in an artificial society of agents. | M Azfar Nisar | May 26, 2014 |
| Thoughtless conformity and spread of norms in an artificial society This model is based on Joshua Epstein's (2001) model on development of thoughtless conformity in an artificial society of agents. | M Azfar Nisar | May 26, 2014 |
| Agent-based Simulation Models of the College Sorting Process We explore how dynamic processes related to socioeconomic inequality operate to sort students into, and create stratification among, colleges. | R Baker | May 23, 2014 |
| A test-bed ecological model This is a multi-patch meta-population ecological model. It intended as a test-bed in which to test the impact of humans with different kinds of social structure. | B Edmonds | May 04, 2014 |
| Nepali Village Model The model implements a model that reflects features of a rural hill village in Nepal. Key features of the model include water storage, social capital and migration of household members who then send remittances back to the village. | J A Janmaat | Apr 17, 2014 |

Computational Model Library

- Integrated strategy for knowledge dissemination
 - Open-access publishing and preservation of scientific code (handles, licenses)

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Village Ecodynamics Project

Submitted By: ipem
Submitted: Sep 21, 2011
Last Updated: Mar 23, 2013
62 Downloads (9 Downloads in the last 3 months)

This project uses agent-based modeling to investigate where prehistoric people of the American Southwest would have situated their households based on both the natural and social environments in which they lived.

We seek to understand general processes in the environments of southwestern Colorado between A.D. 600 and A.D. 1300. Agent-based models allow us to study a system characterized by high degrees of interaction between the landscape as it was affected by climate change and by the actions of farmers, and among the farmers themselves, as they sought to make a living in this marginal farming area.

Please see the [research plan](#) for more information.

[Instructions for downloading and configuring swarm](#).

This model also requires a [very large dataset](#).

The model is also available in a preconfigured [virtual machine](#) that contains the model in executable form, all data files, and a simple development environment that allows you to experiment directly. This is the preferred method to explore the Village model. You may find more information and download the appliance directly from the [appliance page](#).

Cite This Model:
ipem (2011, May 27). "Village Ecodynamics Project" (Version 2). CoMSES Computational Model Library. Retrieved from: <https://www.openabm.org/model/2518/version/2>

Model Version: 2 [Latest] Model Files

Version Notes:

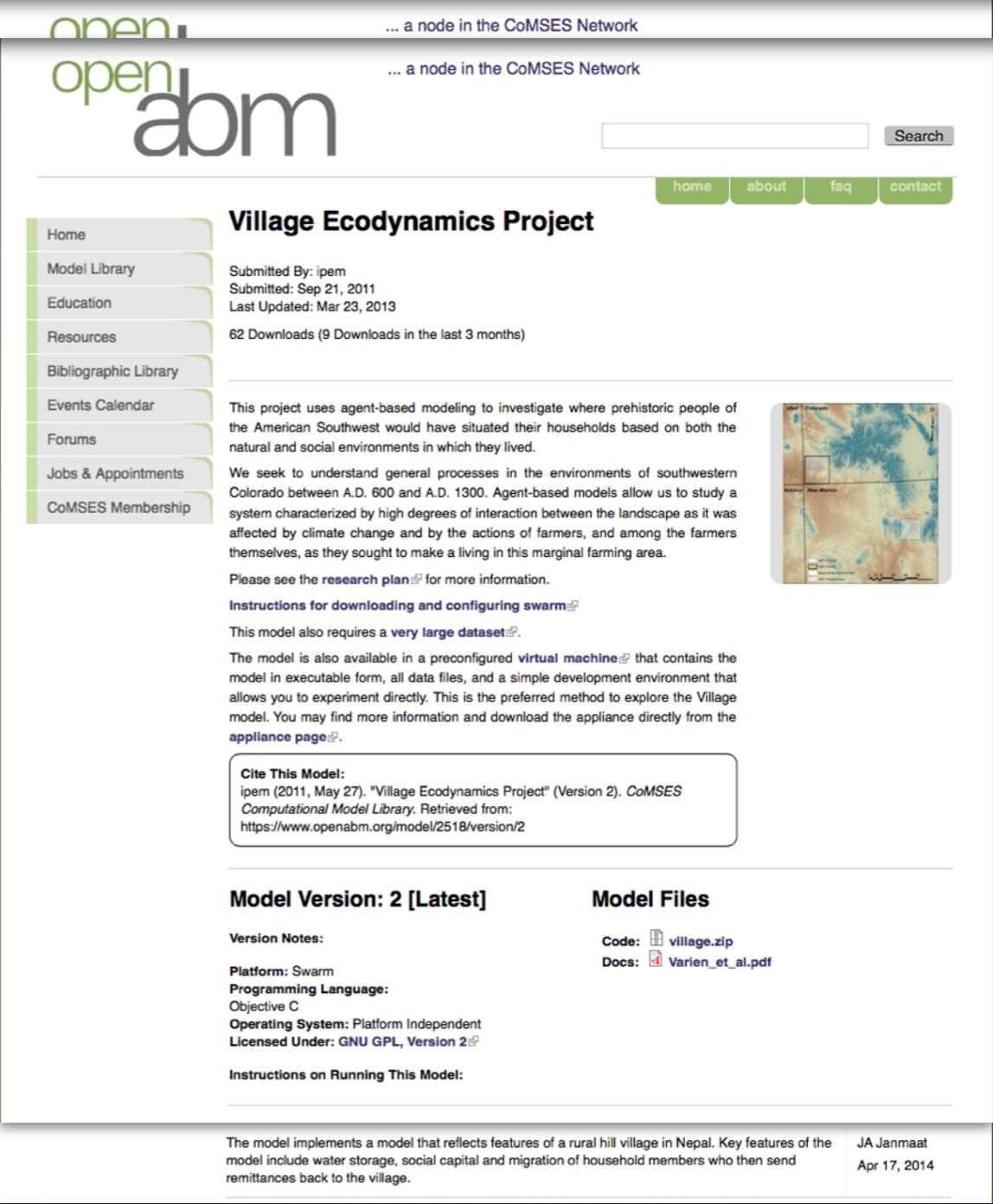
Platform: Swarm
Programming Language: Objective C
Operating System: Platform Independent
Licensed Under: GNU GPL, Version 2

Code: [village.zip](#)
Docs: [Varien_et_al.pdf](#)

Instructions on Running This Model:

The model implements a model that reflects features of a rural hill village in Nepal. Key features of the model include water storage, social capital and migration of household members who then send remittances back to the village.

JA Janmaat
Apr 17, 2014



Computational Model Library

- Integrated strategy for knowledge dissemination
- Open-access publishing and preservation of scientific code (handles, licenses)
- Community standards and best practices for description and citation

The screenshot shows the 'Standards' page of the openabm website. The header features the 'open' logo with three green hexagons followed by 'abm'. The main content area has a sidebar with links: Home, Model Library (highlighted in green), Education, Resources, Bibliographic Library, Events Calendar, Forums, Jobs & Appointments, and CoMSES Membership. The main content area starts with a section about the ODD Protocol, mentioning its proposal by Volker Grimm et al. (2006). It discusses simulation models for autonomous organisms or agents and the lack of a standard protocol. Below this is a list of related resources: 'Using the ODD Protocol for Describing Three Agent-Based Social Simulation Models of Land-Use Change', 'Volker Grimm's ODD Site', 'ODD Discussion Forum (offsite)', and 'ODD Preprint (Updated on September 2010)'. There is also a link to log in or register to post comments. A comment from Volker Grimm dated August 2009 is shown, updating the ODD protocol manuscript. The footer contains a note about a model for a rural hill village in Nepal and a copyright notice for JA Janmaat, April 17, 2014.

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Standards

The ODD Protocol was proposed by Volker Grimm *et al.* (2006) because:

Simulation models that describe autonomous individual organisms (individual based models, IBM) or agents (agent-based models, ABM) have become a widely used tool, not only in ecology, but also in many other disciplines dealing with complex systems made up of autonomous entities. However, there is no standard protocol for describing such simulation models, which can make them difficult to understand and to duplicate.

(Grimm, V. *et al.*, 2006, p.115)²

The ODD is organized around the three main components to be documented about a model: Overview, Design concepts, and Details. These components encompass seven subelements that must be documented in sufficient depth for the model's purpose and design to be clear and replicable for a third party: Purpose, State Variables and Scales, Process Overview and Scheduling, Design Concepts, Initialization, Input, and Submodels.

In addition to the original 2006 publication, Grimm *et al.* have continued to publish updates to the protocol with examples of its application to research projects:

- Using the ODD Protocol for Describing Three Agent-Based Social Simulation Models of Land-Use Change³
- Volker Grimm's ODD Site⁴
- ODD Discussion Forum (offsite)⁵
- ODD Preprint (Updated on September 2010)⁶

Log in or register to post comments

Comments

August 2009: Update of ODD protocol (manuscript)

Submitted by Volker Grimm
Sat, 08/22/2009 - 12:31

Hi,
We just (August 2009) submitted an updated description of the ODD protocol to "Ecological Modelling". This manuscript is available at: <http://www.ufz.de/index.php?de=10466>⁷.
ODD did not change very much, but we completely rewrote (and hopefully improved) its description, including some changes that should make ODD easier to use by modelers from social sciences.
Although the ms might of course still change a lot during the review process, we thought it would be good to make it available as soon as possible, so that ODD users can take advantage of the improved description.
Volker

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JA Janmaat
Apr 17, 2014

Computational Model Library

- Integrated strategy for knowledge dissemination
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- Community standards and best practices for description and citation
- Peer review of models and code

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JA Janmaat
Apr 17, 2014

Computational Model Library

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 - Open-access publishing and preservation of scientific code (handles, licenses)
 - Community standards and best practices for description and citation
 - Peer review of models and code
 - Academic credit and incentives for model authors

The screenshot shows the 'Pumpa irrigation model' page on the CoMSES Computational Model Library. The top navigation bar features the 'open abm' logo and links for 'home', 'about', 'faq', and 'contact'. A search bar is also present. The main content area displays the model's details: title ('Pumpa irrigation model'), author ('Irene Perez Ibarra, Marco A. Janssen'), submission date ('Submitted By: ireperez'), last update ('Submitted: Feb 18, 2013'), and last updated ('Last Updated: Jan 24, 2014'). It also shows download statistics ('85 Downloads (12 Downloads in the last 3 months)'), a rating section ('★★★★★'), and a 'CERTIFIED' badge. The model description states it is a replication of the Pumpa model for Nepal, analyzing robustness to disturbances. Below the description is a 'Keywords' section with terms like 'climate change adaptation', 'irrigation', 'institutions', and 'social-ecological system'. A note indicates it is a replication of a previously published model by Cidaloz et al. (2010). A sidebar on the right contains a 'Cite This Model' section with the citation information and a 'Model Certification' section with a detailed description of the certification process.

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open abm

Search

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Pumpa irrigation model

Irene Perez Ibarra, Marco A. Janssen

Submitted By: ireperez
Submitted: Feb 18, 2013
Last Updated: Jan 24, 2014

85 Downloads (12 Downloads in the last 3 months)

★★★★★
All Versions: 4/5 (1 ratings)

CERTIFIED

This is a replication of the Pumpa model that simulates the Pumpa Irrigation System in Nepal (Cidaloz et al., 2010). The purpose of this model is to analyze the robustness of this small-scale irrigation system to two scenarios of disturbances to the natural resource (discharge reduction and time shift in water supply), and two scenarios of disturbances to the physical infrastructure (canals and gates) using five possible irrigation policies (open flow, sequential rotation, optimized sequential, 24-hour rotation, and 12-hour rotation).

Keywords:

climate change adaptation irrigation institutions social-ecological system

This is a replication of a previously published model:
Cidaloz O., Regmi A., Andries J.M., Rodriguez A.A. 2010. Robustness,

Cite This Model:
Perez Ibarra, Irene, Janssen, Marco A. (2013, January 9). "Pumpa irrigation model" (Version 1). *CoMSES Computational Model Library*. Retrieved from: <http://hdl.handle.net/2286.0/oabm:3580>

Model Certification

This model has been Certified that it meets the CoMSES Guidelines for Modeling Best-Practices. Certification involves a review process by which a model is examined to ensure it has been coded and documented according to the community's best-practices. For more information on the Model Review process and Certification:

[Read more](#)

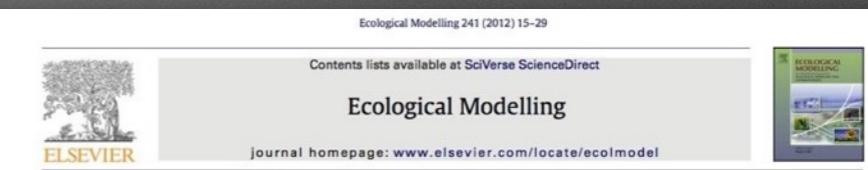
Collaboration with Journals

- Establishing peer review protocols
- Promoting citation and crediting of models
- Providing infrastructure for reviewing code with manuscripts
- Providing infrastructure to store and access code

Copyright © 2013 by the author(s). Published here under license by the Resilience Alliance.
Watkins, C., D. Massey, J. Brooks, K. Ross, and M. L. Zellner. 2013. Understanding the mechanisms of collective decision making in ecological restoration: an agent-based model of actors and organizations.
Ecology and Society 18(2):32. <http://dx.doi.org/10.5751/ES-05497-180232>



Research
Understanding the Mechanisms of Collective Decision Making in Ecological Restoration: An Agent-Based Model of Actors and Organizations
Cristy Watkins¹, Dean Massey², Jeremy Brooks³, Kristen Ross² and Moira L. Zellner²



Exploring complexity with the Hohokam Water Management Simulation: A middle way for archaeological modeling

Advances in Complex Systems
Vol. 15, Nos. 1 & 2 (2012) 1150003 (24 pages)
© World Scientific Publishing Company
DOI: 10.1142/S0219525911003359



AGENTS OF CHANGE: MODELING BIOCULTURAL EVOLUTION IN UPPER PLEISTOCENE WESTERN EURASIA

JASSS

Jan C. Thiele, Winfried Kurth and Volker Grimm (2012)

Agent-Based Modelling: Tools for Linking NetLogo and R

Journal of Artificial Societies and Social Simulation 15 (3) 8
<<http://jasss.soc.surrey.ac.uk/15/3/8.html>>

Environmental Modelling & Software 61 (2014) 59–64

Contents lists available at ScienceDirect
Environmental Modelling & Software
journal homepage: www.elsevier.com/locate/envsoft

A Computational Model Library for publishing model documentation and code



● Pageviews

20,000

10,000

10,000

CoMSES Net Stats

last year

October 2013

January 2014

April 2014

July 2014

282 models in Computational Model Library

| Page Title | Pageviews | Pageviews |
|--|---|---|
| Total visits to CoMSES Net | 167,707 % of Total: 100.00% (167,707) | 167,707 % of Total: 100.00% (167,707) |
| 1. Open Agent Based Modeling Consortium ... a node in the CoMSES Network | 23,128 | 13.79% |
| 2. CoMSES Computational Model Library Open Agent Based Modeling Consortium | 15,804 | 9.42% |
| 3. Jobs and Appointments Open Agent Based Modeling Consortium | 8,381 | 5.00% |
| 4. Search Open Agent Based Modeling Consortium | 5,906 | 3.52% |
| 5. Introduction to Agent-Based Modeling Open Agent Based Modeling Consortium | 4,337 | 2.59% |
| 6. Model Library Open Agent Based Modeling Consortium | 3,523 | 2.10% |
| 7. Education Open Agent Based Modeling Consortium | 3,385 | 2.02% |
| 8. Resources Open Agent Based Modeling Consortium | 2,749 | 1.64% |
| 9. Modeling Platforms Open Agent Based Modeling Consortium | 2,427 | 1.45% |
| 10. User account Open Agent Based Modeling Consortium | 2,005 | 1.20% |

● Pageviews

20,000

10,000

10,000

CoMSES Net Stats

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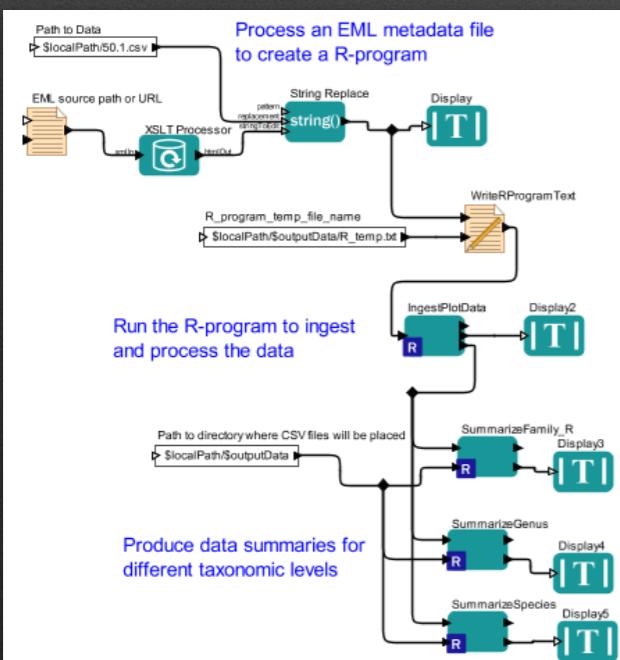
MIRACLE Project

- Mining Relationships Among Variables in Large Datasets from Complex Systems
- Digging Into Data international consortium research
 - Social Sciences and Humanities Research Council (Canada)
 - National Science Foundation (USA)
 - Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Netherlands)
 - Jisc (UK)

MIRACLE Project

- Cloud-based, community tools for management and analysis of large, high-dimensional data resulting from computational models of complex socio-ecological systems
- Reproducible workflow
- Next phase for computational transparency and open science

Kepler



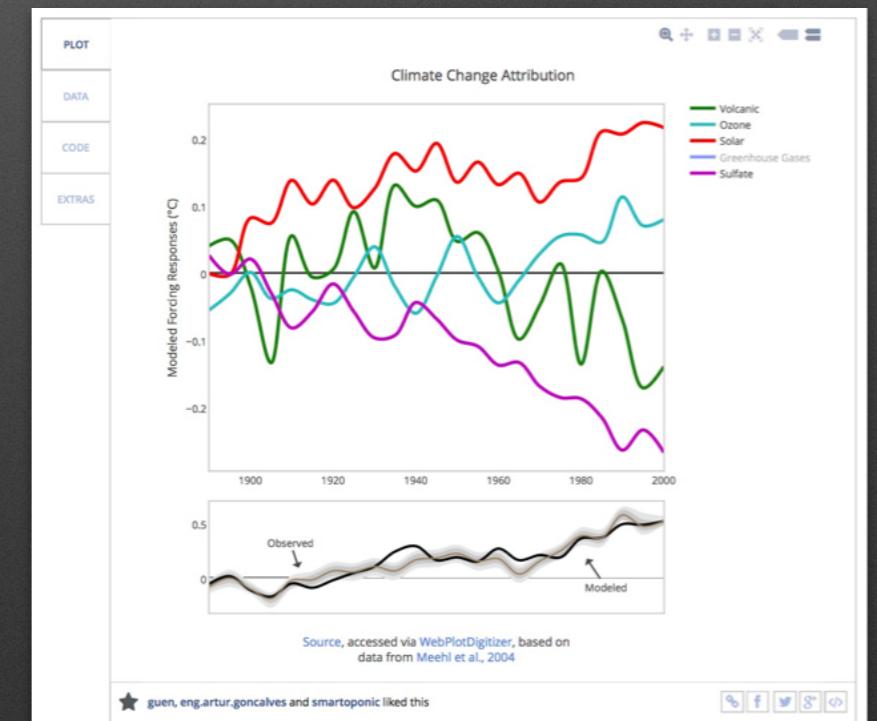
An IPython notebook titled 'IP[y]: Notebook' is shown. The notebook contains the following R code:

```
In [1]: X = c(0, 1, 2, 3, 4)
In [5]: Y = c(3, 5, 4, 6, 7)
In [7]: resid(lm(Y~X));
      1   2   3   4   5
     -0.2  0.9 -1.0  0.1  0.2
In [8]: coef(lm(X~Y))
      (Intercept)      Y
                 -2.5       0.9
In [9]: plot(X,Y)
```

Below the code, there is a scatter plot with X and Y axes ranging from 0 to 4.

Domino

Plotly



Acknowledgements

- NSF Human Social Dynamics Program, grant BCS-623162
- NSF Coupled Natural and Human Systems Program, grant GEO-909394
- NSF Digging Into Data, grant SMA-1430411

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