High-end computing support for large-scale agent-based modelling

Challenges & opportunities

Gary Polhill

The James Hutton Institute

Thanks to…
Alison Heppenstall, Mike Batty, Richard Milton, Doug Salt, Matt Hare, Ric Colasanti, Kieran Jarrett

Outline

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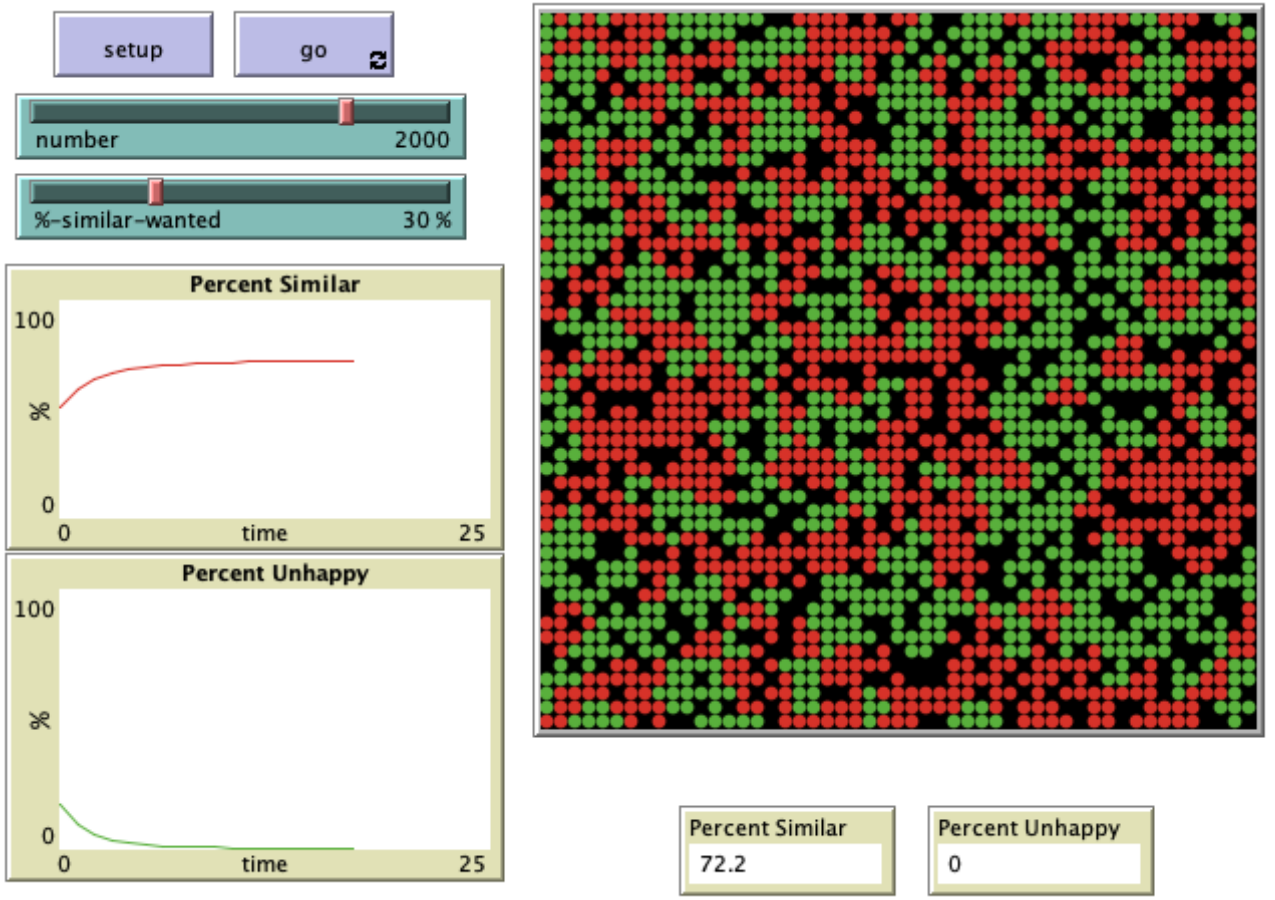
- A very short history of ABMs
- Empirical ABMs need HPC
  - But not routinely used
- Challenges and opportunities for making HPCs suitable for ABM
  - Institutional and technical

From…



Schelling-Sakoda ABM of Social Segregation

...to

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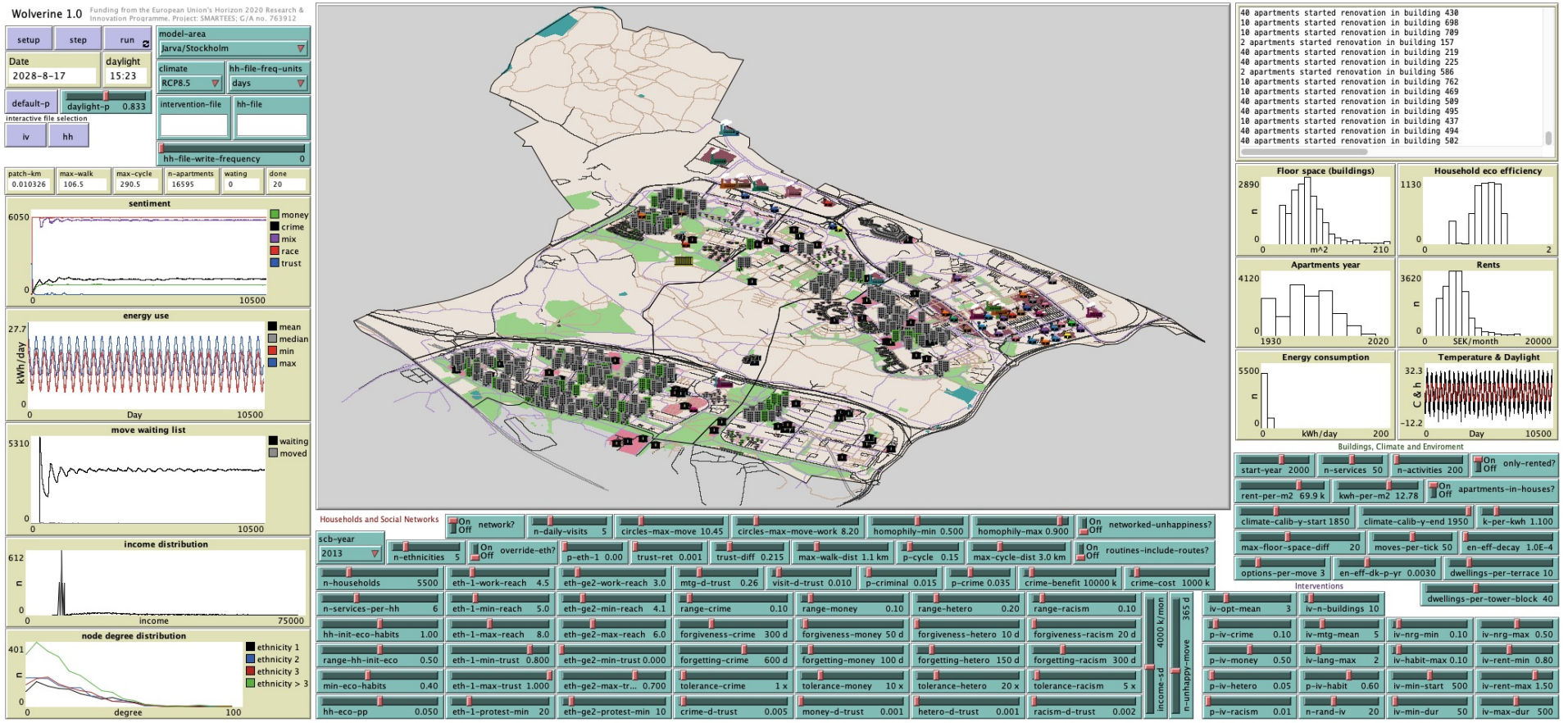

District Regeneration in an Area of Stockholm

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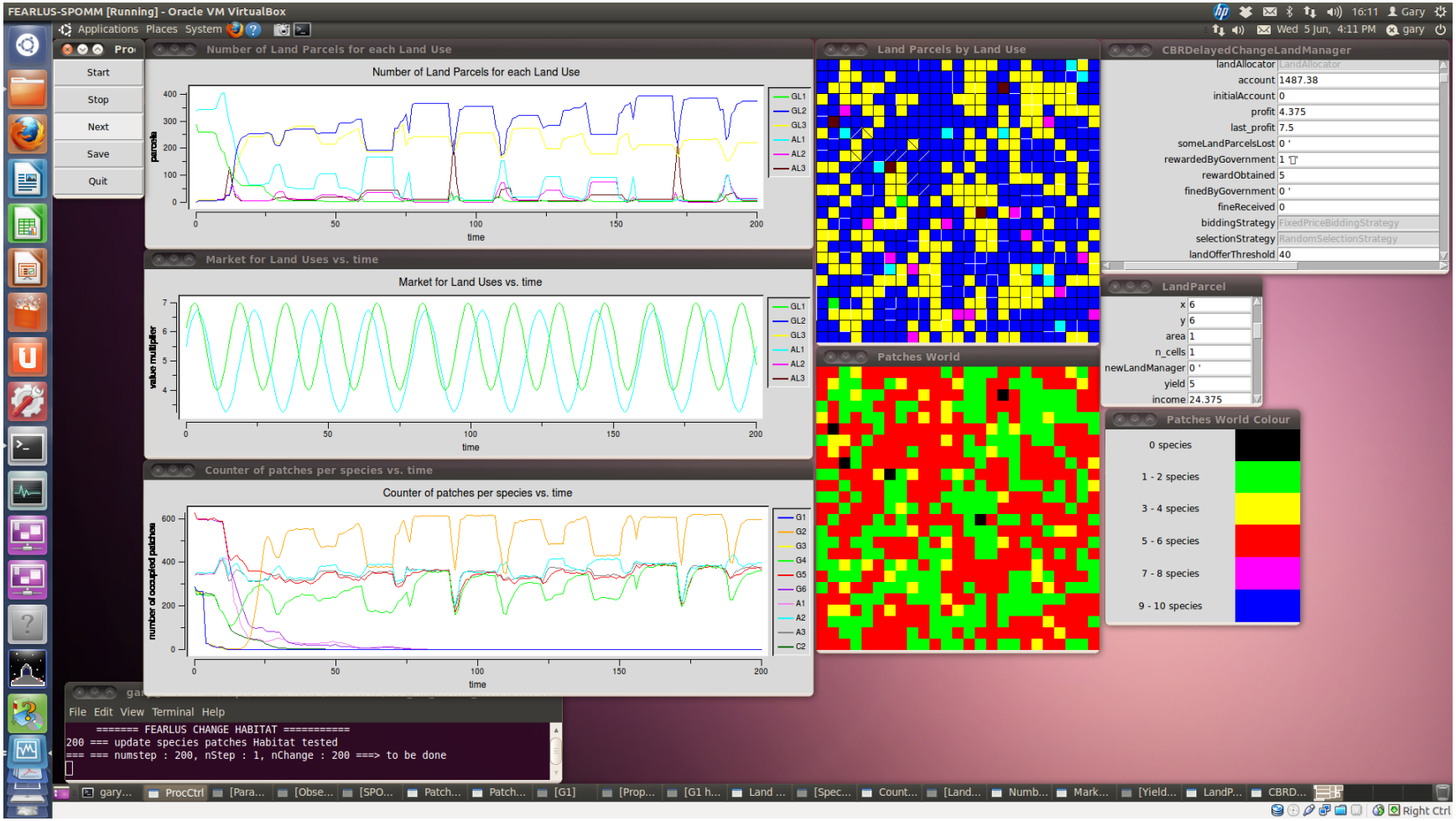
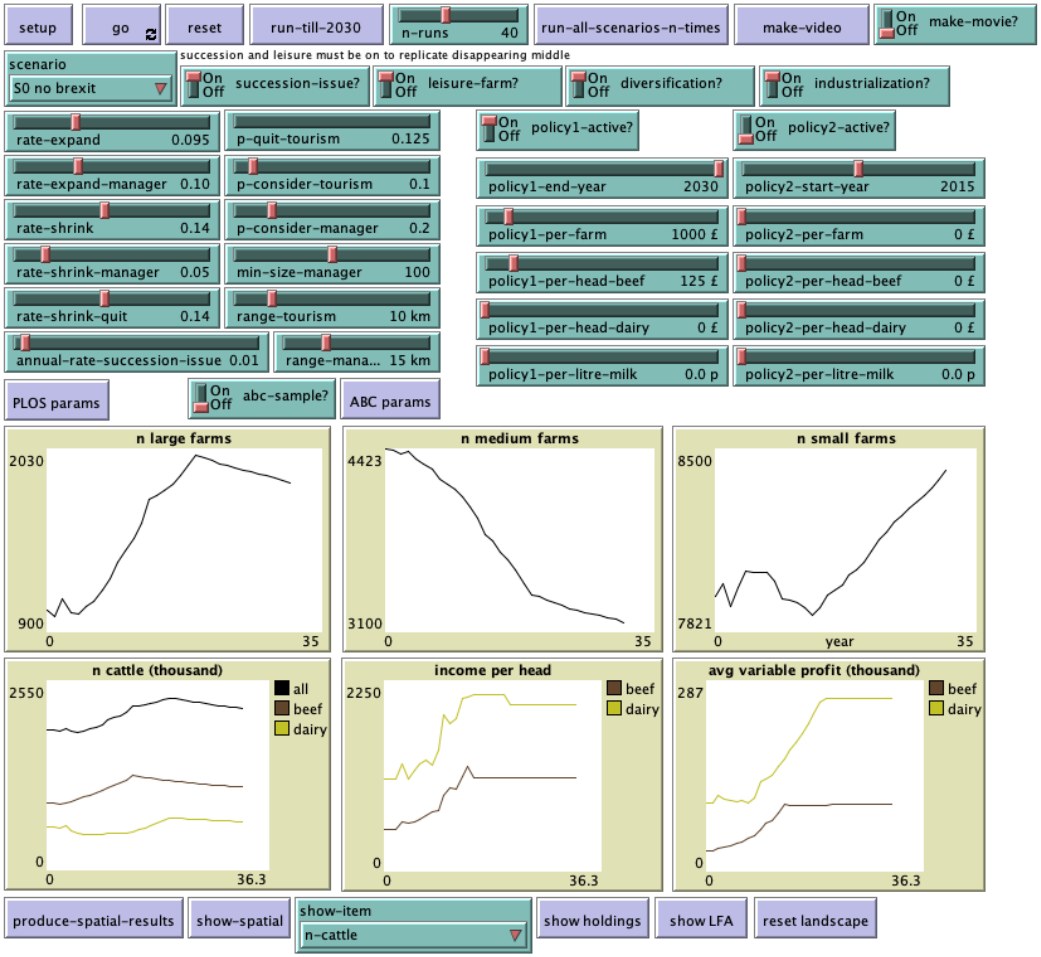
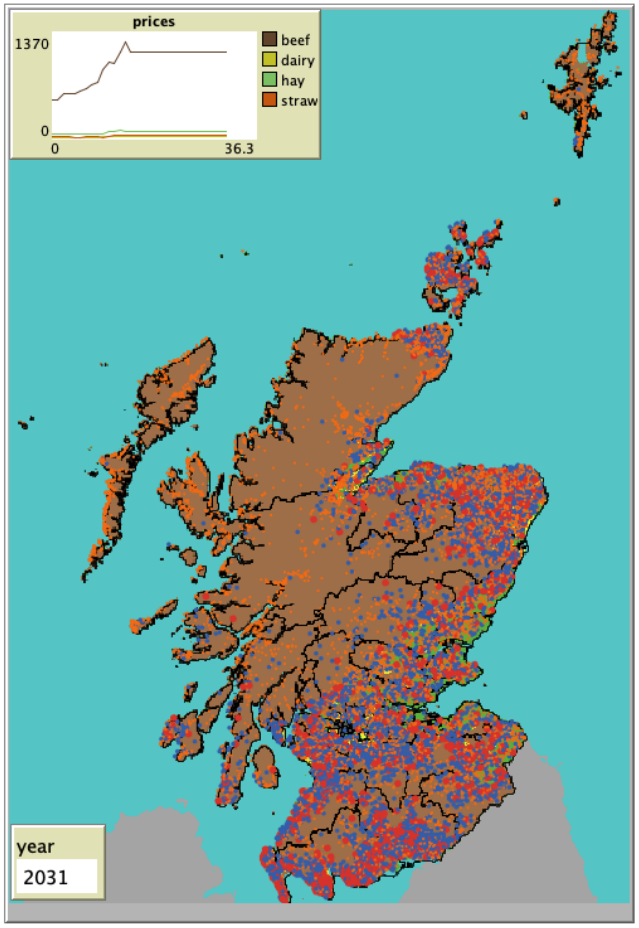


FEARLUS-SPOMM: biodiversity and agricultural land use change (stylized)

...to





Cattle farmers in Scotland and potential responses to Brexit

From…

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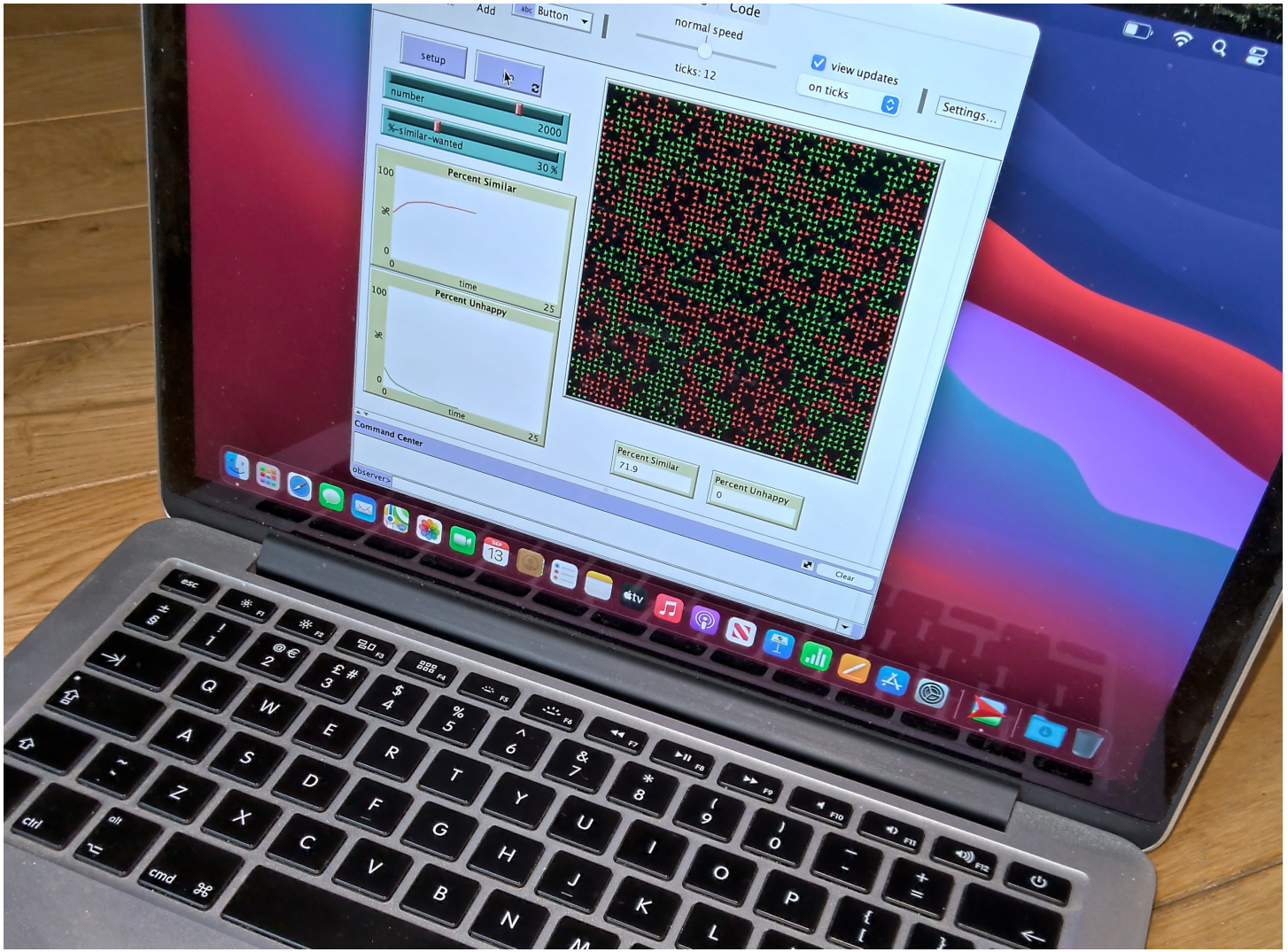
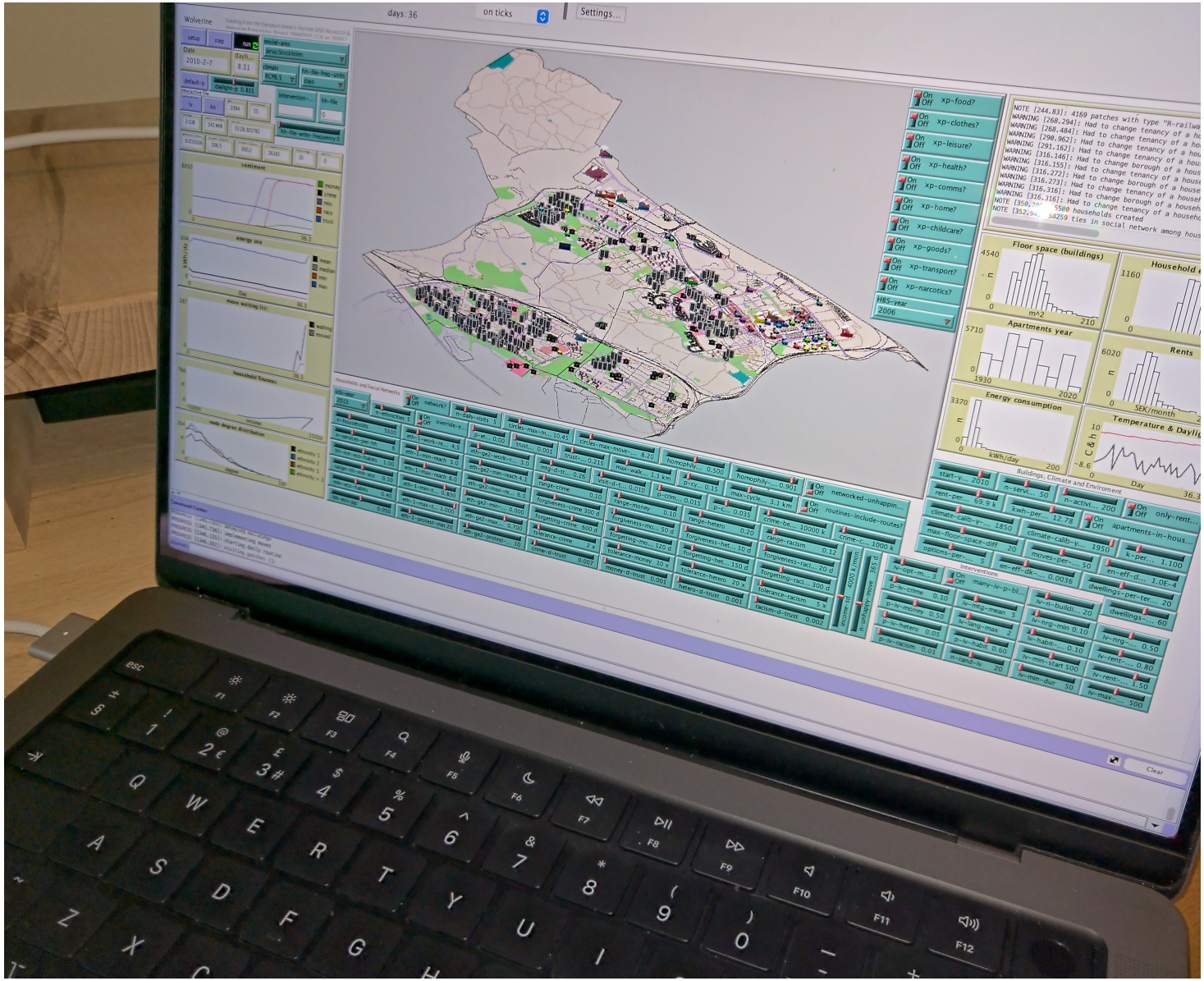


...to!?



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Empirical ABM…

- Growth in use cases
- Easier for non-experts
- Take advantage of ‘ontological realism’
- Loads of data
  - Input and Output
- Require more complicated models
- Need more runs
  - Calibration/Validation
  - Equi-/multifinality
- Need HPC

Ecology & Society

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E&S HOME > VOL. 11, NO. 2 > ART. 37

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The following is the established format for referencing this article:
Janssen, M. A., and E. Ostrom. 2006. Empirically based, agent-based mode
http://www.ecologyandsociety.org/vol11/iss2/art37/

Guest Editorial, part of Special Feature on Empirical based agent-based

Empirically Based, Agent-based models

Marco A. Janssen [1] *and Elinor Ostrom* [2]

[1]Arizona State University, [2]Indiana University and Arizona State University

ELSEVIER

Environmental Modelling & Software

Volume 86, December 2016, Pages 56-67

Simple or complicated agent-based models? A complicated issue

Zhanli Sun [a], Iris Lorscheid [b], James D. Millington [c], Steffen Lauf [d], Nicholas R. Magliocca [e], Jürgen Groeneveld [f g], Stefano Balbi [h], Henning Nolzen [f], Birgit Müller [f], Jule Schulze [f], Carsten M. Buchmann [i j]

Show more

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https://doi.org/10.1016/j.envsoft.2016.09.006

Why don't ABMers routinely use HPC?

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- Steep learning curve
  - Yet another bit of unstable CS tech for social scientists to learn
  - Alessa et al. (2006)
  - An et al. (2020)
- 'HPC snobbery'
  - 'Embarrassingly parallel' multiple parameter samples
- Resource needs unpredictable…

CONTENT

ANTISOCIAL SIMULATION: USING SHARED HIGH-PERFORMANCE COMPUTING CLUSTERS TO RUN AGENT-BASED MODELS

DECEMBER 14, 2022 THESUBMISSIONAUTHOR LEAVE A COMMENT

By Gary Polhill

Information and Computational Sciences Department, The James Hutton Institute, Aberdeen AB15 8QH, UK.

Interlude: the Wolf-Sheep model

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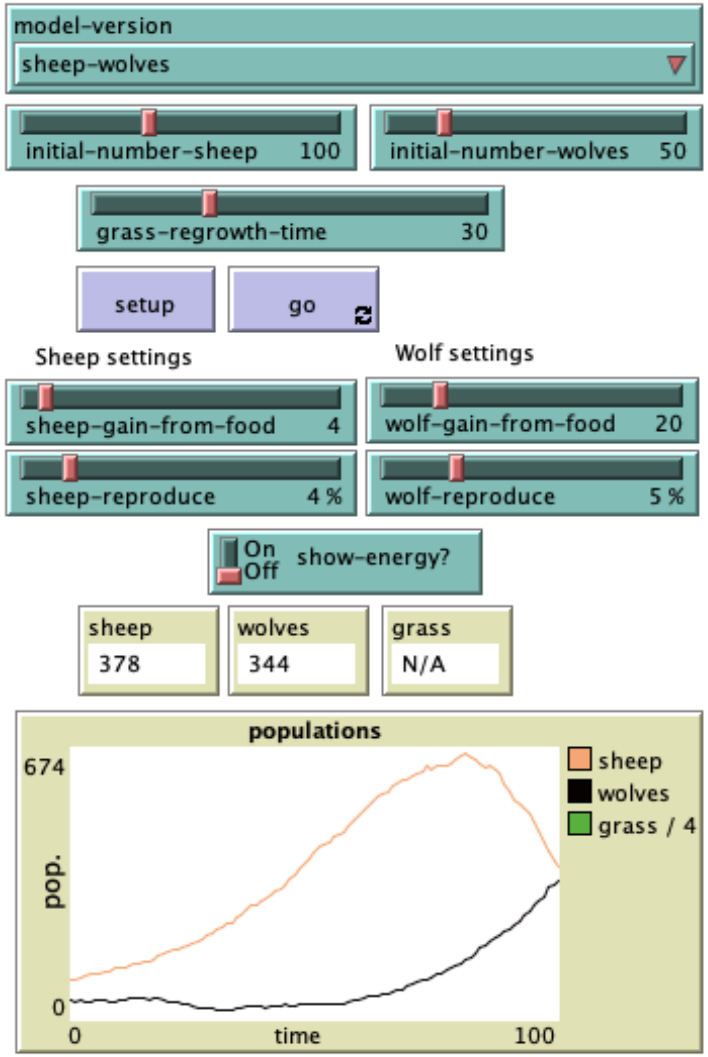

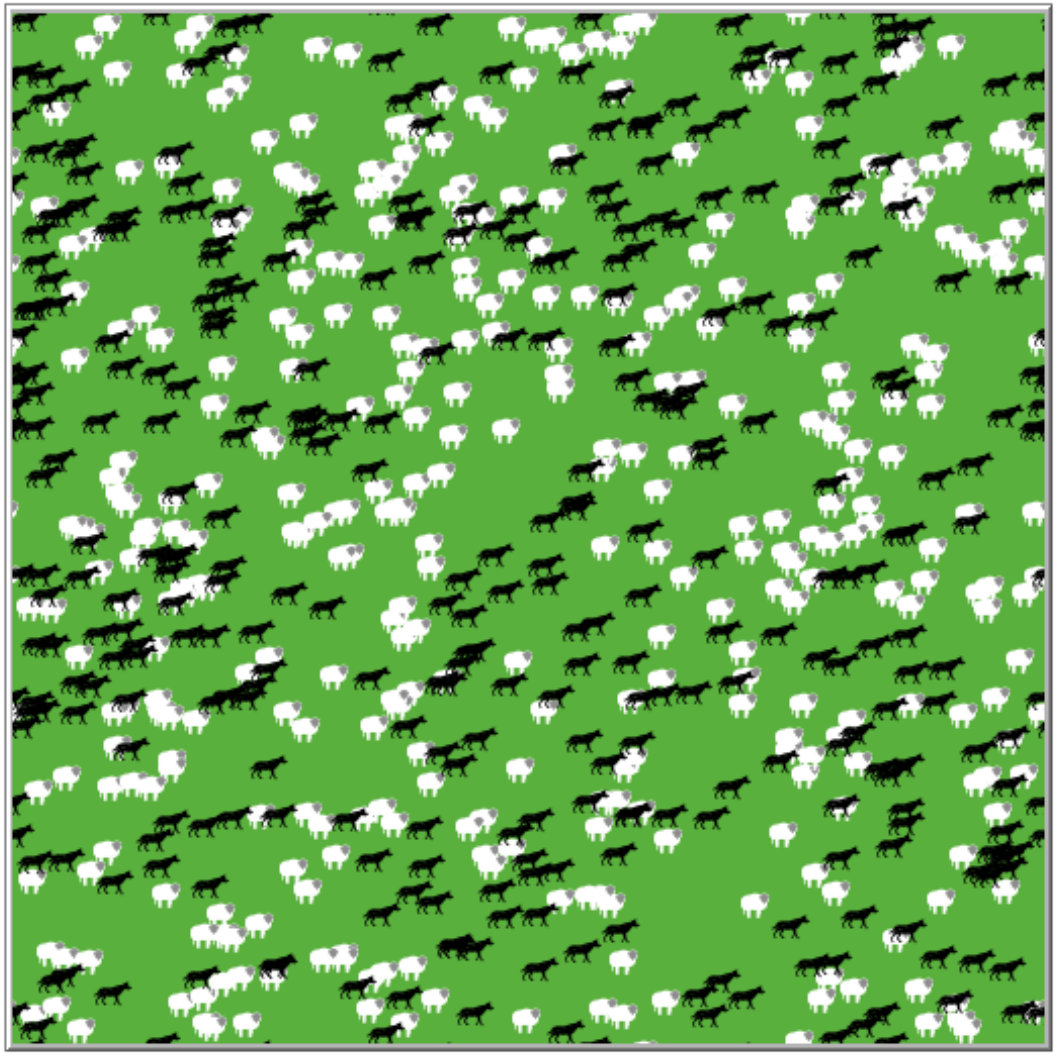

Wolf sheep model

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- Simulates predator prey dynamics
  - Sheep reproduce and are preyed on by wolves
  - Wolves reproduce and eat sheep
- Stops when all the sheep are dead
- Populations of sheep and wolves depend on each other and where they are
- N.B. Lotka-Volterra model classic in ecology
  - Regular population cycles
  - Deterministic

$$\frac{\partial \text{sheep}}{\partial t} = \zeta \times \text{sheep} - \eta \times \text{sheep} \times \text{wolves}$$

$$\frac{\partial \text{wolves}}{\partial t} = \theta \times \text{sheep} \times \text{wolves} - \lambda \times \text{wolves}$$

Change 1: Fix the seed before setting up

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```
1  globals [ max-sheep ]  ; don't let the sheep population grow too large
2
3  ; Sheep and wolves are both breeds of turtles
4  breed [ sheep a-sheep ]  ; sheep is its own plural, so we use "a-sheep" as the singular
5  breed [ wolves wolf ]
6
7  turtles-own [ energy ]       ; both wolves and sheep have energy
8
9  patches-own [ countdown ]    ; this is for the sheep-wolves-grass model version
10
11 to setup
12   clear-all
13
14   random-seed 123456789
15
16   ifelse netlogo-web? [ set max-sheep 10000 ] [ set max-sheep 30000 ]
17
18   ; Check model-version switch
19   ; if we're not modeling grass, then the sheep don't need to eat to survive
20   ; otherwise each grass' state of growth and growing logic need to be set up
21   ifelse model-version = "sheep-wolves-grass" [
22     ask patches [
23       set pcolor one-of [ green brown ]
24       ifelse pcolor = green
25         [ set countdown grass-regrowth-time ]
26       [ set countdown random grass-regrowth-time ] ; initialize grass regrowth clocks ra
27     ]
28   ]
```

Line 14:

`random-seed 123456789`

Change 2: Use an arbitrary seed after

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```
44    [
45      set shape "wolf"
46      set color black
47      set size 2  ; easier to see
48      set energy random (2 * wolf-gain-from-food)
49      setxy random-xcor random-ycor
50    ]
51    display-labels
52    reset-ticks
53
54    random-seed new-seed
55  end
56
57  to go
58    ; stop the model if there are no wolves and no sheep
59    if not any? turtles [ stop ]
60    ; stop the model if there are no wolves and the number of sheep gets very large
61    if not any? wolves and count sheep > max-sheep [ user-message "The sheep have inherite
62    ask sheep [
63      move
64
65      ; in this version, sheep eat grass, grass grows, and it costs sheep energy to move
66      if model-version = "sheep-wolves-grass" [
67        set energy energy - 1  ; deduct energy for sheep only if running sheep-wolves-gras
68        eat-grass  ; sheep eat grass only if running the sheep-wolves-grass model version
69        death ; sheep die from starvation only if running the sheep-wolves-grass model ver
70      ]
71
```

Line 54:

`random-seed new-seed`

Time (in the model)

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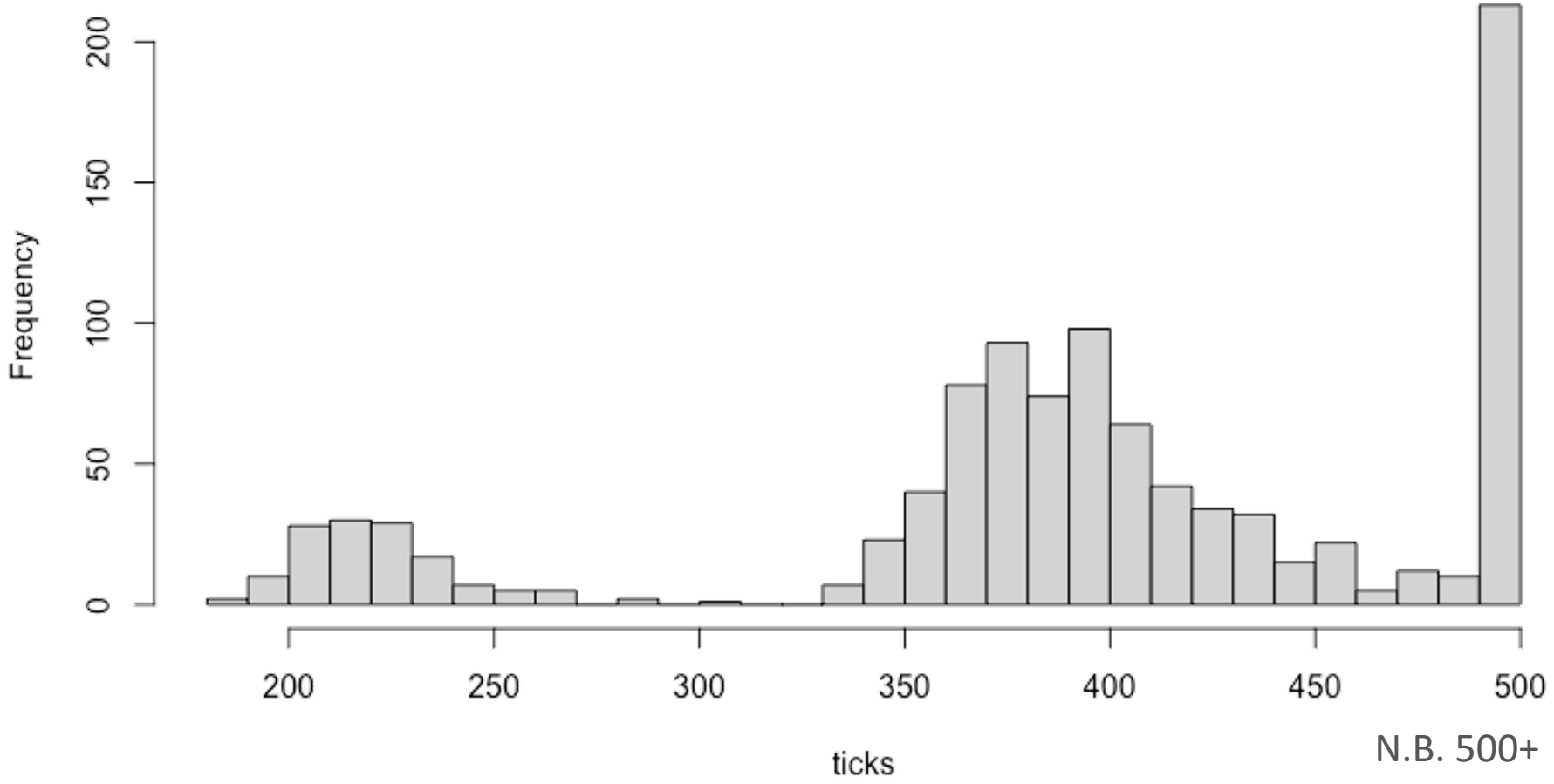
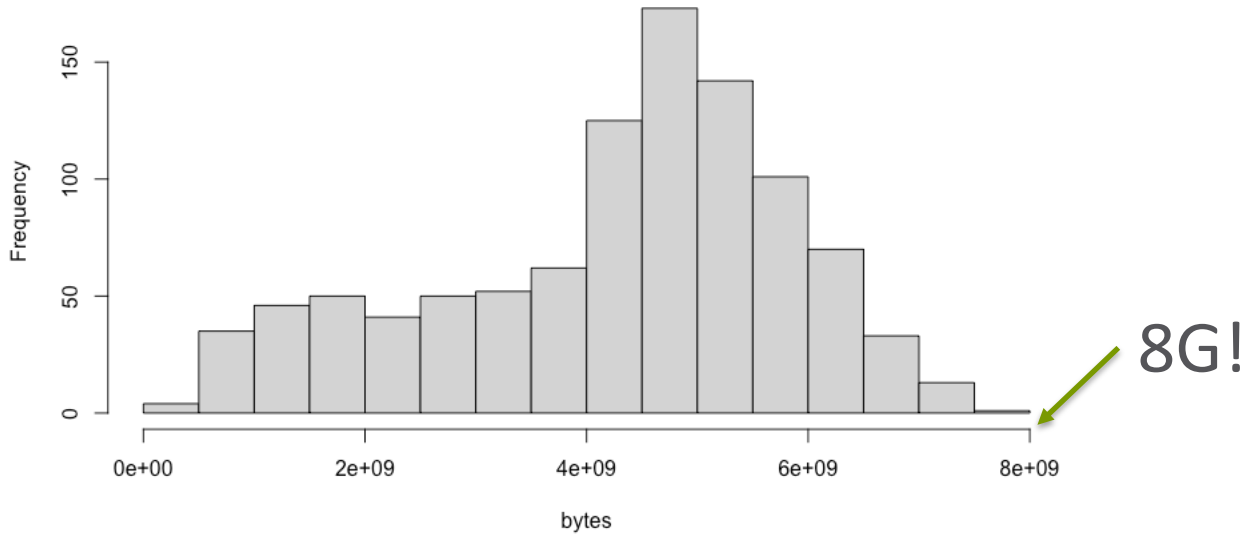


N.B. 500+

Memory use



- Simple, canonical model
- Identical initial conditions and parameters
- Huge variation in memory requirements
- Huge variation in CPU time needed

Features of ABMs affecting computing

- Population change
  - Extinction
- Interactions when social networks not fixed
- Agents having memories
  - Lists grow and shrink
- Contextually sensitive decision-making
  - e.g. Consumat (Jager 2000)
- Qualitatively different behaviour at large scales
  - e.g. Gotts & Polhill (2010)

Uncertainty	Needs Satisfaction: High	Needs Satisfaction: Low
High	Do what most others do	Do what others like me do
Low	Do what I did last time	Maximize utility

Advances in Complex Systems
| Vol. 13, No. 04, pp. 453-467 (2010)

SIZE MATTERS: LARGE-SCALE REPLICATIONS OF EXPERIMENTS WITH FEARLUS

NICHOLAS M. GOTTS and J. GARY POLHILL

https://doi.org/10.1142/S0219525910002670 | **Cited by:** 7

‘Technical Assessment’ form for ARCHER2

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Please see notes in the Service Specification document regarding the maximum amounts of time that can be applied for and technical specifications.

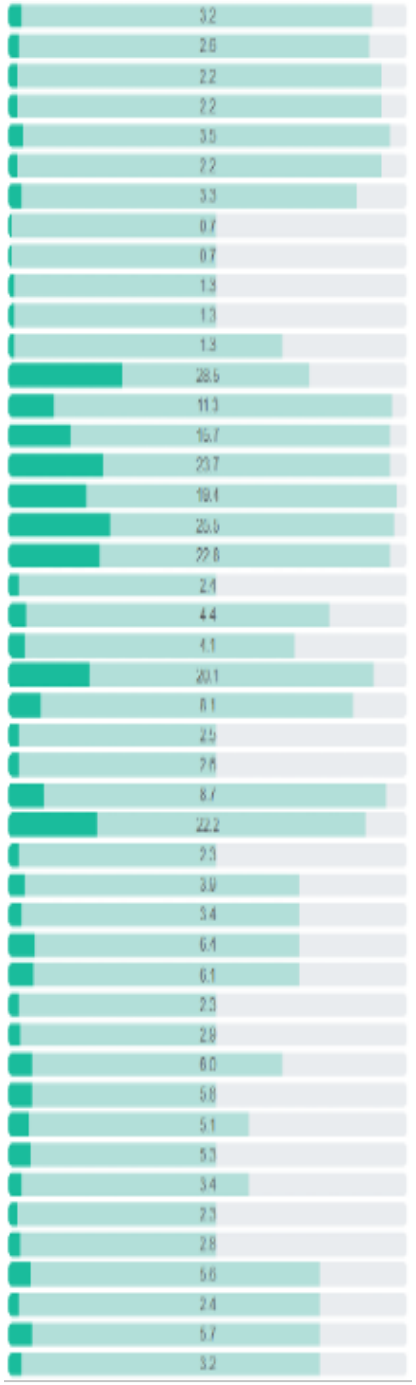
	Largest Job	Typical Job	Smallest Job
Number of nodes	[Please Complete Table]		
Number of cores/GPUs used per node			
Wallclock time for each job*			
Number of jobs of this type			
Memory per node required.			

*The maximum permitted wallclock time per job is a function of local Service centre policy.

Rice, H. G. (1953) Classes of recursively enumerable sets and their decision problems. *Transactions of the American Mathematical Society* **74**, 358-366. https://doi.org/10.1090/S0002-9947-1953-0053041-6

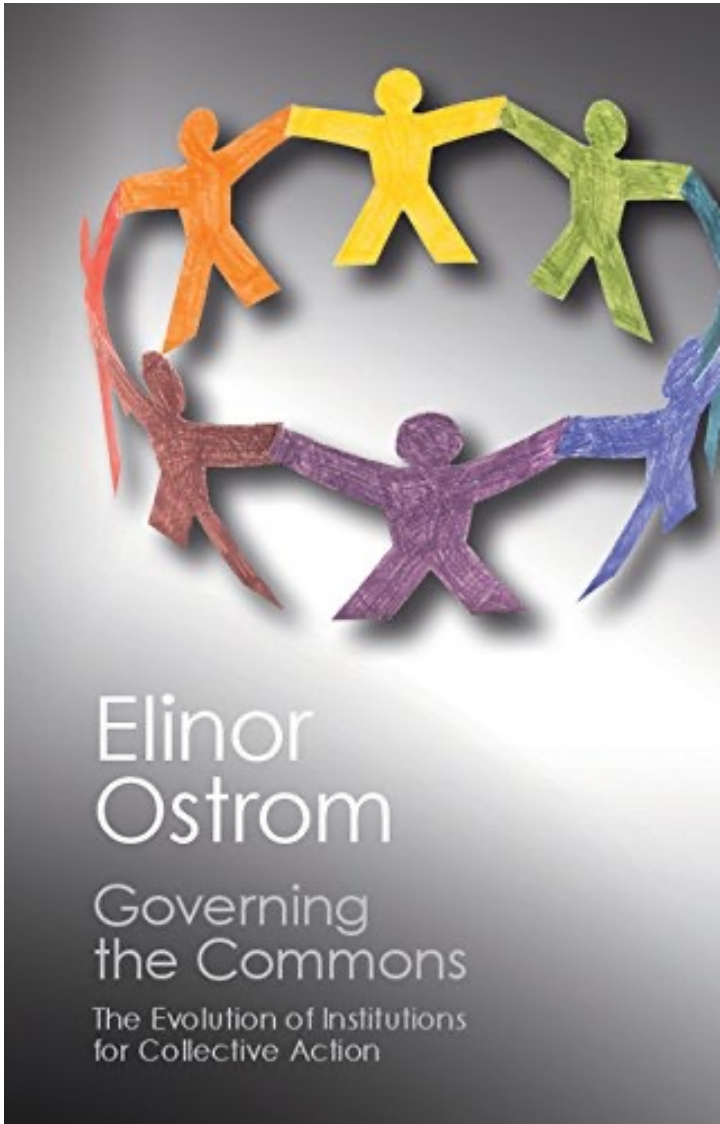
Can I once again remind everyone to please be sensible (and considerate) in your allocation of memory for jobs on the cluster. We now have a situation on the cluster where jobs are unable to run because large amounts of memory have been requested yet only a tiny amount is actually active - check the attached image, where light green shows allocated and dark green shows used.

Over allocating resources can block the cluster for others, as well as waste a huge amount of energy as additional machines need to power up unnecessarily.



The ‘other side’…

- HPC equipment is expensive and needs to be justified to the funder
  - i.e. tax-payer
- Scientists are *impossible* to manage!
- Shared resource needs *some form* of governance
  - But we have adopted a managerialist / ‘leviathan’ approach…
    - Ostrom: other options exist…



HPC as a social dilemma

- Suppose no-one can predict their resource use accurately
  - Only the most boring computational problems are predictable
    - Complexity snobbery ☺
- If I underestimate I will not get my results at all
- If I overestimate I will get my results
- If too many people overestimate, it will take ages to get my results
  - Too much computing time needed
- Long history of applying ABM to common pool resources…

Regular Article

Modelling individual behaviour and group performance in an intelligent agent-based simulation of the tragedy of the commons

P.J. Deadman

Segismundo S. Izquierdo, Luis R. Izquierdo and Nicholas M. Gotts (2008)

Reinforcement Learning Dynamics in Social Dilemmas

Journal of Artificial Societies and Social Simulation vol. 11, no. 2 1 <https://www.jasss.org/11/2/1.html>

Using HPC effectively: opportunities

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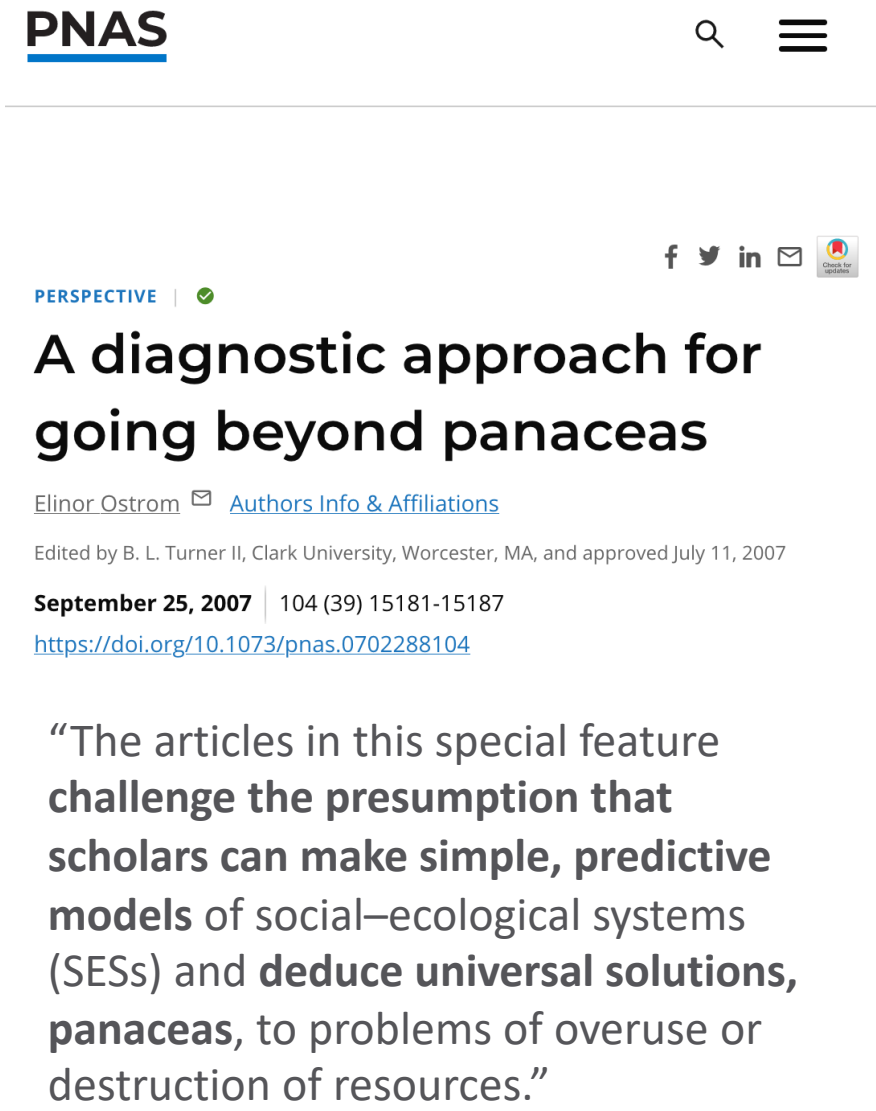
- Study HPC use with ABMs!
  - Which policies work?
  - Can users exploit them?
- Draw on social sciences
  - Governance and institutions
  - Mindfulness of power dynamics
    - Gender/ethnicity/class dimensions
  - Critiques of hegemonistic managerialism
- Fun computing science!
  - Adaptive HPC schedulers?
  - Automatic parallelism?
  - Encryption for confidentiality?
    - Memory space, data in/out, …



PNAS

PERSPECTIVE

A diagnostic approach for going beyond panaceas

Elinor Ostrom | Authors Info & Affiliations

Edited by B. L. Turner II, Clark University, Worcester, MA, and approved July 11, 2007

September 25, 2007 | 104 (39) 15181-15187

https://doi.org/10.1073/pnas.0702288104

"The articles in this special feature **challenge the presumption that scholars can make simple, predictive models** of social–ecological systems (SESs) and **deduce universal solutions, panaceas**, to problems of overuse or destruction of resources."

Exascale computing…

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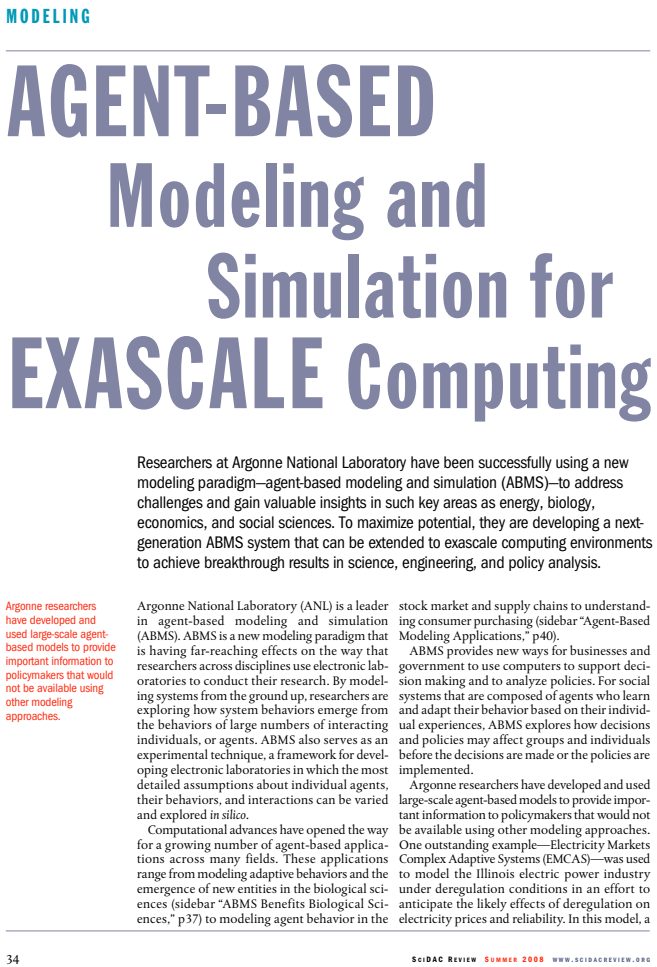
- 10^18 FLOPS
  - ~ A billion laptops
  - ~ A million clusters
  - ~ A thousand clouds
- First exascale computer in 2022
  - Frontier, USA
  - ~600k CPU cores; ~8M GPUs
    - N.B. massive parallelism
  - 21 MW of power
- Macal & North 15 years ago!
  - But interactions kill parallelism…
- UK and EU both planning one



MODELING

AGENT-BASED Modeling and Simulation for EXASCALE Computing

Researchers at Argonne National Laboratory have been successfully using a new modeling paradigm—agent-based modeling and simulation (ABMS)—to address challenges and gain valuable insights in such key areas as energy, biology, economics, and social sciences. To maximize potential, they are developing a next-generation ABMS system that can be extended to exascale computing environments to achieve breakthrough results in science, engineering, and policy analysis.

Argonne researchers have developed and used large-scale agent-based models to provide important information to policymakers that would not be available using other modeling approaches.

Argonne National Laboratory (ANL) is a leader in agent-based modeling and simulation (ABMS). ABMS is a new modeling paradigm that is having far-reaching effects on the way that researchers across disciplines use electronic laboratories to conduct their research. By modeling systems from the ground up, researchers are exploring how system behaviors emerge from the behaviors of large numbers of interacting individuals, or agents. ABMS also serves as an experimental technique, a framework for developing electronic laboratories in which the most detailed assumptions about individual agents, their behaviors, and interactions can be varied and explored *in silico*.

Computational advances have opened the way for a growing number of agent-based applications across many fields. These applications range from modeling adaptive behaviors and the emergence of new entities in the biological sciences (sidebar "ABMS Benefits Biological Sciences," p37) to modeling agent behavior in the stock market and supply chains to understanding consumer purchasing (sidebar "Agent-Based Modeling Applications," p40).

ABMS provides new ways for businesses and government to use computers to support decision making and to analyze policies. For social systems that are composed of agents who learn and adapt their behavior based on their individual experiences, ABMS explores how decisions and policies may affect groups and individuals before the decisions are made or the policies are implemented.

Argonne researchers have developed and used large-scale agent-based models to provide important information to policymakers that would not be available using other modeling approaches. One outstanding example—Electricity Markets Complex Adaptive Systems (EMCAS)—was used to model the Illinois electric power industry under deregulation conditions in an effort to anticipate the likely effects of deregulation on electricity prices and reliability. In this model, a

Summary

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- Empirical ABMs need HPC
- HPC needs new institutions and software
  - Don’t hamstring expensive equipment so it can only solve (computationally) easy problems…

- ExAMPLER project (EPSRC: Jun 23 – Nov 24)
  - Exploring transformative potential of exascale computing for empirical ABM
    - Exascale computing is fast enough to experiment with large-scale ABMs in under a second
    - Imagine being able to explore options to handle a developing crisis without waiting a month for your ABM results…

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https://exascale.hutton.ac.uk/
https://large-scale-modelling.hutton.ac.uk/

Agent-based modelling work at The James Hutton Institute has been funded by the Scottish Government, the European Union, the Macaulay Development Trust, the Economic and Social Research Council, the Engineering and Physical Sciences Research Council, and the Research Council of Norway

Scottish Government
Riaghaltas na h-Alba
gov.scot

MACAULAY DEVELOPMENT TRUST

UKRI Economic and Social Research Council

UKRI Engineering and Physical Sciences Research Council

With funding from The Research Council of Norway

SYSTEM CERTIFICATION ISO 14001 SGS

SYSTEM CERTIFICATION ISO 9001 SGS

ECU GENDER CHARTER Athena SWAN Bronze Award

Stonewall DIVERSITY CHAMPION SCOTLAND

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