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engage
Engaging research with
e-Infrastructure

Using Research Software to ask new questions

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UNIVERSITY OF
Southampton

MANCHESTER
1824



Engaging Researchers with e-Infrastructure



- Original goal:

“Make high-end computational tools available to more researchers”

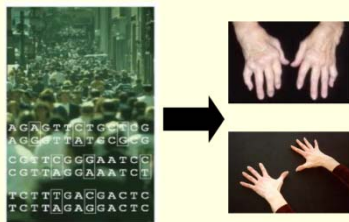
- *Trivial barriers often seem insurmountable*

Engaging Research with e-Infrastructure



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JISC



An Examination of Mr. Hume's Objection to Miracles.
MR. HUME, in his celebrated Essay, *Narr. R.* defines a miracle "A transgression of a law of nature, would undoubtedly silence all opposers, namely, that a greater miracle must be wrought to prove the existence of a lesser one, &c. in other words, that a miracle is the only criterion by which to prove or judge of the existence of miracles. The credit due to them, it is admitted, rests entirely upon testimony; but the specious objection to it, from the supposed incompleteness of human testimony, is invalid, and at most a mere begging of the question. Nevertheless, it must be remembered, that the failure of six witnesses suffices to prove a negative by an excess establishes the converse, an affirmative. On the present occasion, therefore, it will not be irrelevant, and, perhaps, the only satisfactory reply to an objection of this sort, not merely to silence the objections, but also to attempt upon adequate evidence to substantiate the affirmative. The prime support attempted to be derived from the subsequent enlightenments contained in the Essay, such as the notion of an hypothetical array of conflicting testimonies, the want of an uniform experience, &c. &c. will in due time be adverted to, but not much enlarged upon, volumes having already been ably



Interviews

Engaging research with e-Infrastructure

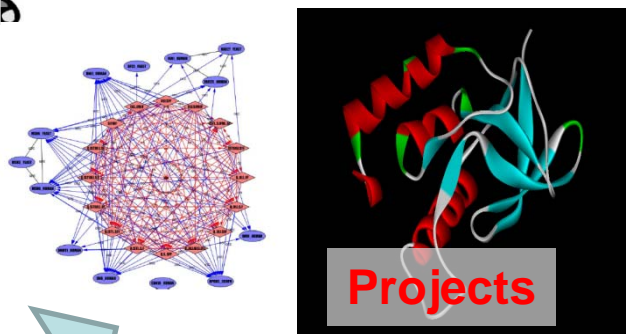
This website provides information to help the research community use and engage with computing infrastructure (e-Infrastructure) in the UK, including workshops, events and success stories.



Learn about how computing has enhanced the work of researchers in Archaeology in the first of a series of video case studies.

If you are a researcher wanting to make use of computing tools and technologies but don't know where to start, you've come to the right place. Use the navigation tabs above to get more information on news, events, and projects.

Wider deployment

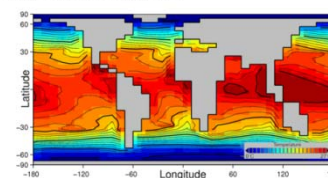


Projects

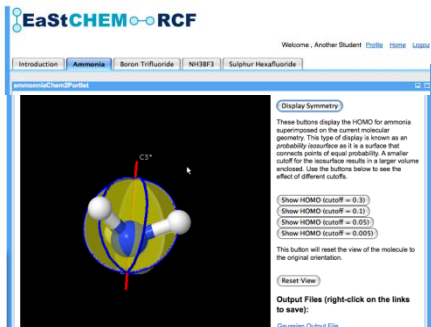
OMII-UK NEWS

March 2009

Making climate modelling accessible



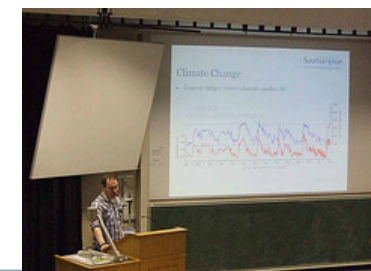
Dissemination



New requirements



Adoption



Engaging Researchers with e-Infrastructure



- Adjunct outcome:

“Make high-end computational tools available to students”

- *Enable students to ask new questions*

Asking questions of the weather

- How can students benefit from utilising the same approaches used in top end research?

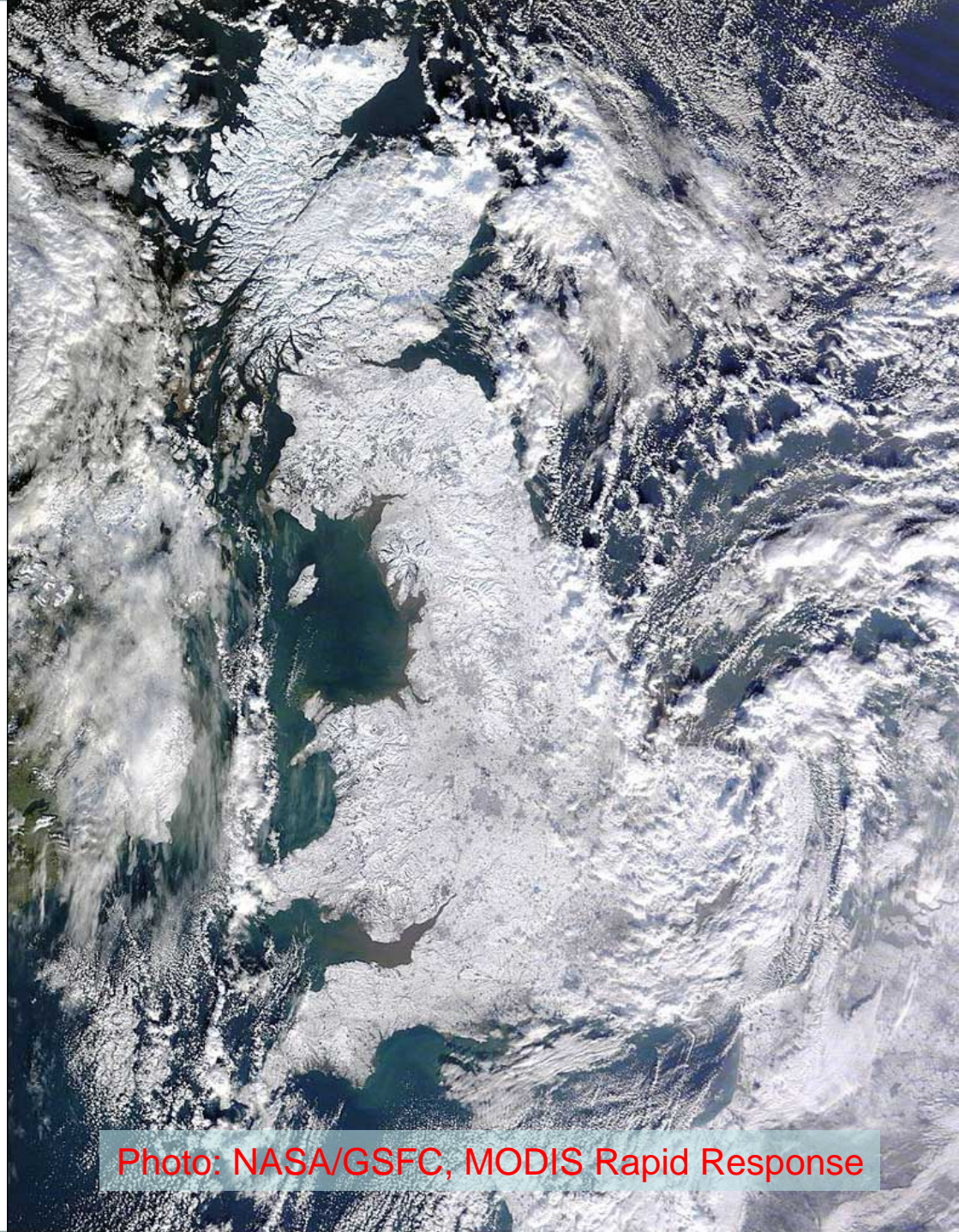
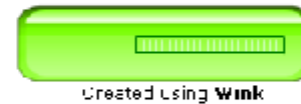


Photo: NASA/GSFC, MODIS Rapid Response

Earth Systems Modelling

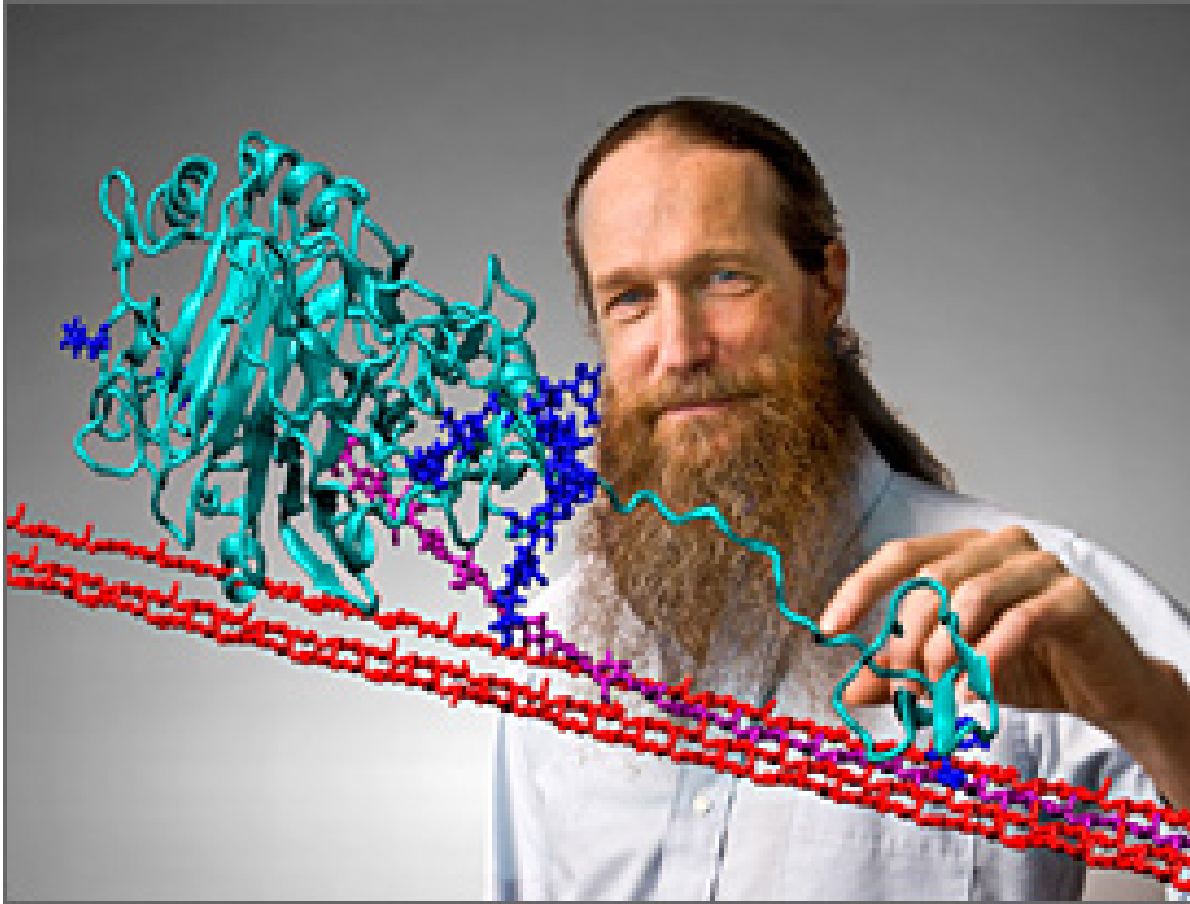


- Easier interface to state of the art earth systems models
- Desktop access



The Open University

Walking with Dinosaurs?



- Michael Crowley, NREL
- Simulation of Cel7A – plant decay
- Efficient biofuels

Protein Simulation



- Carbohydrate recognition
- Chaining several complex tools

The screenshot displays a software interface for protein simulation, likely CCP4. It features two side-by-side 3D molecular models of a protein structure, each with a corresponding control panel on the right. Below the models are two Ramachandran plots showing the distribution of phi (Phi) and psi (Psi) angles for the protein. The interface includes various toolbars and menus for file operations, editing, and visualization.

Left Panel (Kinematic #1):

- File M1
- mainchain
- Calphas
- sidechain
- IFs
- all
- chain A
- chain
- hets
- chain B

Right Panel (Kinematic #1):

- File M1
- mainchain
- Calphas
- sidechain
- IFs
- all
- chain A
- chain
- hets
- chain B

Bottom Left Plot (All data):

- Decorations: Grid, Labels, Axes
- All data
- General
- Glycine
- Proline
- Pre-proline
- Data pts
- Favored
- Allowed
- Titles
- Outlier Lbls

Bottom Right Plot (All data):

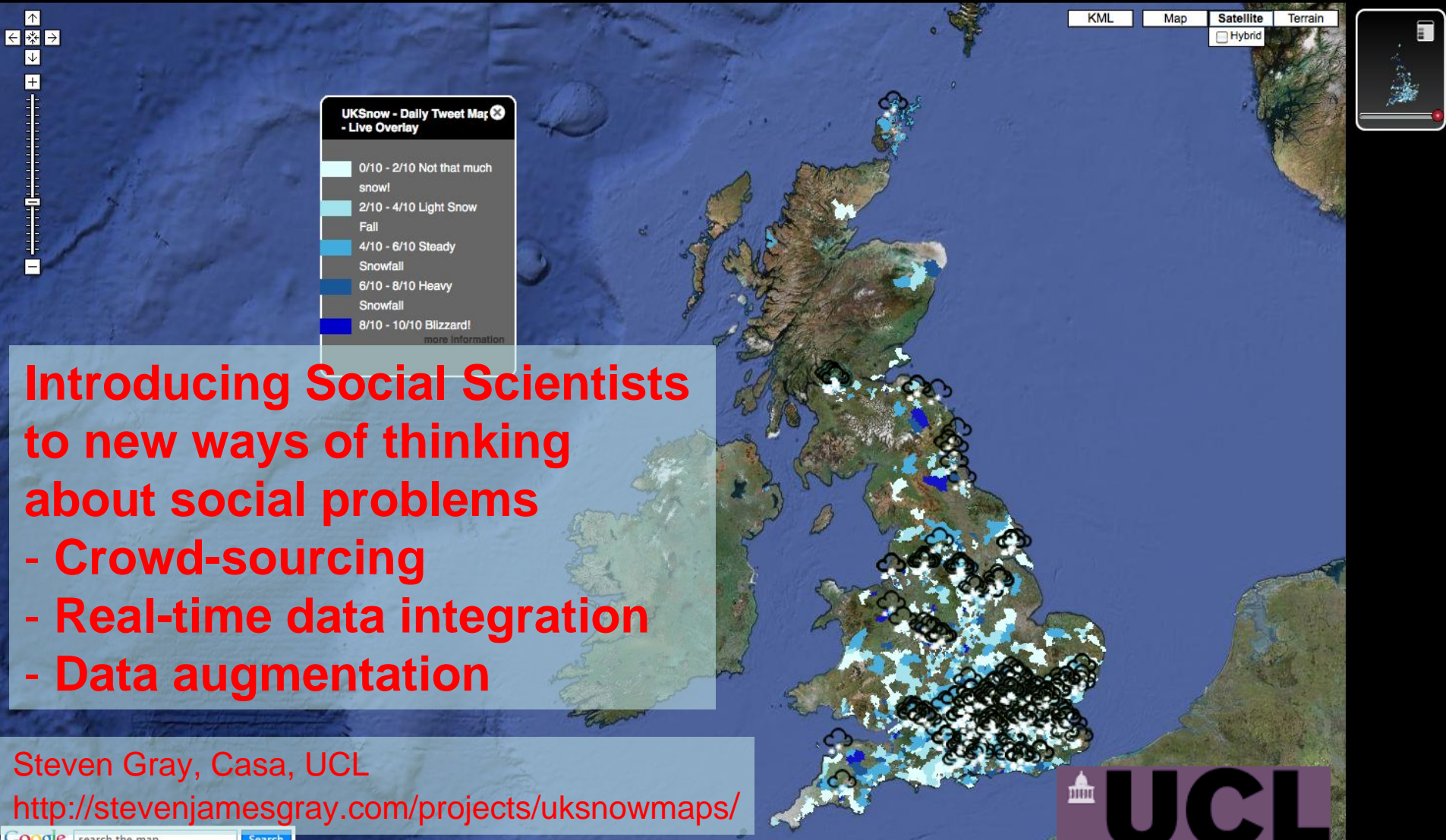
- Decorations: Grid, Labels, Axes
- All data
- General
- Glycine
- Proline
- Pre-proline
- Data pts
- Favored
- Allowed
- Titles

Bottom Status Bar:

All-Atom Contacts	Clashscore, all atoms:	197.07	41 st percentile* (N=222, 0.85Å - 1.35Å)
All-Atom Contacts	Clashscore, all atoms:	178.82	41 st percentile* (N=222, 0.85Å - 1.35Å)

Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.

NeISS: UKSnow-MapTube



Introducing Social Scientists to new ways of thinking about social problems

- Crowd-sourcing
- Real-time data integration
- Data augmentation

Steven Gray, Casa, UCL
<http://stevenjamesgray.com/projects/uksnowmaps/>



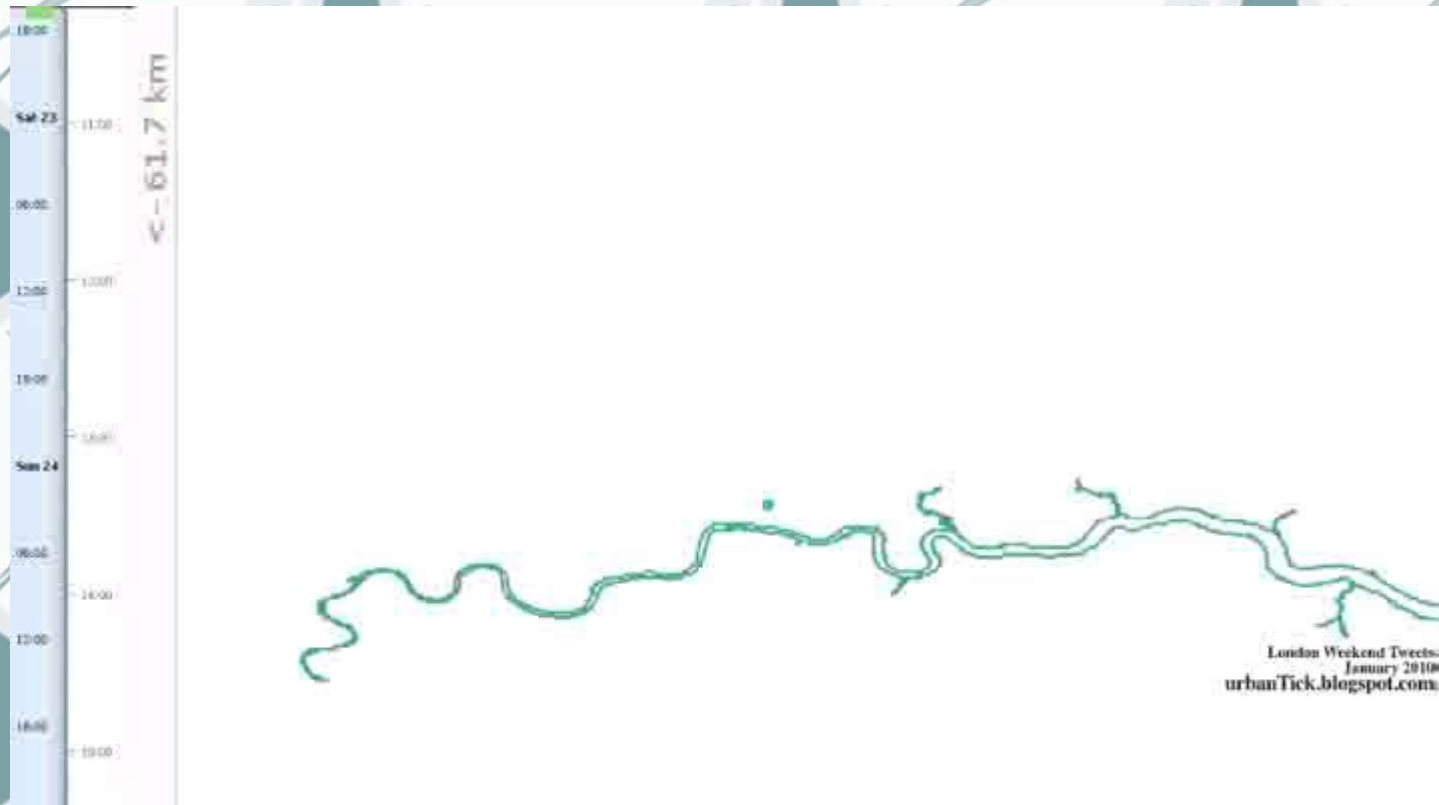


Tweet-o-Meter

NeISS: Tweet-o-Meter



The power of data is what you can do with it



Steven Gray, Casa, UCL
<http://www.casa.ucl.ac.uk/tom/>



Research Computing in the future



- Researcher-led, student-driven simulation



- Make leading research available through the right technology
 - Accurate
 - Appealing
 - Appropriate
 - Accessible

