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Elements of a computational infrastructure for social simulation

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Applications of simulation modelling in social science domains are varied and increasingly widespread. The effective deployment of simulation models depends on access to diverse datasets, the use of analysis capabilities, the ability to visualize model outcomes and to capture, share and re-use simulations as evidence in research and policy-making. We describe three applications of e-social science that promote social simulation modelling, data management and visualization. An example is outlined in which the three components are brought together in a transport planning context. We discuss opportunities and benefits for the combination of these and other components into an e-infrastructure for social simulation and review recent progress towards the establishment of such an infrastructure.

Keywords: social science; simulation models; e-infrastructure; scenario planning

1. Introduction

Recent years have seen a big upswing of interest in simulation for the natural and physical sciences. Some commentators have emphasized how simulation embodies the transition from science *in vitro* to science *in silico* and argue that this signals the emergence of a new scientific paradigm where the focus is on data exploration, rather than hypothesis or experimentally driven research:

The world of science has changed, and there is no question about this. The new model is for the data to be captured by instruments or generated by simulations before being processed by software and for the resulting information or knowledge to be stored in computers. Scientists only get to look at their data fairly late in this pipeline.

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One contribution of 16 to a Theme Issue ‘e-Science: past, present and future I’.

The techniques and technologies for such data-intensive science are so different that it is worth distinguishing data-intensive science from computational science as a new, fourth paradigm for scientific exploration.

(Bell *et al.* 2009)

This trend towards simulation-based methods can also be seen across a range of social science disciplines. Social simulation applications can be characterized as wide-ranging in both method and subject domain, as policy and theory relevant and as short- and long-term. They are typically data-rich, evidence-based, often computationally intensive and are of communal interest. Both micro-simulation and agent-based modelling—for which Epstein (2007) has coined the term ‘generative social science’—have been widely adopted within economics, sociology and geography. Simulation models have also provoked high levels of interest in healthcare research, anthropology and political science. For example, in economics, simulation approaches have been applied to derive the nature of market behaviour from the interactions between individual consumer and producer ‘agents’. These approaches are characterized by an acceptance of disequilibrium behaviour and heterogeneity, both in contradiction of traditional normative economic assumptions (Arthur 1999). In the field of epidemiology, similar agent-based models have been used to model the transmission of illness across a population, with alternative policy interventions to control resistance (i.e. vaccination) or social mixing (Ferguson *et al.* 2005). Long-term projections of the composition and behaviour of populations are increasingly of great importance to planners and policy-makers with an interest in the increasing mass, ethnic diversity and age profile of the population in developed countries—for example, the implications of increased dependency of a growing elderly and retired population on a shrinking cohort of economically active workers (<http://www.lse.ac.uk/collections/MAP2030/>).

New approaches to social simulation are going some way to address longstanding reservations among social theorists about the limitations of quantitative approaches. A representative early example is provided in the critique of Lee (1973), whose ‘seven deadly sins’ convey a sense of unease about the social physics of human systems modelling, and which is embellished in Sayer’s (1979) appeal for a clear distinction between an understanding of the city itself and its representation as an abstract mathematical model. Many of Lee’s reservations about first-generation urban models (in particular, the sins of ‘hungriness’, ‘mechanicalness’ and ‘expensiveness’) are addressed quite directly by the e-infrastructure concept: the lack of data and computational power are not such impermeable barriers to effective social modelling as they once were.

Social simulation has been an important focus for the UK e-Social Science programme (Halfpenny *et al.* 2009). In particular, three projects—DAMES (<http://www.dames.org.uk>), MoSeS (<http://www.ncess.ac.uk/research/geographic/moses>) and GeoVUE (<http://www.ncess.ac.uk/research/geographic/geovue>)—have targeted complementary stages of the simulation research life cycle: data management and integration; mathematical modelling and analysis; and visualization, respectively. Building on these foundations, the National e-Infrastructure for Social Simulation (NeISS; <http://www.neiss.org>) project is undertaking a coordinated programme of productionizing services and community

engagement to create a sustainable, world-class social simulation capability, supporting the entire research life cycle and with potential for major impact, both in the UK and internationally.

The NeISS seeks to provide production-quality services for social simulation that will enable researchers to take full advantage of data-intensive methods. Exploiting the capacity that the new generation of simulation tools and infrastructure have for generating large volumes of data is not, by itself, sufficient to maximize their benefits: the aim of NeISS is to support the entire simulation research life cycle, from data management and population generation through to model building and execution, visualization, analysis, publication and archiving of the entire process for future discovery and re-use. Further, NeISS aims to build community capacity in the use of social simulation by promoting a sharing of simulation methods, models and results among social scientists and broadening the user base to include commercial and public sector decision-makers and the general public.

In this paper, we discuss the motivations for providing computational support for social simulation and then describe some of the important developments to date in the NeISS project. An example scenario will be articulated, and we consider the scope and benefits of an integrated e-infrastructure platform.

2. NeISS motivation and overview

The benefits of the NeISS can be viewed from a number of perspectives, but what is most important is the way in which it aims to bring together a range of services in order to provide integrated support for the whole simulation research life cycle. The NeISS aims to introduce social scientists to new ways of thinking about social problems and provide new services, tools and research communities to support them. These tools will be capable of being deployed for a diverse range of social research domains: they will enable users to create workflows to run their own simulations, to visualize and analyse results and to publish them for future discovery, sharing and re-use. NeISS will facilitate development and sharing of social simulation resources within the social science community, encourage cooperation between model developers and researchers and help foster adoption of simulation as a research method in the social sciences and as a decision support tool in the public and private sectors.

The computational requirements of simulation can be rather extensive. In the work on the transmission of avian bird flu, Ferguson (2005) observed that ‘to do these runs quickly, the model needed . . . huge amounts of memory—20 times that found on a typical PC. In fact, the team hooked up ten high-powered computers in parallel, but even then the final runs took more than a month of computer time’. The suitability of social simulation models for massive parallelization has also been demonstrated previously (George *et al.* 1997). Computational support for decision-making with social simulation has been explored through a series of projects funded through the UK e-Social Science programme (Birkin *et al.* 2005; Townsend *et al.* 2009).

Visualization is intimately linked to simulation as the means by which complex model outputs can be easily digested and interpreted. In addition, the visual representation of geographical information—as maps—provides a

standard for decision-support in applied contexts, from emergency planning to retail management. McEachren *et al.* (2005, p. 300) explain how visual simulation supports emergency planning in ‘transportation support, search and rescue, environmental protection and fire fighting’ and go on to argue that as decision-making is typically a multi-step, multi-participant process, collaborative environments have major importance. The potential for computational steering, with a (real-time) interaction between computational simulation and policy intervention (e.g. Brodlie *et al.* 2004), also deserves further exploration in the context of social policy. Work in the GeoVUE node has combined the development of a shared repository for spatial data (MapTube) and more innovative and experimental approaches through mechanisms such as ‘Second Life’.

The importance of simulation modelling as a means for combining evidence at alternative levels of aggregation, or from complementary sources, has long been recognized in the domain of micro-simulation, and a range of techniques have been developed for data merging (e.g. Merz 1986) to support micro-simulation. Increasingly, the relationship between theory and evidence and the issues of model validation and verification are seen as crucial questions for agent-based social simulation (Manson & O’Sullivan 2006). Social simulations typically require the use of multiple data resources that are heterogeneous in both scale and formats and subject to varying access constraints (while a simulation itself can also generate further data resources relevant to subsequent analysis). Moreover, it is increasingly recognized that the most important data have a rich, complex longitudinal character (Wolfson 2009) that is especially open to further permutations and enhancements. Tools supporting access to and further enhancement of heterogeneous social science data resources are a key component of the DAMES project and have been incorporated into the NeISS.

There are other e-Research components that are potentially of great value for social simulation, but whose potential has not yet been recognized widely. These components may be established in other fields of e-Research, but not yet deployed within social simulation, they may be still evolving as e-Research tools or they may be manifestations of practices that are undertaken within social simulation, but not yet translated into an e-infrastructure environment. Examples include secure, role-based access to simulations, the integration of service components into repeatable (plug-and-play) workflows and the provision of repositories for the archiving and sharing of social simulation models and components.

Finally, ensuring the widest possible take up of NeISS requires raising awareness of social simulation among academic research groups and public and private sector organizations; understanding the requirements of different types of users; building capacity and skills through training programmes; and providing services to facilitate public engagement in research and policy-making.

3. Social simulation services

The UK e-Social Science programme has supported development in three areas that are highly relevant to social simulation and can provide the elements of a much more comprehensive e-infrastructure. These are simulation modelling, data analysis and visualization. Here we present a brief review of progress in each area.

(a) Social science modelling and analysis

Methods developed in the MoSeS project can support the generation of synthetic populations, demographic forecasting and activity analysis. A *population reconstruction model* (PRM) is used to produce synthetic individual and household populations for small geographical areas. In the context of a specific city—Leeds—this means that 705 000 individuals are aggregated into 302 000 households, and each household is allocated to one of the 2400 census output areas. The individuals are synthesized from the UK Census Sample of Anonymized Records (SARs; <http://www.ccsr.ac.uk/sars/>) and therefore represent real people. The PRM uses UK census data for small areas to ensure that real variations are also represented at the local level, for example, heavy concentrations of young people, students and ethnic minorities in the central areas, whereas more affluent families are much more likely to be found in the northern suburbs and commuter villages.

The *population forecasting* process produces annualized ‘future’ versions of the household and individual database for a 30-year planning horizon, starting in 2001. These projections were generated using dynamic models of individual and household demographics to accommodate ageing, morbidity and mortality, as well as household formation and dissolution, new births and the migration of individuals and households between small areas in the city, as well as immigration and emigration elsewhere in the UK and the rest of the world (Wu *et al.* 2008; Birkin *et al.* 2009).

A dynamic micro-simulation model is used, which applies demographic transition rates to individual people and households. These transitions include ageing, migration, household formation and dissolution (leading to the creation and elimination of households), fertility, illness and mortality (leading to the creation and elimination of individuals). The dynamic transition rates are estimated in relation to longitudinal data drawn largely from the British Household Panel Survey (BHPS), but also using other sources including ONS ward-level Vital Statistics, International Passenger Survey and pupil census data (see Wu *et al.* 2008 for more details).

The advantages of this dynamic micro-simulation approach are well known, for example, allowing efficient representation of highly disaggregate large-scale populations and facilitating flexible aggregation to various levels of spatial and sectoral details (van Imhoff & Post 1998). The synthetic data generation approach also facilitates detailed modelling without incurring threats to privacy or the risks associated with the use of personal data.

An example application of population recreation with dynamic forecasting has been prepared in association with Leeds City Council Social Services. A ‘needs analysis’ for social care was conducted to identify high-risk groups. In many cases, for example, to identify multiple deprivation and co-dependency, synthetic reconstruction is required simply to compute current distributions. Estimates for the base year of 2006 and projections to 2016 and 2031 are shown in table 1. Some key policy questions here are whether existing utilization is a fair reflection of need or whether provision drives uptake and how future provision can be optimized or improved in relation to expected change, particularly in relation to an ageing and more ethnically diverse population.

Table 1. Demographic forecasts to support the delivery of social care.

primary care trust	day care		demographics				
	attendance	places	elderly	limiting long-term illness	co-dependents	ethnicity	deprived
2006							
Leeds NW	514	639	21 464	12 837	1931	1200	1506
Leeds NE	298	138	14 465	8720	1323	1136	1022
Leeds E	514	587	20 271	12 152	1843	942	1241
Leeds S	400	431	17 328	10 438	1475	596	1151
Leeds W	343	277	13 685	8096	1168	488	946
2016							
Leeds NW	?	?	23 297	12 234	1662	2146	1104
Leeds NE	?	?	15 457	8182	1199	1962	798
Leeds E	?	?	22 108	11 747	1611	1856	989
Leeds S	?	?	18 972	9980	1316	1167	792
Leeds W	?	?	14 020	7304	997	960	643
2031							
Leeds NW	?	?	29 061	16 015	2308	4719	1191
Leeds NE	?	?	19 662	10 766	1638	3789	913
Leeds E	?	?	26 628	14 709	2240	4518	1058
Leeds S	?	?	25 742	13 974	2048	3112	921
Leeds W	?	?	16 971	9202	1427	2414	700

Activity modelling: the implication of population change for service provision in cities is an important motivation for the MoSeS project. Such understanding requires that demographic projections be combined with models of service utilization and uptake. A powerful approach to this problem, with applications to services as diverse as education, healthcare, retailing, utilities and emergency (Birkin *et al.* 1996), is the application of spatial interaction models, which combine demand for services with the quality, quantity and accessibility of provision to generate modelled flows of products, patients, students and customers within a city region. Such flows can then be aggregated to provide indicators of equity and efficiency in relation to current or future service networks. An example of this technology was provided in an early e-Social Science demonstrator project—Hydra—which considered the optimal location of cancer screening services under alternative scenarios of patient demand and the economics of provision (Birkin *et al.* 2005). Further examples are introduced in §4 below.

(b) *Social simulation data*

An exciting opportunity afforded by more powerful computational infrastructural provision for simulation modelling is the enhanced capacity to conduct multiple analyses in response to plausible variations in the representation of the underlying data. Examples might include re-running simulations using different categorizations of measures of ethnicity or educational qualifications or using

different weighting factors for population subgroups. Across the social sciences, while it is recognized that changes to the data underlying an analysis may have significant consequences upon subsequent results, a lack of suitable tools to manage and analyse the large volumes of data has meant that, nevertheless, it has hitherto been relatively uncommon for researchers to try out numerous different data permutations or to systematically document the options available to them and the choices they made.

The skills and issues associated with (potential) variations in the underlying data are often referred to as those of ‘data management’. They can usually be described as concerning the possibility of recoding or restructuring variable measures or of enhancing data by linking them with other relevant resources. The DAMES project seeks to raise capacity in, and to raise standards in the documentation of, a number of data management tasks associated with quantitative datasets in social science research.

An example of the application of data management to social simulation would be in understanding the long-term impact of demographic changes upon the structure of social inequality. These are likely to be non-trivial because many other consequential social structural outcomes are strongly differentiated by age and birth cohort. For instance, owing to recent expansions in further and higher education, younger age cohorts in contemporary Britain have much higher average levels of educational qualifications, but it might be expected that the long-term benefits of those qualifications, as these cohorts age, may not be as strongly differentiating as has been the case in the past. Other simulation studies have addressed similar themes (e.g. O’Donoghue *et al.* 2009). An innovation of the NeISS project is that its infrastructural resources will (i) support numerous alternative measurement representations of key data on educational qualifications and related socio-economic outcomes and (ii) allow the development of the application in a dynamic spatial model that is sensitive to local level variations, which themselves are of consequence to the age and socio-economic distribution (e.g. Birkin *et al.* 2009).

(c) Social science visualization

We argued in §2 above that visualization is an essential component of a social simulation infrastructure. MapTube (<http://www.maptube.org>) was initially developed as part of the GeoVUE project to allow rapid sharing of thematic maps within an environment that allows simple visual analysis and data overlay. Data are converted via the GMAPCREATOR software suite that allows users to quickly and easily convert geographical boundary data (shapefiles) to a MapTube overlay. In essence, GMAPCREATOR creates a tile-based raster version of any vector dataset, thus allowing data, which may be subject to file size restrictions or indeed copyright issues, in the vector format to be shared online.¹

¹It could be argued that some information is lost in the process of vector to raster conversion. However, it is envisaged that the e-infrastructure will support the export of model data, so that users are equally able to represent the data through vector mapping software if they so desire. A fully functional e-infrastructure would support multiple representations of simulation outputs in both vector and raster formats, and the foundations for this will be laid through the deployment of a ‘Geographic Linkage Service’ elsewhere within the NeISS project.

Figure 1. Snow reports from January 2010: live Twitter feed to MapTube.

Created tiles are hosted on external servers with MapTube collating data via use of XML. MapTube acts as a content creation tool as well as a portal for thematic geographical information.

MapTube's custom tile renderer was developed to extend beyond the ability to convert shapefile file format. Indeed, it is possible to convert almost any format containing geographical information into a map on the system. This is ensured via the creation of geographical boundaries directly on the server so any data linked to boundaries such as postcode districts, census wards, output area and such can be mapped via a simple link to the raw data file. This allows near real-time data collection and visualization with the addition of any relevant geographical tag in the collection process. This aspect of MapTube has been used extensively by traditional media with surveys carried out by BBC Radio 4, BBC South, BBC North West and BBC East all powered by the MapTube system. We are extending this feature set via the NeISS project to create a Web-based service, allowing custom surveys to be set up and mapped in real time with output compatible with higher-end GIS systems.

Initially aimed at social scientists and policy-makers, these crowd-sourced data have notable potential. The system makes use of social networking systems, such as Twitter, to collect data. Currently, in beta testing, a demonstration map integrated with Twitter to display live weather information shaded by postcode has attracted over 20 000 responses a day. The Twitter feed is geo-located and linked to the outlines located on the MapTube server, allowing districts to be shaded according to the response. The map updates itself every 3 min, allowing for time tagged data collection and display. Figure 1 illustrates the demonstration map with Tweets overlaid with the shaded data.

Figure 2. Baseline performance indicators for transport analysis.

4. An example: congestion in Leeds in the year 2031

In this section, we describe an example of the application of the NeISS service components to a problem involving the development of the transport system in Leeds from the period 2001 to 2031.

(a) Population reconstruction and transport generation

We used the PRM described in §3*a* to generate a base population of the city of Leeds for the year 2001.

Transport demand was estimated from the combination of individual level data from the SARs with travel demand data from the BHPS (now enhanced to the UK Household Longitudinal Study; <http://www.iser.essex.ac.uk/survey/ukhls>). It includes many behavioural and activity variables, including, for example, political voting patterns, leisure activities and membership of sporting clubs, income and expenditure, as well as duplicating most census variables.

We have used a synthetic matching procedure in order to link individual records from the PRM to a similar record in the BHPS on the basis of five shared characteristics (age, ethnicity, gender, social class and economic activity). Although this procedure is well defined and robust, it is also arbitrary

and a number of questions merit substantial further exploration, concerning aggregation, variable and data selection. For example, should higher (or lower) levels of aggregation be applied to variables such as ethnicity? Which variables should be selected for matching, and could alternative statistical matching algorithms be deployed? Should an alternative source such as the National Travel Survey (Department of Transport 2009) be used? Furthermore, questions also arise in whether the procedure is free from biases between rural and urban areas owing to differences in accessibility and travel mode variations. By providing an infrastructure to support multiple analyses after the re-specification of data resources, the DAMES contribution to NeISS (as described in §3*b* above) seeks to address such questions. This could ultimately lead to a better understanding of aggregation effects and to give NeISS users some practical recommendations about levels of aggregation for different kinds of analyses. The representation of entities at individual and household levels also promotes the investigation of questions of spatial aggregation. For example, can we identify particular scales at which concepts such as ‘neighbourhood’ or ‘community’ become manifest, which forms part of an ongoing work package in the Genesis project (www.genesis.org).

(b) Trip behaviour

A simple social simulation model of urban travel behaviour is used to generate estimates of the volume of flows on the traffic network, which arises from our estimates of travel demand, as described in §4*a*. The model assumes a simplified transport network that has both public and private transport components. A coarse spatial zoning into 33 census wards was adopted and the distances between each pair of zones generated from a simplified set of routes between neighbouring wards. Trip destinations were estimated as a function of workplace locations as captured within the 2001 Census Special Workplace Statistics. For this purpose, we used a doubly constrained spatial interaction model that was calibrated in order to produce estimates of the average trip distance by both public and private means and a model split between trips equivalent to those derived from the 2001 census for the city of Leeds (Birkin *et al.* 2009).

(c) Model indicators and visualization

The outputs from the trip modelling process are based on three key performance indicators (KPIs): the level of congestion as measured by the average time spent in travel (to the workplace) by residents of each area; the level of pollution given as a linear function of the number of private and public trips in each ward normalized by the physical area of each zone; and the number of road accidents given as a linear function of the total trip distance in person kilometres by both public and private transport in each ward.

In order to visualize the outputs of the modelling process, we export data in CSV format files of the KPIs into the MapTube map generator, as described in §3*c* above. Three sets of outputs are shown in figure 2 with a Google Maps representation, which indicates a broadly concentric pattern of pollution with its focus in the centre of Leeds, and thumbnails of both average journey time and road accidents. Not surprisingly, the distribution of pollution, road accidents and accessibility all follow a strongly urban–rural pattern.

Note that although we have presented these outcomes as a simple and limited set of indicators (3 KPIs and 33 wards: 99 values in total), one of the beauties of the simulation modelling approach is that extensive disaggregation is a straightforward matter. For example, if we were to examine the trip patterns of eight different age groups with four ethnicities and four social groups in both public and private modes and to disaggregate spatially down from 33 census wards to 2400 output areas, then we would now have more than 600 000 values ($8 \times 4 \times 4 \times 2 \times 2400$) for each indicator, which is roughly equivalent to the population of Leeds. The opportunity and challenge of flexible aggregation to appropriate levels of detail are a well-known and important property of social micro-simulation modelling in this style (e.g. [van Imhoff & Post 1998](#)).

(d) Model scenarios

The real power of social simulation becomes evident when alternative scenarios and future projections are examined. In this work, we performed the following simulation experiments. First, we projected the population of Leeds over a 30-year period from 2001 to 2031.

Second, we ran ‘what if?’ simulations of trip behaviour assuming:

- no change in the underlying transport network;
- the introduction of a Supertram into Leeds between 2011 and 2014;
- adoption of a congestion charge in the central areas from 2009 onwards;
- and
- the introduction of uniform road pricing in all areas of the city from 2009 onwards.

Figure 3 shows the effect of the road pricing and congestion charging scenarios on the pattern of air pollution, which was seen earlier. Road pricing effects a general softening in the impact of air pollution by encouraging a city-wide redistribution from private to public transport, whereas congestion charging has big benefits for the central areas but some displacement of externalities to neighbouring zones.

A fuller set of scenario illustrations can be found at the MapTube website, at <http://maptube.org/map.aspx?mapid=773> up to <http://maptube.org/map.aspx?mapid=791>.

5. Discussion

In §4, we looked at an example of a social simulation model in the context of transport scenario analysis for the city of Leeds. The example combines building blocks from existing e-social science activities in data management, spatial modelling and visualization. At present, these components are loosely coupled to the extent that interactions are essentially flows of data between them. In this section, we consider the framework for the articulation of a more tightly coupled e-infrastructure that combines these elements, and we use this as the basis for a discussion of development priorities for the NeISS.

A generalized description of a social simulation scenario is provided in figure 4. The combination of constituent services into a tightly coupled infrastructure could provide the capability for repeated simulations across different local areas

Figure 3. Impact on air pollution of alternative transport scenarios: (a) congestion charge and (b) road price.

(i.e. repeat models for congestion charging in Leeds, Manchester, Nottingham, etc.), for revised scenario analysis across different time periods (e.g. impact of road charging in 2012, 2015, 2018 and so on) and even the execution of

Figure 4. Components of an e-infrastructure for social simulation.

different models at various levels of refinement (e.g. coarse-grained analysis of alternative road-pricing structures as the basis of selection of a candidate policy and fine-grained analysis of impacts across different occupations, age bands and ethnic groups for local neighbourhoods). Flexible data inputs could support various different substantive application domains: thus in moving from transport to healthcare simulations, one might substitute health-based constraints in the population reconstruction, merge lifestyle and morbidity variables in place of trip behaviour and apply interaction models to patient flows or general practitioner visits rather than journey-to-work trips, but the overall simulation architecture would be very similar.

For the transport application, the social simulation tools of figure 4 comprise a set of spatial interaction models. The development of a more extensive set of tools including analytics such as pattern detection is envisaged within NeISS, and in the longer term, the provision of standards to allow external simulation tools to be imported and integrated could greatly extend its capability. The integration of NeISS with the UK National Grid Service creates the possibility for the definition and execution of simulations across a wide-ranging parameter space or group of ‘what if?’ scenario options (for example, show me projections of my local area under assumptions of high/medium/low economic growth, free movement/restricted migration and so on), where such model variants might be executed under something like a parameter sweep of the type popular in e-Research applications in the physical sciences and realized in projects such as nanoCMOS (Walker *et al.* 2010).

With standardized licensing and security, it would be possible to access European data repositories and to integrate distributed datasets. This would allow the investigation of, for example, social research problems that require modelling of population movement across European boundaries. Given the computational intensity of these activities, it is likely that tackling such problems will call for access to international scale compute resources. We observe that

the European Grid Initiative (<http://web.eu-egi.eu/>) architecture of federated National Grid Initiatives maps well to a wide range of problems involving spatially based analysis, where the requirement for scalability can be satisfied by federating national-scale simulations.

Another promising application area for the NeISS lies in ‘near real-time’ forecasting in support of emergency planning and management. Emergency planning demands the prediction of the impact of foreseeable events on populations, physical and social infrastructure and the formulation of ways to deal with them. Emergency management requires access to up-to-date situational data and the means to revise predictions on a moment-by-moment basis. For example, planning for and managing the outbreak of an epidemic may require decisions about optimal locations for mass immunization facilities and the capacity to track and predict the probable patterns and rates of infection transmission. Effective emergency planning and management calls for multi-faceted models that can capture relevant features of population behaviour and physical infrastructure and can be adapted in the light of real-time data. Planners need to be able to explore different scenarios and use simulation predictions to devise optimal plans, test them under realistic conditions and train personnel to react. Managers need to be able to collect situational status information from diverse, distributed sources, to visualize data in meaningful ways and to update simulations so as to predict how an emergency will unfold.

The integration of Taverna functionality into the NeISS (<http://www.taverna.com>) is underway to allow the development of portlets with JSR 168/286 compliant components that provide access to enactment, management, monitoring and creation of workflows. At present, work is underway on the disaggregation of MapTube thematic visualizations in this framework, so that a single workflow can be used to generate a variety of representations of a single data field according to the selection of colours, shading styles, the number of intervals and boundary selection method. The higher level task of combining workflows in the generation of scenarios will be achieved in part by re-purposing of services from myExperiment (De Roure *et al.* 2009), a virtual research environment for the social curation and sharing of scientific research entities, especially workflows and *in silico* experiments, facilitating their integration into a portal. An important focus will be the incorporation of social networking functionality to provide extended archiving and documentation capability for social simulations, and early progress on this theme is illustrated in the Twitter application described in §3c. A persistent repository of social simulations is being designed around the notion of Research Objects, aggregations of resources (datasets, analysis methods, workflows, results and people) that tell a particular story about an investigation, experiment or process and capture key information about the life cycle of the investigation (for example, provenance information about analyses), facilitating re-use of results and repeatability of experiments.

For many users of the NeISS, access to social simulation resources could be mediated solely through repositories of simulation resources. This is the case for existing demonstrators that have been developed for policy users (Townend *et al.* 2009) and for level 2 undergraduate teaching of urban simulation at the University of Leeds. Our collaborators include city councils with an interest in the

provision of social services, housing, transportation and economic development, including simulation perspectives on proposed ‘eco-towns’, as well as the Royal Town Planning Institute with interests in planner education. We see considerable scope for public engagement through this process. For example, in relation to the transport demonstrator, social simulation could be used as a means to enable the public to understand the long-term implications of continuing existing travel patterns and to explore for themselves the effects of possible changes of behaviour. The fourth group of ‘research’ users in [figure 4](#) could typically be expected to have a much more wide-ranging interest in the development and deployment of social simulation services.

6. Summary and conclusions

In recent years, substantial intellectual progress in the domain of social simulation has been complemented by the deployment of social science models, data management and visualization through Web portals. The work of the NeISS project to incorporate and extend these components within an e-infrastructure for social simulation will make them easy to access, use and share for diverse strategic applications including health and social services, transport, land-use and economic development and potentially for real-time issues such as emergency planning and disaster management. Development priorities include the combination of services into workflows, the creation of persistent repositories and the deployment of social simulation tools through secure portals. Applications are expected to benefit a heterogeneous user community of researchers, policy-makers and citizens.

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References

- Arthur, W. 1999 Complexity and the economy. *Science* **284**, 107–109. (doi:10.1126/science.284.5411.107)
- Bell, G., Hey, T. & Szalay, A. 2009 Beyond the data deluge. *Science* **323**, 1297–1298. (doi:10.1126/science.1170411)
- Birkin, M., Clarke, G., Clarke, M. & Wilson, A. G. 1996 *Intelligent GIS: location decisions and strategic planning*. Cambridge, UK: Geoinformation International.
- Birkin, M., Dew, P., Macfarland, O. & Hodrien, J. 2005 Hydra: a prototype grid-enabled spatial decision support system. In *Proc. 1st Int. Conf. on e-Social Science, Manchester, UK, 23 June 2005*. Available at http://www.ncess.ac.uk/events/conference/2005/papers/papers/ncess2005_paper_Birkin.pdf.
- Birkin, M., Wu, B. & Rees, P. 2009 MoSeS: dynamic spatial microsimulation with demographic interactions. In *New frontiers in microsimulation modelling* (eds A. Zaidi, A. Harding & P. Williamson), pp. 53–77. Farnham, UK: Ashgate.
- Brodlie, K., Wood, J., Duce, D. & Sagar, M. 2004 gViz: visualization and computational steering on the grid. In *Proc. UK e-Science All Hands Meeting, September 2004*, pp. 54–60.
- Department of Transport. 2009 *National travel survey, 2002–2006*, 3rd edn. Colchester, UK: UK Data Archive.

- De Roure, D., Goble, C. & Stevens, R. 2009 The design and realisation of the myExperiment virtual research environment for social sharing of workflows. *Future Gen. Comp. Syst.* **25**, 561–567. (doi:10.1016/j.future.2008.06.010)
- Epstein, J. M. 2007 *Generative social science: studies in agent-based computational modelling*. Princeton, NJ: Princeton University Press.
- Ferguson, N. 2005 Making the paper: what would happen if a flu pandemic arose in Asia. See <http://www.nature.com/nature/journal/v437/n7056/full/7056xia.html>.
- Ferguson, N. M., Cummings, A. T., Cauchemez, S., Fraser, C., Riley, S., Meeyai, A., Iamsirithaworn, S. & Burke, D. S. 2005 Strategies for containing an emerging influenza pandemic in Southeast Asia. *Nature* **437**, 209–214. (doi:10.1038/nature04017)
- George, F., Radcliffe, N., Smith, M., Birkin, M. & Clarke, M. 1997 Algorithms for solving a spatial optimisation problem on a parallel computer. *Concur. Pract. Exp.* **9**, 753–780. (doi:10.1002/(SICI)1096-9128(199708)9:8<753::AID-CPE246>3.0.CO;2-Q)
- Halfpenny, P., Procter, R., Lin, Y. & Voss, A. 2009 Developing the UK e-social science research programme. In *e-Research: transformation in scholarly practice* (ed. N. Jankowski). London, UK: Routledge.
- Lee, D. 1973 Requiem for large scale models. *J. Am. Plan. Assoc.* **39**, 163–178. (doi:10.1080/01944367308977851)
- Manson, S. & O'Sullivan, D. 2006 Complexity theory in the study of space and place. *Environ. Plan. A* **38**, 677–692. (doi:10.1068/a37100)
- McEachren, A., Cai, G., Sharma, R., Rauschert, I., Brewer, I., Bolelli, L., Shaparenko, B., Fuhrmann, S. & Wang, H. 2005 Enabling collaborative geoinformation access and decision-making. *Int. J. Geogr. Inf. Sci.* **19**, 293–317. (doi:10.1080/13658810412331280158)
- Merz, J. 1986 Structural adjustment in static and dynamic microsimulation models. In *Microanalytic simulation models to support social and financial policy* (eds G. Orcutt, J. Merz & H. Quinke), pp. 423–446. Amsterdam, The Netherlands: North-Holland.
- O'Donoghue, C., Leach, R. H. & Hynes, S. 2009 Simulating earnings in dynamic microsimulation models. In *New frontiers in microsimulation modelling* (eds A. Zaidi, A. Harding & P. Williamson). Farnham, UK: Ashgate.
- Sayer, R. A. 1979 Understanding urban models versus understanding cities. *Environ. Plan. A* **11**, 853–862. (doi:10.1068/a110853)
- Townend, P., Xu, J., Birkin, M., Turner, A. & Wu, B. 2009 MoSeS: Modelling and Simulation for e-Social Science. *Phil. Trans. R. Soc. A* **367**, 2781–2792. (doi:10.1098/rsta.2009.0041)
- Van Imhoff, E. & Post, W. 1998 Microsimulation methods for population projection. *Popul. Engl. Select.* **10**, 97–138.
- Walker, J. A., Sinnott, R., Stewart, G., Hilder, J. A. & Tyrrell, A. M. 2010 Optimizing electronic standard cell libraries for variability tolerance through the nano-CMOS grid. *Phil. Trans. R. Soc. A* **368**, 3967–3981. (doi:10.1098/rsta.2010.0150)
- Wolfson, M. 2009 Orcutt's vision 50 years on. In *New frontiers in microsimulation modelling* (eds A. Zaidi, A. Harding & P. Williamson), pp. 21–30. Farnham, UK: Ashgate.
- Wu, B., Birkin, M. & Rees, P. 2008 A spatial microsimulation model with student agents. *Comp. Environ. Urban Syst.* **32**, 440–453. (doi:10.1016/j.compenvurbsys.2008.09.013)