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The pilot Environmental Virtual Observatory, EVOp, a proof of concept project to develop new cloud-based applications for accessing, interrogating, modelling and visualising environmental data, by developing a series of exemplars, EVOp has demonstrated how cloud technologies can make environmental monitoring and decision making more efficient, effective and transparent to the whole community.
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Final Report
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The Annex to this document can be found online at http://www.evo-uk.org
Executive summary

The EVO Pilot (EVOp) was an ambitious two year project to test the value of new cloud technologies for connecting and integrating fragmented data, models, and tools to deliver new holistic approaches to environmental challenges. The need for such an approach has become increasingly clear as we seek to improve food, water and energy security. These all require a new way of working which spans disciplines and organisations, and that breaks down science-culture boundaries. If successful, the project would demonstrate the vision and opportunities for further funding, attract academic, policy, industry, and global partners, and create a step-change in the way that NERC science is delivered and exploited.

The final deliverables were -

- A tested web service using local, national and global exemplars
- Future funding
- An informed and engaged community

This was achieved through establishing a project team which had a mix of computer specialists, environmental scientists (from across 13 organisations) and an end-user stakeholder group covering a range of organisations. The work was organised into a series of packages which cooperated closely to deliver the overall vision. The packages covered; leadership and management; cyber infrastructure; modelling; and tested exemplars.

The exemplars were chosen to engage with end-users and explore barriers and opportunities at three spatial scales; local, national and global, focused on such topics as flooding, diffuse pollution and uncertainty in climate change projections. Thus the project combined a 'narrow and deep' testing using these exemplars with more 'broad and shallow' explorations of issues such as vocabularies and semantics, data security and legal issues. Many briefings and presentations of the project were given via meetings and workshops throughout the lifetime of the project to potential end-users ranging from Defra and public agencies, to the water industry, academic audiences, and industry bodies such as the Information Assurance Advisory Council. A major conference was organised in Oct 2012 to showcase opportunities for national and international initiatives working in this area at the Royal Geographical Society. The project’s Stakeholder Group provided guidance and support throughout the project, ensuring that this was not another IT 'white elephant' but of real value to organisations that are challenged daily with tackling complex environmental problems.

All the deliverables have been achieved with a community of postdocs, academics and end-users who are all now familiar and excited about the opportunities of the approach. New funding is in place from a variety of sources including the Government's Big Data Initiative, the international Belmont Forum and the NERC-TSB joint Environmental Data call, all of which have acknowledged the role of the EVOp in securing the funding. A final report including experiences of barriers and opportunities encountered during the lifetime of the project is available on the EVOp website (www.evo-uk.org) providing a legacy to be exploited by the whole community as they explore the potential of application of these new cloud technologies for environmental science.

The opportunities are many, and other initiatives that are already in progress include: real-time integrated monitoring of the environment to produce real-time alerts; modellers ‘cloudifying’ their models and creating user-friendly web interfaces for increased accessibility and testing; work to establish international standards and vocabularies; software developments to enhance inter-operability, and much, much more.
1 Overview of the EVOOp Project

There is an emerging and urgent need for new approaches to environmental challenges in the broad context of sustainability. Scientists, businesses and policymakers are asking questions that are far more interdisciplinary than in the past. Unfortunately, an unexpected outcome of the explosion of data and associated information is the growing disconnect between and within the supply of scientific knowledge, and the demand for that knowledge from the private and government sectors. NERC commissioned the Environmental Virtual Observatory pilot project to explore the question:

"Is there a way of providing the 'wiring' to help people access the resources they need, be they a scientist, policy maker, industrial body, regulator or member of the public?"

1.1 The hypothesis

The hypothesis to be explored was that novel cloud computing technologies could be exploited to increase accessibility in a data-intensive world to "filter" and integrate this information to manageable levels as well as provide visualization and presentation services to make it easier to gain creative insights and build collaborations. This has been called the 4th paradigm (Gray, 2007; Hey et al, 2009). The ultimate aim was to make NERC science more efficient, effective and transparent. The transparency issue has been highlighted in a recent Royal Society report as requiring urgent attention to increase public confidence in the process of translation of scientific evidence through to policy making (The Royal Society, 2012).

1.2 Beyond data

A second hypothesis was to test if there is value going 'beyond data' to include models which are effectively a synthesis of current understanding and one of the main tools NERC scientists use to integrate complex data, upscale and make projections under future scenarios. Within the terrestrial and freshwater communities many models address environmental questions concerning soil and water quality, flood and drought risk, and ecosystem structure and function (e.g. Defra recently identified ca. 60 models currently used in diffuse pollution modelling alone). These models simulate complex physical, chemical and biological process interactions. There is a challenge however in gaining access to these models, linking them together to deliver more holistic outputs and objectively testing to the level needed by end-users who need to make policy or management decisions based on their outputs. This leads to the second question to be tested:

"How can we create a culture of more open and rigorous testing and evaluation of the current models necessary to improve process understanding, process representation in models and thus model forecast accuracy?"

Two main challenges currently limit this ongoing model development; the spatial/temporal limitations of our observational capacity and the lack of integration of data, models and visualisation tools across the air-land-water domains. However, recent advances in technical methods allow for detection of real-time changes in biogeochemical, hydrological and ecological functioning (e.g. molecular markers, isotopic and spectroscopic approaches, land and space-based observational techniques). Given a platform where these observations could be explored, accessed and integrated with models across domains, a fast and more informed analysis of system change would emerge, leading to tools which identify options for immediate, targeted and thus more cost-effective management interventions.

The EVOp project therefore needed to develop a platform for both data and models to answer these two questions. The approach taken was to represent data and models as services in a secure cyber-infrastructure. In the long term there would be a need to ensure it possessed a robust architecture, standards, and global access linking private and public clouds, GRID and HPC environments where appropriate. Such a platform would directly address the two challenges, leading to improved exploitation of NERC data and models, and a more integrated response to urgent environmental challenges. The alignment of science supply and demand in the context of continuing scientific uncertainty will depend on seeking out new relationships, overcoming language and cultural barriers to enable collaboration, and merging models and data to evaluate scenarios.

The £2 million pilot Environment Virtual Observatory pilot (EVOOp) project was commissioned by NERC in January 2011 to test these two hypotheses and identify opportunities and challenges that might lead to a potentially far greater investment by NERC in partnership with stakeholders into the future.

1.3 Building the EVOOp team

NERC recognized the project required a community-led cyber-infrastructure development and new
approaches to scientific workflows that describe, compose, model and execute ensembles of data, models, tools and visualisations on distributed resources with global access. The EVOp team therefore required a mix of IT and computer specialists, a test research community of scientists and a potential future end-user community drawn from government, regulators and industry. A sandpit was organized which brought together a community from which a single large project consortium representing 12 institutions emerged incorporating a mix of IT specialists and soil-water scientists (see online Annex), later this would be supplemented by additional involvement from individuals from other organisations Soil-water science was proposed by NERC as an ideal community to test this approach as it is experienced in cross-disciplinary working, has a good range of well-tested models and is well-linked to a range of end-users tackling significant environmental challenges such as flooding, diffuse pollution and climate change. The consortium elected a leadership team to represent the different communities needed to deliver the pilot project spanning IT specialism (Robert Gurney), basic research (Bridget Emmett) and industry needs (Adrian McDonald). A Project Advisory Group was established covering a wide range of potential end-users including representatives from government, industry, regulators, policy makers and funders (see online Annex).

1.4 Project Structure

A major objective of the consortium from the beginning was to ensure that the work programme was science and end-user led underpinned by a robust exploration of the available IT technologies. Five principal areas of activity were identified, some requiring narrow and deep testing of the approach across different operational scales (i.e. data and model application from local to global scale) whilst other areas needed a broad and shallow exploration across a range of challenges (i.e. IPR and data security). The five areas were:

i. legal and security issues associated with security of data handling and consumption ensuring the EVO can scale rapidly without compromising the integrity of data;
ii. data licensing, platform hosting and licensing, and use of the platform taking into account the range of data initiatives including data.gov.uk;
iii. options for cloud infrastructure with security-by-design inbuilt;
iv. development of standards and inter-operability;
v. case studies focused on soil-water process understanding and management at three scales (local, national and global).

Six work packages were developed involving overlapping teams to cover these areas of activity:

i. WP1 Leadership and management (covering legal, security, outreach issues, future funding and responsibility for commissioning and delivery of the global exemplar in Year 2);
ii. WP2 Cloud infrastructure (data licensing, platform hosting, cloud infrastructure, inter-operability, standards);
iii. WP3 Modelling in the cloud;
iv. WP4 Local Exemplar;
v. WP5 National Exemplar (hydrological and biogeochemical exemplars);
vi. WP6 International engagement.

1.5 Deliverables

The high level deliverables reinforced the pilot status and the expectations placed on the project. They were selected to facilitate advances in understanding about the issues and feasibility of delivering such a service to the community. The development process was therefore experimental and although some useful and interesting science emerged and technology solutions generated, the resulting service was not envisaged to become operational as an outcome of the pilot project. In recognition of this status, emphasis was placed on identifying future ways to progress the EVO concept. Furthermore, throughout the project, the team endeavoured to raise awareness about the EVO beyond those communities already familiar with the potential capability provided by IT. The deliverables were:

i. A tested web service providing web based environmental models and data across a limited number of exemplars at a variety of scales. The nominal scales used are referred to as local (catchments in the range 10 to 200 km²), national with some sub-national division and global.

ii. An identification and analysis of barriers and opportunities revealed in the development of deliverable (i). The barriers considered range from technical feasibility, ownership, governance and financial through to the to the legal and liability issues. Opportunities range from improved science (both in new questions and new solutions) because of the better data and modelling synthesis and the resulting communication through improved public awareness to financial opportunities and market leadership.

iii. A skilled and engaged community is, in part, a direct outcome of deliverable (ii). In a pilot project, engagement is more easily achieved than the ‘skilling’ up of many groups of stakeholders because the product is not created until a considerable way through a project. The skills development is therefore not seen as a technical training skill but as a higher-level conceptual and vision framework - the skill to recognise the opportunity and potential and to contribute to the
moulding of the future information framework. Within the team, translation across the science/IT interface inevitably resulted in improved skill sets.

iv. Funding and partners in place. The final deliverable is the positioning of the EVOp for further development. To strengthen partnerships through membership of important cross-disciplinary alliances such as LWEC, contributions and organisation of national and international conferences and the partnership with industry and across research agendas.

1.6 End-user engagement and the use of storyboards

A major innovation of the project as a whole was to use storyboards to ensure the exemplars were grounded in real questions/challenges by end-users. Potential end-users were considered to cross a wide range of communities from governments to public, and industry to regulators. Initial scoping of likely questions from a range of stakeholders are indicated in Figure 1.1, a full list is provided in the online Annex.; these were developed with, and approved by, our Project Advisory Group. Single specific questions and storyboards were then developed for the local, national and global exemplars. These are summarised in Figure 1.2, with the fully annotated storyboards provided in the online Annex. A requirement of these storyboards and exemplars was to test particular aspects of the data IPR, model operability in the cloud and critically different elements of the cyber infrastructure as indicated in Figure 1.3.

Figure 1.1 Exemplar questions provided by a range of EVO stakeholders.
### Figure 1.2 Mapping of exemplars to users and issues.

<table>
<thead>
<tr>
<th>End product</th>
<th>Local hydrology</th>
<th>National hydrology</th>
<th>National biogeochemistry</th>
<th>Global</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local catchment flow and water data and user-friendly interface for modelling tools to forecast flood risk</td>
<td>Selection tool for modelling water resource; Alert tool for industry as to when weather conditions may threaten energy production due to drought</td>
<td>Modelling tool to quantify nutrient fluxes for a range of catchments and marine water bodies at different scales</td>
<td>GCM analogue tool linked to impact assessment model to quantify global regions where uncertainty in change of soil C are greatest</td>
<td></td>
</tr>
</tbody>
</table>

| User | Farmers and local stakeholders; insurers | Power companies primarily, but other alerted stakeholders associated with abstractions | Government departments and agencies | NERC scientists; DECC |
| Issue | Flood risk | Drought | Water Framework Directive compliance and OSPAR reporting | Uncertainty in GCMs and soil C |
| Unique data needs OS / NERC / EA / Met | Live and historical flow data; Local webcams | Live EA data; Access to forecast products | Global databases and driving variables |
| Science demonstrated | Linking sensors, data and visual data together; Land management decision support tool; Preparedness assessment tool | Multiple model application for hydrology; Uncertainty; Model selection tool; An ensemble of coupled predictive capability | Multiple model application for biogeochemistry; Uncertainty; Regional modelling framework; Model selection tool; Data rich to data poor catchment | Sensitivity to climate change impact models to uncertainty between different GCMs and speed in assessing different emission ‘storylines’ |
| EVO ‘added value’ | Access to data and models; Integration of functionality | National security; Alerts for end-users; Old and new data view and model forecasts for multiple sites; An exemplar for a real time security management issue for important national infrastructure for multiple pressures | Online scenario testing; Ensemble macronutrient modelling; Scaling and multiple metrics | Access to climate change impacts assessment tool with increased capacity and faster working |
| Future potential | Adaptive modelling’ for local conditions; Ask an expert blog; Preparedness tool | Approach shows data/model cloud resources for identifying forecast alerts for any environmental threshold | Reverse engineering’ tools to find solutions; Dynamic coupling with hydrological modelling | Linking to other land-atmosphere models; Addition of valuation tool |

### Figure 1.3 Date security.

<table>
<thead>
<tr>
<th>Framework properties</th>
<th>Local hydrology (Eden)</th>
<th>National hydrology</th>
<th>National biogeochemistry</th>
<th>Global</th>
</tr>
</thead>
<tbody>
<tr>
<td>Essential infrastructure properties</td>
<td>Everything as a service</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>Sharing of everything</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>Openness and interoperability</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>Transparency</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>Ease of use by different communities</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<tr>
<td>The cloud as a utility</td>
<td>Alternative business models</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>Elasticity</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<td></td>
<td>The managed cloud</td>
<td>O</td>
<td>O</td>
<td>O</td>
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<tr>
<td>Enhanced management</td>
<td>Tailored management models</td>
<td>O</td>
<td></td>
<td></td>
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<tr>
<td>Web 2.0 techniques</td>
<td>Multi-cloud management</td>
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<td></td>
<td>Supporting mashups</td>
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<td>Supporting workflows</td>
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<tr>
<td></td>
<td>Service discovery</td>
<td>O</td>
<td></td>
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<tr>
<td>Systems of systems</td>
<td>Enhanced discovery</td>
<td></td>
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<td></td>
<td>Combining with ubiquitous computing</td>
<td>O</td>
<td></td>
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<tr>
<td></td>
<td>Combining with mobility</td>
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</tbody>
</table>

O = major effort, o = some effort, • = left for full EVO
O = completed, O = required
1.7 Data security
Concerns over data security were identified as a critical issue for many potential providers. Within the EVOp project a scoping exercise was undertaken through a workshop approach led by the data security industry. A report was delivered to the EVOp leadership team to help inform NERC of future needs, should a fully operational EVO be commissioned. The EVOp Cyber Security Advisory Board proposed six key areas that would require further consideration should the EVO concept be commercialised. Details are contained in the report provided in the online Annex, and can be summarized as:

i. Striking the right balance (confidentiality, integrity and availability): A clear understanding of the core principles and their corresponding priorities is important in the ‘Security by Design’ approach. Additional core principles that should be considered include non-repudiation, authentication and privacy. It is also clear that the importance of each core principal will vary based on security standards, classifications and the target audiences for each model, tool and data set.

ii. Cloud Security: Considerations associated with cloud security fall into two areas. These are related to cloud providers and customers (i.e. the EVO). In the continuously evolving domain of cloud security, the Cyber Security Advisory Board will provide important guidance to ensure the right cloud providers are chosen and all cloud security issues are considered.

iii. Data Protection Methods (encryption and other): Perimeter or layer protection methods (i.e. firewalls and IDS/IPS) are common focal points in the protection of data. Whilst these methods serve their place, an additional consideration for the EVO is security of the systems that will store and process the most sensitive data. Implementation of appropriate encryption methods may be a suitable method for ensuring that data is protected within the data centre(s), not just at the perimeter. Understanding the ideal encryption methods and how and when to implement them is vital in maintaining the high performance of EVO virtual modelling and the transmission of live data (such as river levels, real-time temperatures, etc.).

iv. Application Security: Whenever an EVO application interacts with suppliers and customers (end users), both the data and the application itself must be protected. As the EVO is expected to allow end-users to create data workflows to modify how data is analysed, it will be important to keep an audit trail of user activities and alert on behaviour which falls outside the norm. Just as important is the need to have an audit trail for all activities undertaken on any database which stores critical EVO information.

v. EVOp Portal Security: The EVOp portal will aggregate content from all of the EVOp systems providing a means for users to explore a variety of data sources and execute simulations and models in the cloud. It is vital that portal security ensures that only an authorised user can generate requests to the applications server(s).

vi. EVOp Security Resource Considerations: A core team will need to be assigned with responsibility for developing a Security Policy Framework and driving cyber security as a business as usual function.

While the six key areas cover the key cyber security considerations such as legal implications and the interaction between these topics; alignment to current security standards and their robustness within a rapidly evolving sector, the legal implications on security, and domain specific; security considerations are also in need of further investigation.

1.8 Legal Issues
A preliminary report on legal issues was prepared by The London Institute of Space Policy and Law (ISPL) and Edwards Wildman as an output of an EVOp-convened workshop. The white paper is split into three parts:

i. Data Collection and Licensing Issues: There will be a number of issues to consider in respect of the collection of the underlying data to be populated in the EVO platform. These include issues arising out of the use of third party intellectual property rights or underlying data that is otherwise in the public domain.

ii. The EVOp Platform: There will be a number of issues associated with the hosting of the EVO platform itself and of the development of new tools and applications. This includes issues arising out of the use of cloud computing technology.

iii. The use of the EVOp Platform and Licensing Issues: There will be a number of issues associated with the use of the EVOp platform, including the onward licensing of the output data and the EVOp platform's potential liability for any reliance placed on such output data.

The legal implications for development of the EVO were considered in parallel to the cyber security considerations. The interdependency of these two areas was acknowledged and further consideration on how to remain joined-up would be required if EVO were to become operational.

1.9 Outreach and community building
One of the deliverables of the EVOp project was to help develop an engaged and educated community. Members of the team were enthusiastic in this endeavour and participated in a wide range of activities including briefings, workshops, summer schools and conferences.

1.9.1 Briefings and conferences
Members of the team were active in promoting the EVOp vision and key outputs within different forums. A summary of interaction with key stakeholders and
events where EVOp featured are provided in the online Annex.

1.9.2 Training
Training was achieved in several ways throughout the course of the project:

i. Seminar on cloud computing: Representatives from WP2 organised a seminar for EVOp team members and staff at Lancaster University during the early stages of the project to provide a foundation level of knowledge and consequently, a baseline for communication.

ii. Involvement of early career scientists: Fourteen Post Doctoral Research Assistants and Research Assistants were employed across science and technology work packages.

iii. Summer School: The leadership team initiated a summer school at Istituto Veneto in Venice sponsored by NERC. The focus of the 2011 summer school was closely aligned to the EVOp and the six EVOp PDRAs that attended received an overview of cloud computing and the type of models that have been used already in environmental sciences in cloud services. Students with no previous advanced computing experience were able to design a working web service in three days, or carry out new work in data assimilation. These activities demonstrate the EVOp, or an allied concept, could be rolled out to the science community, and also the operational community, without a very high training barrier. In particular, the summer school illustrated that it would be possible to develop a training course, possibly on-line or through webinars, to deliver the necessary training quickly and without considerable expense for scientists to appreciate the potential of the approach. It must be noted however that professional trained computer scientists are essential to design and implement the actual cyberinfrastructure. Indeed, one of the main issues during the EVOp project was the over-reliance by scientists on too few computer specialists. Any future related activities would need to correct this and provide a more balanced distribution of skills within the team.

1.9.3 Project Advisory Group
The project benefited from the input from an Advisory Group which met on four occasions (approximately every six months). Membership of the Project Advisory Group was diverse and incorporated representatives from the water and IT industry, regulatory bodies, government, and academia (see online Annex); they were extremely supportive of the potential and need for an EVOp approach to gain greater efficiency, effectiveness and transparency of NERC science.

1.9.4 Alignment with other UK national initiatives
Awareness of aligned initiatives was essential in identifying how a future fully operational EVO could co-deliver more efficient, accessible and transparent data and models. We identified the following aligned initiatives and held various briefing/meetings with key participants including NERC Theme Leaders and Principal Investigators:

- Data: NERC has invested National Capability funding in an array of Data Centres which ensure secure long-term storage and access to data resources. Any future EVO platform would need to work together with the Data Centres and develop a clear interface to these as well as other initiatives such as data.gov.uk, the UK locator programme and those ongoing in the Met Office and Ordnance Survey. This would increase uptake of current investment and enhance ongoing work on international standards and data access. Testing of links to some Data Centres were explored within the Pilot and links and discussions with other data providers will inevitably be ongoing in future EVO-related initiatives.

- Science: A range of research investments are in place which cross the air, land, water, geological and climate communities providing resources and researchers actively pursuing the integration of NERC science. Of particular relevance to the EVO activities are the Programmes which seek to bring together the biogeochemical-hydrological and ecological communities (e.g. Macronutrients, BESS, Changing Water Cycles and Network of Sensors). These programmes all seek to improve the science which underpins the sustainable exploitation of our natural capital therefore providing a wealth of resources to underpin future EVO activities.

- Modelling: NERC’s Integrated Environmental Modelling Initiative which emerged from NERC’s proposed Modelling Strategy seeks to identify benefits of improved model integration and data exchange tools. Running concurrently to EVOp, a web portal, or ‘Experimental Zone’ was initiated under the NERC PURE programme to facilitate the sharing and fusion of models and data from a variety of different sources information to practitioners in environmental risk management.

- Tools: The Environmental Science to Services Partnership (ESSP) is a joint initiative by NERC, the Ordnance Survey and the Met Office to develop new products from current data and knowledge to improve uptake and impact of environmental science. Thus there is input by Defra, the EA and NERC capabilities through CEH and BGS.

1.9.5 Alignment with other international initiatives
In addition to the array of data, standards and climate initiatives ongoing in the European and global arena the following have made specific links to the EVOp team and indicated their interest in joint future collaborations:

- NSF EarthCube: Developing a framework to create and manage knowledge in geosciences to understand and predict the Earth system. There are opportunities to move forward in the short-term with joint legal workshops where EarthCube can
learn from our current knowledge and in turn, NSF can fund future joint workshops together with joint SAVI grants.

- **NSF Neon**: A continental-scale research platform for understanding and forecasting the impacts of climate change, land use change and invasive species, on ecological processes and on interactions of the biosphere with the geosphere, hydrosphere and atmosphere. NEON will collect data from 106 sites, over the next 30 years, from an investment of $434M.

- **Knowledge Systems for Sustainable Landscape Management Initiative**: An initiative to develop more sustainable integrated land management solutions building upon existing data collections and analysis tools, with investments for the development and deployment of new tools. Partners include USAID, Oak Ridge National Lab, NASA, CGIAR, World Bank, NASA, CSIRO.

- **Belmont Forum**: High level group of the world’s major and emerging funders of global environmental change research and international science councils. NERC International team facilitated participation in activities to define future research agenda.

### 1.9.6 EVOp International Conference

A national conference to explore how new information technologies, in particular cloud computing, could be used in the environmental sector was organised by the EVOp with support from five learned societies (British Ecological Society; British Hydrological Society; Royal Geographical Society; Royal Meteorological Society; and The British Society of Soil Science). The conference, “Harnessing Emerging IT Technology for Environmental Science - A 2020 Vision” was held at the Royal Geographical Society in London on 16 May 2012. The event brought together a diverse range of topics in the form of presentations, interactive demonstrations and posters (see online Annex).

From an early stage in the project, the need for an EVO-led event to provide a dedicated platform where the ambitions and outputs of the pilot could be showcased was apparent. Whilst the team would be active in communicating different aspects of the project within the various academic forums relevant to their expertise, there would be no single academic conference that could adequately represent all areas of interest. It was envisaged that an EVO-led event would be an opportunity where the future horizon for environment science, as influenced by technology, could be explored in addition to raising awareness about the EVOp project.

Although unique at that time in its ambition to combine data, models and tools into a single platform, the EVOp has drawn upon knowledge and links with other international science and technology programmes and initiatives active in generating new standards and new ways of working. Through the conference, the pilot EVO played a role in promoting the need for groups from disparate disciplines to come together and address the following questions:

- How can advances in IT help to solve or ameliorate major environmental issues?
- What are the practical barriers hindering and the opportunities to encourage integration between IT, research and user communities?
- What approaches, individuals and institutions appear to constitute the cutting edge of this IT - environment integration?

Over 160 people attended the event which included 36 posters/demonstrations on relevant topics and sixteen presentations. Each session offered a different perspective, aimed to inform and provoke discussion on the potential links between the environmental science and IT communities both in the UK and elsewhere. Lord Selborne provided the keynote address in which he outlined government policy and the programme landscape. Other speakers included representatives from the EU and UK government, IT industry, academic and research sectors: ARUP Australia, British Ecological Society, CEH, Defra, Dtex, European Commission, Geoscience, Google, Manchester University, Met Office, Microsoft, University of Cambridge, University of Colorado, and Willis Group Holdings.

The full conference programme is available within the online Annex. Recordings have been prepared by the Environmental Sustainability Knowledge Transfer Network and can be viewed on the ESKTN TV YouTube channel. Website, EVO portals and publications

### 1.9.7 EVOp website

A website - www.evo-uk.org - was established early on to advertise the activities and ambitions of the project and to bring in national and international partners. Initial work to scope out a potential landing page and the navigation routes end-users may select was undertaken by the team with design direction provide by website consultants INTRO. A key issue identified was the different ways in which end-users liked to access resources. An attempt to accommodate these different preferences is reflected in a landing page which has options to explore the EVO resources by location, topic and data. For the more experienced user, there is also provision of direct access to models, tools, apps and the workflow library (Figure 1.4).

The current design provides an adequate mechanism for demonstrating the pilot web service to EVO end-users; it was however noted that further work would be needed to develop different portals for different communities should the EVO ever be operationalised. A recommendation from the EVO pilot is that any future related initiative should focus more resources on this aspect and include a separate activity for planning and end-user testing of the portal interface.
1.10 The EVOp legacy

As one of the key aims of the project was to provide information to the wider community on opportunities and barriers in the EVOp approach, a series of legacy publications are provided within the online Annex. Videos of the local, national and global teams talking through the exemplars are also available on the EVOp website along with two-page flyers covering each of the work packages. An international publication summarising the overall project is also available (International Innovation paper - online link). This publication is an open access publication designed to communicate worldwide environmental research and development. The publication is distributed to over 30,000 stakeholder readers at all levels in the government, policy, research and related health stakeholder sectors and communicates the impact and relevance of both fundamental and applied research in the field.

Finally, EVOp has played a role in raising awareness and contributed to establishing an engaged and educated community that are becoming increasingly more open and ready to exploit the advantages new technology holds and benefit from future initiatives. Thus, perhaps one of the most important legacies of the project are the funding opportunities which have emerged from NERC and others.

1.11 Funding landscape and partners

1.11.1 NERC

By early 2012, it became evident that to make the EVO operational would require mixed funding to underpin the complex range of activities spanning: capital, research and private sector investment along with international and stakeholder collaboration. NERC have opted to continue a range of activities under the Environment Information Initiative.

- Environmental Big Data Investments: JASMIN, CEMS, Environmental Research Workbench, Environmental Big Data Capital Call.
- Innovation Activities: NERC Environmental Data: short projects to consider applications, products and services as a precursor to the joint NERC/TSB call, Solving Business Problems with Environmental Data”.
- Belmont Forum: e-Infrastructure Knowledge Hub programme).

Several of these initiatives have adopted approaches that utilise and build upon knowledge acquired during the EVOp explicitly and thus the legacy and value of NERC’s early investment was well founded.

1.11.2 Agencies, government and industry

A forum was convened by NERC to discuss the needs and opportunities for demonstrating tangible economic
Consider the needs of end users and maintain this but in summary:

These are outlined in various parts of this final report but in summary:

- A call for by the EA for requiring cloud-based data, exploration and visualisation approaches for delivering the Water Framework Directive.

- Commissioning of an integrated data and modeling platform for diffuse pollution management and ecosystem services by Defra, the EA, NERC and Scottish Government from a consortium led by CEH, one of the EVOp leadership team.

1.12 Lessons learned, and opportunities and barriers identified

These are outlined in various parts of this final report but in summary:

- Consider the needs of end users and maintain this focus throughout development. Perhaps the most successful part of the EVO project was its strong focus on end users. The advice from the Project Advisory Group to use storyboards to articulate the needs of the user informed both the overall appearance and development of the portal, as well as informing the IT requirements. This approach is now embedded at the heart of other recent funding calls. The AGILE approach was also influential in the project design and encouraged exposure of the developing system to stakeholder input. This aspect is often the most used and communicated part of the project.

- The concept of deploying data, models and tools as services in the cloud was demonstrated to be an effective way forward. A mix of commercial and private cloud providers is likely to be the optimum solution. The cost of commercial providers is likely to be prohibitive for large modeling applications. There is much to be learned from approaches adopted by other communities e.g. the astronomy community and bioinformatics community (e.g. CloudBioLimux) which could accelerate the progress of the environmental community in this field.

- There is a continuing need for international collaboration in the development of standards and interoperability. The EVOp project effectively borrowed from existing activities in this area. The Belmont Forum activities should ensure progress is made in the area in the immediate future.

- It is critical to ensure an appropriate balance and mix of science/IT skills in any future initiatives. The EVOp despite trying to ensure this from the outset had insufficient IT / computer science postdoctoral researchers. There was a pinch-point between the enthusiastic and engaged catchment scientists with many ideas and the capacity to make these operational within the cloud.

- Incorporate a small number of carefully selected exemplars in the early stages of system development. This was a major success of the EVO project to both provide cohesion to the diverse and large team and facilitate outreach to a broad section of the potential end-user community. The pace of development is inevitably enhanced by utilising established science for the exemplars.

- The culture change. One of the areas of the EVOp project of most interest to end-users was the potential for a change in research culture. Could the community move towards a more open and transparent way of working? Would they be willing to web-enable their models and encourage independent testing to gain greater trust by the end-user community. The potential for the EVO-like service to effectively act as a ‘market place’ for models; potentially only those made freely available and web-enabled in the EVO or cloud would gain traction in the end-user community was appealing to some end-users as they sought ways to move forward to develop more tested and integrated modelling approaches to tackle the complex environmental challenges they face.

1.13 Conclusions

Although not operational, the EVOp portal has demonstrated the value of integrating fragmented and widely-distributed public and private sector data, expert knowledge, modelling tools and visualisation services. It has illustrated how cloud computing improves the efficiency, speed and effective use of such resources. Valuable lessons have been learned and key issues identified for future investigation. Out of all the impacts, perhaps most important of all is the support and enthusiasm it engendered from its stakeholder groups, the potential for expansion to other science areas, industry applications and benefits arising from social and economic data were evident. From the outset, the EVOp was purposefully ambitious. It sought to demonstrate new capability and ways of working, to expand the knowledge base and sign post the way for the future. In achieving these aims the EVOp has undoubtedly had a bearing on current...
funding and approaches being taken in this arena. In the context of research programmes, the outputs and impact of this pilot are significant considering the modest investment and timeframe for implementation.

1.14 References
Gray J. 2007 Talk given by Jim Gray to the NRC-CSTB in Mountain View, CA, on January 11, 2007
Hey T, Tansley S, Tolle, K (Eds). 2009 The Fourth Paradigm Data-Intensive Scientific Discovery. Microsoft Research

Related links
NSF EarthCube
http://www.earthcube.org
Earth System Science Partnership (ESSP)
http://www.essp.org
Environment Information Initiative
http://www.nerc.ac.uk/research/capability/
Environmental Sustainability Knowledge Transfer Network
https://connect.innovateuk.org/web/sustainability ktn
ESKTN TV YouTube channel
http://www.youtube.com/playlist?list=PLE862DA5853C19459
Natural Environment Research Council (NERC)
http://www.nerc.ac.uk
London Institute of Space Policy and Law (ISPL)
http://www.space-institute.org
2 Developing the cyber-infrastructure

A key objective of the pilot Environmental Virtual Observatory (EVOp) project was to provide a cyber-infrastructure capable of demonstrating the potentials of a virtual observatory that utilises the powers of the Internet to support uniform and open access to a series of scientific resources, and to therefore support and encourage online experimentation. This aspect of the project aimed to show how the application of new Internet-based technologies, specifically cloud computing, and web portals can facilitate this vision and in particular achieve the integration of a wide variety of information sources (including disparate data sets, sensor data and models applicable at different temporal and spatial scales), together with associated information tools and services, to provide answers to big environmental science questions. From a technological perspective, the challenge was to define the architecture and associated architectural principles underpinning the EVOp, supporting multi-scale experimentation through an open extensible infrastructure, and harnessing existing resources (data, models, etc.). Core to this task was the definition of an overall architectural approach as a refinement of Web 2.0 standards, incorporating mechanisms to deal with meta-data, and the population of the architecture with exemplar services to support the project’s other work packages.

2.1 What is cloud computing?

Cloud computing is core to the EVOp project, providing the underlying technology to implement the required cyber-infrastructure. Cloud computing has emerged as one of they key areas of digital innovation in recent years and the associated technology is having major impact in a variety of areas such as eCommerce, eGovernment and smart cities. The goal of EVOp was to investigate the potential impact of cloud computing on the Environmental Sciences and indeed on science more generally.

In general terms, cloud computing is a shift from resources being on individual computers towards having these services available in the greater Internet. The classic definition from the National Institute of Science and Technology (NIST) defines cloud computing as follows (??):

“Cloud computing is a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (e.g., networks, servers, storage, applications, and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction.”

Coulouris et al (Coulouris et al., 2011) provide an alternative definition:

“A cloud is defined as a set of Internet-based application, storage and computing services sufficient to support most users’ needs, thus enabling them to largely or totally dispense with local data storage and application software”.

They then go on to refine this vision saying:

“[Cloud computing] also promotes the view of everything as a service, from physical or virtual infrastructure through to software, often paid for on a per-usage basis rather than purchased”.

Cloud computing is better understood as not a single approach but actually a family of approaches and part of the EVOp story has been to work through the different options and the implications for the Environmental Sciences community. In particular, a key defining characteristic is who provides and manages a given cloud infrastructure:

- The first option is to have a private cloud implemented within an organisation for that organisation. This option requires significant up-front investment and the responsibility for managing the cloud rests with that organisation. The organisation though retains control and ownership of the resultant infrastructure and associated cloud services.
- The second option is to opt for a public cloud where the cloud is implemented and managed by a third party provider such as Amazon, Microsoft, or Google and offered through the Internet as services to the greater public (including organisations or private individuals). The advantages here are that the upfront investment and resultant management is delegated to a third party (for a given cost), but with a loss of control over the infrastructure (for example, for data it may not be possible to specify or know where the data is stored).

Hybrid solutions are also common where organisations will adopt a mix of public and private cloud provision. More generally, there is a tendency towards multi-cloud environments where organisations use multiple...
highlights the fact that, in cloud computing, everything is a service and this is the key unifying principle underpinning cloud computing. This encompasses though a variety of approaches, often distinguished as:

- **Infrastructure as a Service (IaaS)** - IaaS is the lowest level of abstraction and refers to access to basic underlying computing resources as a service. The most common example here is to request and be given access to a computer as a service, accessed across the Internet. More specifically, when coupled with virtualisation, you will be given a virtual machine which you can then use as if it is a real, physical machine for your purposes (e.g. to act as a web server or as a hosting environment for models).

- **Software as a Service (SaaS)** - at the opposite end of the spectrum, SaaS refers to being given access to application-level software. This is a very open ended category and includes the availability of a suite of applications that offer classic functionality such as word processing, e-mail, calendars, etc (e.g. Google Apps). This category also includes domain specific software, e.g. an environmental model that you would like to make available as a cloud service.

- **Platform as a Service (PaaS)** - PaaS sits in the middle and refers to services that reside above operating systems and which are useful in the construction of application software. Key examples include software frameworks to support web servers and databases.

A sub-goal of the EVOp project was to understand the full range of approaches under the ‘cloud computing’ umbrella and the implications for the Environmental Sciences community.

### 2.1 Why cloud computing for Environmental Services?

The general benefits of cloud computing are well document, for example see (Zhang et al., 2010). In this section, we focus on the specific benefits in the context of supporting an Environmental Virtual Observatory.

The most profound impact is in terms of supporting a new kind of science:

- **An open science** - whereby open access is provided to a range of environmental assets including data sets, models and supporting assets such as visualisations;

- **A shared and collaborative science** - whereby assets are accessible and shareable from anywhere via the cloud by different stakeholder groups, encouraging collaboration and opening up new avenues such as citizen science;

- **An integrative science** - whereby problems can be studied by bringing together data and models from different disciplinary perspectives, over different geographical regions and at different scales.

In addition to this, we gain a number of key benefits emanating from the cloud computing approach:

- **Everything as a service** - All models and data assets follow a common service model. This offers a level of transparency, by which details of where and how the data are held are hidden from users. This allows for data to be used in models and simulations without necessarily giving it to the users, avoiding some of the delicate issues of ownership.

- **On-demand cloud elasticity** - In cloud computing, it is possible to request resources as and when they are needed and then return them to the cloud provider when no longer needed. Through this approach, resources can grow and shrink to meet current demand (a property known as elasticity). For example, if a user is running a complex climate change model that requires extra virtual machines, these can be requested and returned when the model completes execution.

- **Delegated management** - Managing a cyber-infrastructure is complex, especially when it comes to ensuring key properties such as secure and reliable access to resources. For example, it is important to ensure that data is continually available in spite of the inevitable failure of underlying computing infrastructure, typically achieved through replication of data and the use of protocols to ensure consistency of replicas. By adopting a cloud approach, such management is delegated to the cloud provider meaning users do not need to worry about these key issues.

### 2.2 The EVOp approach

#### 2.2.1 Overall approach

The first key decision was to adopt a multi-cloud approach spanning private and public cloud provision. The private cloud is hosted in Lancaster University and is operated by us using OpenStack, an open source virtual infrastructure management solution. The public cloud resources are provided by Amazon Web Services (AWS). The pairing of OpenStack and AWS is a common one in the cloud computing world: AWS is arguably the most mature and feature rich public IaaS provider, and OpenStack is backed by many (including large organisations like NASA, IBM, and many others) as the de facto open source alternative to the core AWS products, i.e. EC2 (utility computing) and S3 (storage service). This makes it possible, at least in theory, to use the same virtual machine images to start instances in either cloud. In order to promote portability and to avoid being tied in to one provider (vendor lock-in), we adopted cross-cloud library jclouds. This open source software provides abstractions across many of the widely used cloud solutions.

Where possible, we adopt standards to enable interoperability within the architecture. Both AWS and OpenStack adopt web service standards and hence, in EVOp, all services (data, models and other supportive services) offer standard web service interfaces. Again where possible, we adopt a RESTful approach to service APIs, an approach that promotes loose
coupling and consequently major improvements in scalability and manageability (Fielding, 2000). The environmental models are implemented using the OGC (Open Geospatial Consortium) WPS (Web Processing Service) standard that specifies how geospatial inputs and outputs should be.

### 2.2.2 The system architecture

The overall architecture for the system is shown in Figure 2.1.

The Model Library is populated by domain specialists (e.g. hydrologists) in liaison with data providers. The process starts with online calibration and testing of a model against a certain dataset (e.g. TOP-MODEL on the rainfall data of the Eden catchment in the North West of England). The outcome of this process is a virtual machine image optimised to run a fine-tuned set of models that are exposed as web services and equipped with all required data. This streamlined execution bundle is then stored in the library to be instantiated upon demand.

Once a user navigates to one of the models, a connection is created with the Resource Broker module of the Infrastructure Manager. This broker responds with an address of a cloud instance that is suitable for the type of computation required, along with some session information. This communication is done using HTML5 WebSockets, which reduces network overhead and browser memory usage.

The Load Balancer monitors the status of running instances with two objectives: minimise costs and maintain instance responsiveness:

- For the former, user requests are served by default using private instances. Upon saturation of private cloud resources, the load Balancer initiates cloudbursting mode where public cloud instances are used beside private ones. This is reversed upon detecting underuse, migrating users back to use private instances.
- For the latter objective, performance metrics are collected and any notable degradation triggers the Load Balancer to start a new instance, redirecting users that were being served by the seemingly malfunctioning instance to the newly created one.

A number of models were migrated to the EVOp infrastructure. For each model, a bespoke visualisation was developed to suit the particular factors in question. In general terms, models generate one of two types of output: geospatial and time series. Geospatial data is visualised using interactive layers superimposed over maps. Google Maps is used due to its wealth in data, features, and the familiarity of the general public with it. The interactive nature of the geospatial layers allows expansion of the visualisation to include time series graphs over specific map locations.

An emphasis in all models is placed on adjustability and flexibility in order to provide an interactive and configurable user experience. This is achieved via dynamic HTML and HTML5 web elements, AJAX asynchronous communications, and browser scripting using advanced open source JavaScript libraries such as JQuery, Flot, qTip, and Google Maps.

### 2.2.3 The use of agile methodology

The development process in EVOp relied heavily on an agile methodology based on a behaviour-driven design. Requirements were drawn from specific storyboards that were outlined by the domain...
Figure 2.2 The Taverna workflow running the FUSE model as seen in the Taverna Workbench editor.

Figure 2.3 The resulting hydrograph output from a Taverna workflow run within the BioVel interface.
specialist within the consortium. These are referred to as the storyboard owners. Prototypes were developed based on these requirements, and are iteratively improved and built following verification (within the development team) and validation (with the storyboard owners, the wider consortium, and stakeholders) processes.

2.2.4 The portal
The EVO portal provides several means of finding information. The portal front page hosts a selection of paths to content and functionality. Furthermore, there are a myriad of info pages that introduce the models and data hosted on the portal along with associated links, FAQs and tutorials. Examples of the portable can be seen throughout this report (for example, see Figure 1.4 for the entry point to the portal).

The project team also investigated the role of workflows to enhance the capabilities of the portal, allowing scientists to create bespoke experiments connecting data and models together in a desired and repeatable pattern ready for execution in the cloud.

The experimentation focused on hydrological models to enable users to explore different management scenarios that might affect water resources in their location. A number of web services and a bespoke web page to run them were created. Building on this, a more flexible interface was developed using the Taverna Workflow Management System.

Figure 2.2 illustrates an example Taverna workflow that was created in the project. This workflow features a WPS service running an R version of the FUSE hydrological model for stream discharge in a catchment (within the Claudia script). The BioVel EC2 image was configured to run this workflow with the Taverna server to handle input parameters and the data loading. The workflow was then connected to a separate EVOp EC2 image to call the WPS running the hydrological modelling service.

Figure 2.3 illustrates the view for the user of the workflow when loaded into the BioVel Web interface. This hides the details of the connection of different cloud services to run the FUSE model. The resulting hydrograph of stream discharge is saved so that users can review and repeat previous workflow runs.

2.2.5 Exploring semantic links for EVOp data
The team investigated the use of GeoNames ontology and Web accessible database. The GeoNames database provides unique Web URIs for locations that can then be used to link to other web resources using Web APIs. The team entered 25 EVOp related sites in to GeoNames using the EVOP tag. These locations could then be linked through the GeoNames database to other resources such as Wikipedia entries for nearby locations (linked through DBPedia) and to Web services providing local weather readings (located through International Civil Aviation Organization (ICAO) sites in GeoNames). This facility to access related information to EVOp sites was developed as a Javascript tool but not included in the final EVOp portal partly due to the reliability of the GeoNames API during testing.

2.3 References

Related links
The NIST definition of cloud computing
http://csrc.nist.gov/publications/PubsSPs.html#800-145
Apache jclouds
http://jclouds.apache.org/
The Taverna Workflow Management System
http://www.taverna.org.uk/
3 Modelling in the EVOp cloud

The EVOp portal deploys interactive web applications to model local flooding and diffuse pollution. From a user perspective, web-based environmental models do not require any software installation as they are accessed using standard web protocols using an internet connection (e.g., http). As a result, they are platform independent and can be easily integrated in workflows as part of the process of environmental data retrieval, manipulation, visualisation, and communication. To maximize efficiency and interoperability with storage, interaction and visualisation tools, the EVOp team have adopted the Web Processing Services (WPS) standard of the Open Geospatial Consortium (OGC), which consists of a wide range of industry and academic actors. Additionally, several stable software implementations of the OGC standards exist, which greatly facilitated the development of these models.

3.1 Selected models and web service implementation

For the purpose of this project, three different environmental models were implemented as web services:

- **TOPMODEL** (Beven and Kirkby, 1979) was chosen to demonstrate the local exemplar. Topmodel is a widely used and well documented semi-distributed, conceptual hydrological model. It was originally developed for small, upland catchments in a humid environment, and is therefore very suitable for the catchments selected for the local case studies. The model produces a time series of river discharge and spatial patterns of soil moisture.

- **FUSE** (Clark et al., 2008) is a state-of-the-art modelling toolbox which includes well established algorithms including VIC and the Stanford Watershed Model. As a toolbox, it allows combination of many different algorithms, thus creating over 1000 possible model structures. As such, it provides a very flexible solution for the large number of catchments to be modelled in the national case study. The model produces a time series of river discharge.

- **Export Coefficient Model (ECM)** (Johnes et al., 2007) is an established approach to allow prediction of nutrient (nitrogen and phosphorus) flux from land to inland and coastal waters. The predictions are based on agricultural practices, such as stocking densities, fertiliser use and crop types, human population density and atmospheric deposition, hence making the model suitable for rapid mitigation scenario development and testing. The model produces predictions from field to national scale and generates mapped outputs and summary tables of nutrient export by source and practice.

These models were written in different programming languages (C, Fortran, C++, and MS Excel). In order to integrate them into a common web service infrastructure, TOPMODEL and FUSE were integrated in the R data analysis platform, either by wrapping R code around the original implementation (for TOPMODEL), or by re-implementing them directly in R (for FUSE). TOPMODEL is already available as an R package, and FUSE has also been made available. A major advantage of R is its convenient integration with PyWPS, a Python implementation of the OGC WPS. The communication between Python and R is facilitated by an existing connector (RPy2). A local PostgreSQL database was used for data storage because a web-based implementation such as the OGC Sensor Observation Service was deemed unfeasible within the context of the pilot.

The ECM was originally implemented in Excel and hence a new implementation of the model was written for this project in a combination of PHP (on the cloud side) and JavaScript (on the desktop side). This language and platform split in the implementation means that the cloud was able to perform the query of the spatial database for the area of interest and the bulk of the model calculations. The summary tables are then passed to the final calculation in the browser. Keeping the final stage of the calculation on the desktop means that the user can undertake scenario testing, such as altering the livestock numbers in a catchment, with the results being very rapidly calculated and displayed. The main spatial database is stored in a MySQL database and the outputs of the modelling can be rapidly mapped at any spatial scale for visual interpretation of model predictions.
3.2 Workflow integration and applications

The modelling web services were integrated in the workflows of two EVOp applications to showcase their potential. These applications are accessible via the main EVOp portal and focus on simulating the impact of land-use changes on flood risk, and diffuse pollution and water quality.

The communication between client (e.g., modelling web portal) and server is defined by the OGC WPS standard. The web client sends the server a HTTP GET request to execute the process. Once the execution terminates, the server sends back an XML response which is parsed at the client side extracting the simulated time series. Data are retrieved by querying the database in real time while the visualization of time series is based on the Google-charts API and similar libraries.

The flood modelling tool is available at the following four locations:

- River Eden catchment:
  - Dacre Beck at Dacre Bridge, Cumbria, England.
- Dyfi catchment: Dyfi Bridge, Machynlleth, Wales.
- Tarland catchment: Coull Bridge, Aberdeenshire, Scotland.

It consists of the following user-interactions:

i. Selection of the location of interest: Based on the user input, observed river flow and precipitation data, as well as pre-calibrated model parameters are queried from the database.

ii. Modification of the land-use scenario: The user input is then mapped onto modifications of the optimal model parameters. At this stage of the EVOp, this conversion is based on an empirical parameter translation table. However, theoretical research on how to parameterise user scenarios is on-going.

iii. Subsequently, the model is run with the modified parameter values and the results are visualised in the web interface. The model can be run many times with different scenarios. The simulated discharge time series are kept while the user session is active. Multiple simulations can be selected and visualised together to facilitate the comparison of different scenarios. The plotting functionality also allows for the visualisation of an estimate of the streamflow threshold above which the flow spills over the banks causing possible flooding.

The diffuse pollution modelling tool has been implemented at the full UK scale at a spatial resolution of 4km². To run the model, the user makes a series of choices:

- Select an area of interest: These are based on countries, OSPAR zones, coastal drainage zones, River Basin Districts and river or water quality catchments based on the locations of gauging sites.
- For the area of interest, specify various options connected with the model setup, although not all options are enabled in the demo:
  - Selection of the model.
  - Selection of the data set to run of the model, such as land cover data from different years.
  - Selection of the hydrological model.
- For the selected model configuration, the user can choose to run the model with the observed historic land management, or to test a set of mitigation options. The mitigation options are 'Good Agricultural Practice', 'Catchment Sensitive Farming', 'Mitigation through on-farm measures', 'Farming for WFD compliance' and 'Urban Waste Water Treatment Directive Plus (UWwTD+)'. Each of these mitigation scenarios makes suitable adjustments to the configuration of the landscape to represent the change. These mitigation options can be spatially targeted at the level of the geoclimatic region (targeting different measures according to the key characteristics of each region).
- The results are then presented as tables, maps or charts for both the observed historic, and the developed scenario.

3.3 Uncertainties

Uncertainties remain a major issue to tackle. The project reviewed the relevant technologies that are available to document uncertainties in a web services context. One of the most promising initiatives is UncertWEB which aims to provide data models and mark-up tools for the propagation of uncertainties in modelling workflows and communication of uncertainties to the end-user. Experiments are ongoing to integrate uncertWEB (Williams et al., 2010) in the FUSE modelling toolset by means of adding UncertWEB data models to the object-oriented class definitions in the R toolbox.

At the same time, efforts were focused on integrating the major uncertainty quantification methods in the modelling toolbox. The following methods are currently available:

- Generalized Likelihood Uncertainty Estimation (GLUE, Beven and Binley, 1992, Beven and Binley 2013).
- Differential Adaptive DREAM (Vrugt et al., 2009).
- Bayesian Total Error Analysis (Thyer et al., 2009).

These implementations are a combination of efforts from the R development community and the EVOp project.

Lastly, efforts have been aimed at developing an objective model structure selection algorithm, based on methods for data mining of model performances, and the extrapolation of model structures in space and time.
Many of the abovementioned activities need further attention. Even though functional implementations of each of the algorithms exist, major technological and conceptual challenges are still to be overcome. These, and others, should be explored further in eventual follow-up projects to EVOp.

3.4 Opportunities

The future opportunities for linking the hydrological and biogeochemical models can be seen in both research and decision support focused areas. For example, the tighter linkage of the model components or models could help to investigate the grand scientific environmental challenges on, for example, the influence of hydrology on processes controlling losses of nutrients (N, P and other macronutrients) from land to surface waters, the location of critical source areas for diffuse pollution in the landscape and how these export processes and locations may alter under projections of climate change. This need for tighter coupling has been recognised in the EU SEAMLESS project, which is aiming to overcome “fragmentation in research models and data in Europe for assessing agricultural systems”. EVO has an opportunity to integrate more closely with this, and other, projects.

The modelling community is moving from an approach where one model approach / structure was deemed sufficient to understand and predict system properties that could be used by the wider community. Through better sharing of data and approaches (as has been shown in molecular and marine sciences) EVO can act to accelerate progress in the environmental sciences. Taking a high level view of the possible future opportunities, there are many possible ways in which EVO could add value to science and society:

- The range of predictions could be extended through linking other catchment hydrological and biogeochemical models into the framework and allowing the cross comparison between the different predictions. As each new model is included, the potential number of combinations significantly increases, requiring the computation resource available in the cloud. Examples include CAPRI DNDC, PSYCHIC, MITERRA, INITIATOR, INCA, RiverStrahler, CRUM3, SCIMAP and PIHM. Research is required to understand which model couplings yield the greatest information gain and how to interface different type of model output (resolutions and types of predictions)
- Time and space scales. Finer spatial scale models, such as SCIMAP, at the 5x5 metre resolution to compliment national models, such as the current ECM. Temporally dynamic models such as HBV light, INCA or CRUM3. The temporally dynamic models could enable real time flow and or WQ predictions for water companies which could be used in abstraction or discharge planning.
- Testing old models with new data. DTC N and P time series are the required level of resolution to test detailed process catchment models. The DTC datacentre could provide data series as web services (mid 2014) and used to drive simulation models. Linking the data stream with the modelling tools could create a powerful platform to test approaches and hence encourage developers to make their tools compatible with the EVO approach.
- There are opportunities to develop mobile applications that make use of the cloud hosted models to deliver support services for CSFOs or for teaching and learning at all levels of education (flood models, mitigation scenarios and augmented reality).
- There is a growing trend towards open source models and publishable workflows (myExperiment, R and iPython notebook), which share best practice and help others to use techniques. Linking the EVO hydrological and biogeochemical models into these tools increases their accessibility and value.
- Stakeholder engagement earlier in the modelling process. Through having a range of different hydrological and biogeochemical models available, it is possible to work closely with stakeholders to understand their problems and build a tailored solution rather than focusing the current limited set of tools that may be available to that user.

3.5 Barriers

The barriers that have been identified are:

- IP on models and datasets. This cannot be understated.
- The required data may not exist, may be protected by IP, not be publicly available (governmental or commercial issues), or be lost. There is therefore the need to make as much data available as possible and to ensure that the datasets that are collected in the future have maximum information content and well documented metadata.
- Modellers and modelling groups may see the conversion of existing models to a web service approach difficult or not worthwhile. If there could be a modelling portal that had licences for the key datasets (e.g. NextMap 5m product, LCM 2007, geology, soils, rainfall, discharge and water chemistry data), then this would be a significant pull for developers to move their tools to the platform.
- There are significant challenges with linking models together to create a solution. This relates
to the issue that models may have been written for a different reason, work at different space and time resolutions, and the feedback between processes represented in different models may not be captured.

- As models become more advanced, the computational cost increases significantly. The computational resource is there via cloud computing technologies but there needs to be a method to cover the costs of using the resource. Precedents for this exist in HPC (e.g. Hector) although a more dynamic ‘economy’ could be created with ‘rewards’ for sharing and creating tools and computational resources and ‘costs’ for using tools and computational resources.
- There is the issue of standards for model description, parameterisation and output. There are a few standards for model output (e.g. WaterML) but there is no currently defined standard for the communication of the uncertainties in predictions and measurements between models.
- The need for further development of methods to propagate uncertainties within modelling workflows.
- The need for methods to communicate uncertainties to end-users.

3.6 References


Related links
EU SEAMLESS project
http://www.seamlessassociation.org
FUSE
https://f-forge.r-project.org/projects/r-hydro
TOPMODEL R-package
http://cran.r-project.org/web/packages/topmodel/
Uncertainty Markup Language
http://www.uncertml.org/
Uncertweb discussion paper
http://www.uncertweb.org
4 Data

The UK is richly endowed with environmental data that have been collected over many decades for a wide variety of reasons (e.g. research, monitoring change, operational, public safety, legal reporting, and regulatory obligations) by many different organisations. The long tradition of environmental monitoring provides the UK with an enormous reservoir of historical environmental information that also is of huge global importance. People are awakening to the potential that such data possess not only for science but for stimulating economic growth and bringing positive impacts and benefits to society.

4.1 Time to unleash the potential of environmental data

The vast majority of environmental data have been collected over the years through public funding. In its Open Data White Paper (HMG, 2012), the UK Government clearly articulates its commitment to inspire the "innovation and enterprise that spurs social and economic growth" through improved sharing of public data. This is reflected in the new Open Data policies published by all Government departments. The BIS Open Data Strategy (BIS, 2012), for example, states the Department's commitment "both to increasing the economic impact of existing public sector information and also to releasing new public sector information to expand the market". A further driver for Government is transparency: helping people make better choices about public services and holding government to account. In a scientific context, Open Data not only promotes innovation but also provides greater transparency of the research process enabling the provenance of data to be checked and resulting claims and discoveries to be corroborated. The Royal Society, in its recent report, "Science as an open enterprise" (2012), called on scientists to "communicate the data they collect... to allow free and open access, and in ways that are intelligible, assessable and usable."

4.2 Open data beyond the UK

Such ambitions on Open Data are not confined to the UK but are part of a global trend towards realising the value and impact of data. The US Government in its paper, Digital Government - Building a 21st Century Platform to Better Serve the American People (USG, 2012), undertakes to "unlock the power of government data to spur innovation". Similarly, on launching the Open Data Strategy for Europe in December 2011, European Commission Vice President Neelie Kroes stated, "taxpayers have already paid for this information, the least we can do is give it back to those who want to use it in new ways that help people and create jobs and growth."

4.3 Initiatives

A number of initiatives are leading the way in promoting data sharing and derive better impact from environmental data, including: the EC's INSPIRE Directive which aims "to establish an infrastructure for spatial information in Europe to support policies or activities which may have an impact on the environment", and the Defra-led UK Location Programme - a UK pan-government initiative to improve the sharing and re-use of public sector location information; and the Public Data Group (Met Office, Ordnance Service, Companies House, Land Registry), which seeks "to maximise the long term economic and social benefit of data". The Environmental Science to Service Partnership (ESSP) involving Defra, the EA, Met Office, Ordnance Survey and the NERC, aims to "combine data, information, knowledge, and expertise to deliver services for society, private enterprises and government, to inform and support decision making". NERC itself has adopted an open data policy and, through the implementation of its new Science Information Strategy, is enabling improved access to data from the activities it funds.

4.4 Advances

Advances in information and communication technologies are further rapidly transforming the way environmental data are collected, accessed, shared and analysed. Improved capabilities offered by the innovation in cloud computing, smart-phones and collaboration tools all affect how people deliver, receive, and synthesise environmental data and are helping to promote the Open Data agenda. Several
projects and initiatives at national-, European- and global-level have sought (or are seeking) to demonstrate the benefits and potentials of exploiting new technology to derive better impact from data. As well as this project, examples include: the Met Office's Open Platform, the European Commission's Shared Environmental Information System, the EEA's Eye on Earth, the NSF's EarthCube (USA), the Global Monitoring for Environment and Security (GMES), and the Global Earth Observation System of Systems (GEOSS)).

A study undertaken on behalf of Research Councils UK, in partnership with JISC and the Royal Society, explored public views on Open Data in research. The following findings, taken from the study's Final Report (TNS, 2012), provide a series of pointers for EVO as it seeks to develop beyond the pilot:

- whilst openness was believed to promote scrutiny which could help build trust... confusion may arise from multiple interpretations of the same data, which in turn could impact on the trustworthiness of research;
- regarding innovation... arguments around better efficiencies in the research process, potential cost savings and to a lesser extent growth (by utilising datasets to develop new products and services) were accepted;
- the principal benefits of open data were seen to accrue for researchers rather than the public;
- the concept of openness sat uneasily with researchers... there was a strong view that those who had put the effort into developing a dataset should have a period of time to take exclusive advantage of this;
- the most important concern around open data was that it should be promoted when it serves the public interest... defined almost exclusively in terms of data that can help improve human health and, to a lesser extent, the environment;
- data should not be released too early or in a way that would be likely to promote poor decision making or do harm; and
- public funded and academic researchers were generally thought to be more open than those funded in the private sector,... increased commercial funding ... was seen as having the potential to negatively impact.

What is Open Data?
Open Data are defined as data that are:

- accessible, ideally via the internet, at no more than the cost of reproduction, without limitation based on user identity or intent
- in a digital, machine readable format for interoperation with other data; and
- free of restriction on use or redistribution in its licencing conditions.

Source: HMG Open Data White Paper, 2012

Figure 4.1 A glimpse of the environmental data landscape.
4.5 The pros and cons

The Royal Society (2012), whilst claiming open data can increase a published paper’s profile (one case study it refers to showed a 69% increase in citation), acknowledges that protecting IPR around data are still a vital issue for many and concedes that "legitimate reasons for keeping data closed must be respected". However, it asserts "the small percentage income universities derive from IP" should "not work against longer term benefit to the national economy." Clearly further work is needed to strike the correct balance between the two.

The reuse of data provided by individuals for purposes other than those for which they were originally collected raises further issues of confidentiality and privacy and the rights and responsibilities of different data stakeholders, which sometimes may conflict (e.g. the rights of individuals versus "the common good"). It would seem many of the moral and ethical aspects of Open Data remain to be explored.

4.6 Conclusions

Despite recent technological advances, a complex and fragmented environmental data landscape persists comprising many different organisations and initiatives all seeking to provide environmental data and associated information (see Figure 4.1). Scientists, students, consultants, environmentalists, politicians and members of the general public alike regularly have difficulty in obtaining relevant data, which, even when successful in identifying, often are returned in unintelligible or unusable form. Such fragmentation and heterogeneity is inefficient and confusing and remains a huge barrier to science, innovation and economic growth.

From a technical viewpoint, implementation of Governments' Open Data policies requires data of many different types and formats to be made accessible in a standard way, through common, standards-based tools and services. EVOp, albeit in a relatively small way, has attempted to tame some of the technical challenges of bringing environmental data, models and tools together as services in a cloud environment, demonstrating the potential benefits to a range of stakeholders. Progressing beyond the pilot, Open Data will provide the EVO with opportunities to exploit, and derive impact from, an increasingly wide range of data types. But in so doing, the EVO will itself be at the vanguard of Open Data implementation and will be forced to address many of the technical and non-technical issues that have been set-out in this section.

4.7 References


5 Local exemplar

The development of the local exemplar has been undertaken in three largely rural catchments based in Scotland, England and Wales, with a team from three universities and one research institute. The project focused on soil and water issues, and this has led to the development and trialling of visualisation of the linkages between hydrology, land use and flooding in the rivers Dyfi, Tarland and Eden. An important aspect of the work has been the consultation with a wide range of potential users in each of these catchments.

5.1 The Catchments

Three catchments were used. Their locations can be seen in Figure 5.1.

5.1.1 The Dyfi

The River Dyfi is located north of Aberystwyth in mid-Wales and its catchment drains an area of 671 km². The Dyfi and its tributaries form a dense, dendritic drainage network with a total channel length of over 1,500 km. Rainfall in the upland areas is on average 2000 mm per annum, falling to ~1000 mm on the coast. Land use in the catchment is dominated by agricultural activity, whereas slate quarrying and metal mining were historically prevalent. Virtually the whole Dyfi catchment has been given some form of conservation status, including the Snowdonia National Park, 23 SSSIs and being designated as a UNESCO biosphere reserve.

5.1.2 The Dee

The River Dee in northeast Scotland has multiple high level habitat designations (Natura 2000, SAC) for species such as Freshwater Pearl Mussel and economically-important Salmonid fish species. Tarland Burn, situated centrally in the Dee, is the first tributary with intensive land use and first point of nutrient-impacted waters entering the oligotrophic main river. Rainfall is approximately 1000 mm with long periods of winter snow. The Tarland catchment (100 km²) includes the village of Tarland and Aboyne (populations 600 and several thousand). The Tarland Burn suffers diffuse pollution and morphology issues with pressures from farming, urbanization and septic tanks. It is currently described as Poor-Moderate under the WFD and is a Priority Catchment for SEPA. Additionally, the community has suffered recent flooding and, in response to these many impacts, has shown some excellent examples of community led initiatives in natural flood management and riparian habitat improvement. A decade of research into both the natural functioning and improvements in the catchment has given a wealth of data and knowledge that will enable testing of models for biophysical and socio-economic aspects of catchment management.

5.1.3 The Eden

The Eden catchment in northwest England is a mixed grassland area, with an area of 2398 km² and a main channel length of 130 km. Agriculture in the catchment is characterised by mixed dairy and livestock farming, and comprises both rough grazing and improved grazing with some arable land use towards the north and on the richer soils of the River Eden floodplain. Average rainfall across the catchment is ~1700 mm per year; however this masks rainfall gradients associated with much higher rainfall on the uplands of the Lake District and Pennine fells. The catchment has several designations for SSSI and SAC status, for the
range of habitats and species it supports, and the river passes through two National Parks, two AONBs and a World Heritage Site. The Morland sub-catchment of the Eden is 10 km$^2$ and is located in the southwest of the main catchment. Pressures in the Morland sub-catchment and Eden are predominantly flooding and diffuse pollution.

5.2 Development of the exemplar
The development of the Local Exemplar for EVOp is outlined below, through the storyboard development, steps taken in implementation, evaluation of the work with stakeholders, and the potential for the future. Each catchment developed a storyboard that reflected the needs of the different stakeholders based around the theme of flooding and these are presented individually.

5.3 Storyboard description and stakeholders

5.3.1 Tarland
The community in Tarland - that includes farmers and the dominant land owner) have worked with researchers to understand how to adapt and mitigate against extreme hydrological events linked to other issues such as the channelisation of streams, diffuse pollution management, and habitat loss. Actions coalesced following major flooding of the village centres and prime arable land several times in 2002 (Figure 5.2). Co-constructional problem solving with stakeholders has led to trial catchment schemes of stream remeandering, several ponds and wetlands, point source mitigation, and knowledge contributing strongly to the sustainable approaches enshrined in the Flood Risk Management (Scotland) Act 2009. What the community have sought during this development has been access to local data and knowledge to inform them and their decision making. The static tools provided by the agencies did not adequately provide dynamic information such as live data feeds and interpretation of flood risk management in their landscape. The storyboard for Tarland concentrated on this stakeholder need (see online Annex).

The project built on existing monitoring platforms at 1 and 50 km$^2$ catchment area stream stations to bring live feeds to the catchment website. EVO has broadened the sensor network in Tarland and this feeds into live modelling within EVOp. The project has also brought hydrology and water cycles into education by hosting weather stations at three local primary schools. The children take manual measurements (raingauges, snow stick, temperature) and record and compare these to Davis Vantage automated electronic met stations located on the school sites.

The EVOp project has followed the timeline of an EU project in Tarland Aquarius - Farmers as Water Managers. As part of this considerable effort was made to bring a flood mitigation measure upstream of Tarland village. The Aquarius project finished in 2011 with a fascinating socio-economic-biophysical knowledge of the barriers to natural and engineered flood mitigation measures in the catchment, yet no measure had been achieved. The proposed engineering structure was large and unacceptable to the farmers involved and stalemate had been reached between the local Council, regulator and land managers.
As part of the EVOp development, Aberdeenshire Council commissioned work to improve the live sensing network as part of the ongoing EVOp developments and skills demonstrated in bringing live information onto web-based services. This has been implemented in three further stations and now provides the Council with early warning information for planning and emergency provision. One of the stations has been intentionally located at the farm site of the failed flood storage measure. The provision of information is helping this farmer understand the water volumes involved, likely storage depths, and risks to his cattle and infrastructure.

Further to this, flooding scenarios were applied to this farmland using the hydraulic model TUFLOW, and TOPMODEL. These were calibrated with the longer-term hydrological stations’ data to bring an application to the web based services in EVOp (Figure 5.3). The visualisations developed as part of the EVOp web tool (Figure 5.4) have now been used to open dialogue between the farmer, the EVOp project staff, and the local Council. It is reasonable to believe that the use of the full range of live data informing and interpretive tools, brought together under the local EVOp banner, are enabling a process of realising a better informed community (farmers, regulators, responsible authorities in flooding such as Aberdeenshire Council and school children - filtering up to their largely farmer parents). These better-informed stakeholders are prepared now to act differently and more favourably with regard to catchment based water quantity (and quality) solutions.

5.3.2 Dyfi

The Dyfi Catchment team developed an integrated storyboard to meet the needs of two key audiences, namely the insurance industry and local stakeholders. A semi-structured qualitative discussion was held with participants to meet the following storyboard objectives to:

i. introduce EVO and assess reactions to its goals as well as present and invite feedback on a draft storyboard as developed by the Dyfi team. Community feedback resulted in a substantially revised storyboard - available in the online Annex;

ii. critically evaluate the storyboard’s Integrated Flood Risk Management Tool;

iii. gather feedback on EVOp data and communication needs.

The storyboard approach was to co-develop the EVOp interface with potential end-users to reflect stakeholder needs. This co-development approach identified several unique EVO offerings, including many beneficial tools that could only be offered with a cloud-based platform:

- **Mapping Tool**: The Dyfi Storyboard mocked-up a mapping tool that was received very well by stakeholders. They were particularly interested in the geomorphological vulnerability point maps, as well as the ability to integrate these data with other layers from an EVO database, including LiDAR, socio-economic data, and infrastructure.
- **Timeline Tool**: Potential timeline tool, using slider technology, was recommended by stakeholders for EVO's flood management interface, with recommendations that it should be split into two different sections, namely (i) flood timeline and (ii) analysis tools. This has been illustrated on the storyboard with a SWITCH button. Stakeholders want a simple timeline, e.g. ‘Past, Now, Current and Future’ to replace original presented options that included Holocene, historical, and future flood predictions.

- **Live Data Tool**: A storyboard mock-up of how a live data tool could operate within EVOp was developed. It uses Google Earth as the backdrop. This shows how georeferenced SMS text inputs could be streamed to the interface to communicate live stakeholder flood updates as well as integrating the EA flood gauge levels.

- **Offer Choice**: Stakeholder feedback demonstrates that different users have different preferences to launch an EVO enquiry. Some users, particularly non-technical audiences prefer to search via location and want to immediately know which databases are available to them for their specific region. Other, more technically minded users are more issue- or tool-driven, e.g. a consultant wanted to immediately know whether Environmental Impact Assessment tools would be available to him, or whether the appropriate datasets were available to conduct the EIA. Therefore the four steps, illustrated in the storyboard, should receive equal weighting when landing on EVO platform: (i) Location; (ii) Tools; (iii) Issues; and (iv) Help. The Help function would use an information filtering system to deliver the best options to match the user’s needs.

- **Video Tour**: A video tour of EVOp should be prominently displayed upon arrival. A three minute duration was identified by stakeholders as the optimal video length.

### 5.3.3 Eden

The basis for the storyboard in the Eden centres on the potential conflict between increasing food production and changing upstream land use to mitigate against downstream flood risk. The full storyboard can be found in the online Annex. EVOp would be used to demonstrate how different scenarios of future land use and land management would potentially impact on the flood risk posed by a particular stream by dynamically running hydrological and hydraulic cloud-based models of that catchment and creating different visualisations in the form of hydrographs and inundation maps. This information could then be combined with other data sources on housing stock and farm land lost to provide an economic cost-benefit analysis of the different scenarios. For example, this could be in terms of houses inundated, property damage costs, loss of farmland, costs of forgone production. The information provided by the EVOp would enable the community to debate what kind of future they want to see and show justification for the funding of flood mitigation measures on farmland, providing farmers with incentives to adopt natural flood management measures. Further information on interpreting model results, their uncertainties and how the models are set up would also be provided to assist users in their understanding of the issues. The opportunity would also exist for users to provide feedback on their interpretation of the model results. This might raise issues relating to the social acceptability of certain scenarios or the accuracy of the model predictions versus local knowledge of how the landscape works. The final stage in the storyboard is the ability to save or share model outputs using a cloud-based user account.

The situation that was the basis for the storyboard is a real problem of ‘muddy flooding’ that occurs in the sub-catchment of Morland Beck in the river Eden. The hypothetical situation used came from a catchment flooding workshop attended by local farmers and landowners, in which the EVOp was being demonstrated as a device for explaining the linkages between activities on the land and consequent flood risk in the river downstream.

### 5.4 Steps taken in implementation

The implementation of the local EVOp online demo has occurred in iterative stages over the course of the project. The Eden storyboard was selected to be developed as the online demonstrator initially, with functionality added to the other catchments over the course of the project. There were two main strands to the process, the development of the web interface and visualisations and the development of the cloud modelling across different catchments. These two strands combined at a later stage in the process as the modelling work was integrated into the web interface.

### 5.5 Web interface

The initial development of the web interface focused on the development of visualisation tools and providing the user with the ability to explore their local catchment. The basis for this work was the use of Google Maps API as background mapping due to its familiarity for users, free accessibility, and widespread development of supporting applications. A map interface was chosen to provide a user interested in a particular geographical area the opportunity to explore data availability in that location (Figure 5.5).

The ability to view and visualise ‘live’ data was highlighted as an interest of local stakeholders when considering the topic of local flooding in the Eden. The sources of data on river level were taken from the EA’s river and sea levels data (Figure 5.6). For the pilot, it was agreed simply to use the image take directly from their website but, with data access agreements, this information could be brought into the EVO cloud as raw data thus greatly expanding the ability of the user to manipulate and visualise it as required. Other live data was provided by the Eden Demonstration Test Catchment project including live rainfall, webcam and stream water quality information. This data was used to develop a second visualisation type to assist users with
interpreting the data they were looking at. Line graph plots of stream temperature and turbidity (an indicator of stream flow) were combined with webcam images over the period, allowing the user to scroll over the graph and see how the stream change related to what was being measured in the stream (Figure 5.7).

5.6 Cloud modelling

Initially, hydrological modelling of a sub-catchment of the Eden - Blind Beck - was developed using data from the CHASM project. TOPMODEL, a very well established hydrological model was used, as it has been implemented as a web service. Model setup was carried out offline to ensure that the input data and parameters were in the correct format and the model could reproduce observed discharge at the outlet of the catchment adequately. The model output is a hydrograph of stream discharge for a storm event. This output can be modified by running the model under the different scenarios to compare the stream’s response to changes to land use and land management.

Once the model was successfully running offline, steps were taken to ‘cloudify’ the model and its outputs by linking a database containing the input data, the web processing service, and a web-based model interface linked to the map page (Figure 5.8). This control panel enables the user to select scenarios to run, change parameter values, and run the model in real time.
Following the success of modelling Blind Beck, three further sites (Dacre Beck [Eden], Coull Bridge [Tarland] and Dyfi Bridge [Dyfi]) have been added to the database to enable the modelling tool to be exploited in all three catchments.

Scenarios of land use and land management change were developed with the help of the local community in Morland (see Section 5.9). Four scenarios were used to illustrate how changes to land use and land management practices are likely to impact on flood risk at the catchment outlet. Uncertainty in the model outputs was also included in the control panel through the use of sliders for the most sensitive parameter values in the model. These sliders default to the settings for each scenario to allow a user to compare how changes to these values alter the model outputs.

In addition to the functionality provided by the modelling control panel, help texts and diagrams have been prepared to provide background information and explanation for the main features of the page (see Section 5.8).

5.7 Unique parts of the design

The unique parts of the design are:

- Two part interface - map and modelling pages take the user from a catchment overview to more focused and complicated modelling processes.
- Viewing live data from different sources - access to data can be a significant barrier for a whole range of user groups, the demo utilises data from five different sources (Environment Agency, Eden DTC, James Hutton, CHASM, BADC) to produce visualisation and run models.
- Combining different types of data together - understanding data outputs for non-scientist users can be challenging. By providing the means to combine different data sources together, such as water quality sondes and webcams, the task of interpreting data can be made more user friendly.
- Development of scenarios for land use and flood risk - the use of scenarios encapsulates some of the complexities of model and parameter setup into descriptions that are more easily understood by people with no, or limited modelling experience. They can be used to demonstrate the linkages between processes in the catchment and effects on water in the stream.
- Dynamic and elastic cloud modelling across two sites in the Eden catchment - rapid, on-demand model runs using a cloud-based model.
- Learning and explanatory materials based on EVO website and as dynamic pop-ups to illustrate how the model represents the landscape - materials developed to facilitate the use of the cloud-based modelling tool for non-specialists.

5.8 Help systems

The help systems in place are:

- Help text and a dynamic cartoon relating a storm event on a hillslope to the discharge seen in the stream are used to illustrate how TOPMODEL conceptually represents hillslope runoff processes (Figure 5.9). The user can mouse over the graph in sequence and view how the rainwater moves through the surface and underground to reach the river. Text is added to explain some of the different concepts incorporated in the model.
- The descriptions of scenarios are provided along with the parameter values used for each scenario and how the parameters represent the changes in process. For example, under the increased woodland scenario, the m parameter - which reflects the how quickly water moves through the catchment - is increased to reflect the greater water storage capacity that woodland land use represents.
5.9 Evaluation
The evaluation process has been an important component of the activities carried out by the work package. Several opportunities were created to raise EVO awareness, gather stakeholder feedback and generate research questions across the three catchments including:

- Three Evaluation Workshops, held in Machynlleth (22 attendees) where several potential EVO end-users attended, including: State government (Countryside Council for Wales), representatives from local environmental groups, e.g. UNESCO Biosphere, Dyfi Woodlands, Centre for Alternative Technology, and the Centre for Public Policy Research, as well as local consultant scientists, environmental artists, residents and a local school teacher. Participants ranged in age from mid-twenties to retirement age.

- Online media, e.g. a Flickr site, twitter account and project website, www.dyfivo.org.uk have been developed, the latter receiving over 1,000 unique visitors.

- Stakeholder Community events, namely the launch of the Dyfi Catchment and Woodland Research Platform (a collaborative research venture between Aberystwyth University and Forest Research) which attracted over 100 scientific and policy making end-users, including the Welsh Government Minister for Environment, and a “Night on the Dyfi” community event attended by over 100 local people, which was sponsored and hosted by the Dyfi Virtual Observatory.

- A short questionnaire survey was carried out with the local residents of Morland village in the Eden to gauge the level of interest in the environment, the types of issues of interest, what questions people had about the environment and, their use of the internet. In total, 37 questionnaires were completed. The survey was not intended to be a representative sample for the village but a snapshot of people’s views. It was also used to recruit people to attend future workshops for the development and evaluation of the local scale EVO demo.

- Development meetings - two meetings in the Morland area during the development phase of the local EVO demo; the first with farmers in June 2011 (Figure 5.10) and the second with local residents and farmers in October 2011.

- Evaluation meetings - four meetings with a range of different stakeholders were carried out from July to October 2012 in the Eden and Tarland. Feedback on the demo development was gathered through a discussion session and questionnaire survey. A copy of the questionnaire used is viewable in the online Annex.

5.10 Issues identified through evaluation
5.10.1 Research Issues
Listening to stakeholder feedback indicates there is a wide range of issues that should be tackled by the EVO. These included:

- biodiversity (including invasive species) and habitat conservation
- river flooding and sea level rise
- climate change and energy security
- food security and natural resource scarcity, including drought
- waste minimisation
- diffuse pollution
- marine health and fisheries

The storyboard developed for the Dyfi reflects this wide range of identified issues. Unprompted, a participant also raised the need to have access to cultural data. This led to several participants widely airing the need for socio-economic data in general to be incorporated
into the EVO platform to allow a 'whole systems' approach.

Furthermore, stakeholders stated the need for the necessary tools to investigate these issues in an integrated fashion. As the EVO demonstration portal currently stands, there is no capacity to integrate flood modelling with diffuse pollution; instead, these modules currently sit side by side. For the EVO platform to genuinely assist the breakdown of 'silto' management of environmental issues, the stakeholder feedback should be heeded. Results from the questionnaire survey show that the 'environmental' issues of interest to the local residents of Morland varied widely. However there were a number of issues raised that many respondents had in common: recycling, wildlife or biodiversity, energy, weather, and climate. A number of respondents also mentioned flooding and water quality, when asked directly about these issues, but levels of concern varied from those who thought it was not a problem for them or their local area, to people who had been directly affected by flooding or felt that there were problems with pollutants getting into the local Beck. A number of environmental questions were raised by the questionnaire respondents, relating to both local, national and international issues, these are summarised in Section 5.10.7. Of those surveyed, 89% had access to the internet either at home, work or through the library, indicating that delivery of environmental information using a web based platform would be able to reach the majority of these people.

5.10.2 Scale of Enquiry

It is clear from stakeholder feedback in Machynlleth that the EVO portal needs to adopt a far more flexible approach to allow inter-scalar enquiries. For instance, one participant asked: "What is a river catchment?" Currently the EVO platform is set up to run enquiries at the river catchment or basin scale, yet the research indicates in this study and elsewhere that river catchment awareness is typically low among citizen audiences. Indeed, the question outlined above, once raised, was echoed across the workshop room. While a simple descriptor could be hot-linked to a "What is a river catchment?" pop up to aid understanding, research indicates that enquiries would be better facilitated if they could be run at any scale chosen by the end-user, e.g. by using a lasso tool to capture their region of interest. Different enquiry scales identified from stakeholders included:

i. neighbourhood, e.g. an individual concerned with their local river's potential to flood and use live data
ii. habitat wide, e.g. Cors Fochno by CCW
iii. river catchment scale, e.g. for users such as the UNESCO recognised Dyfi Biosphere Partnership
iv. at a UK wide scale, as communicated by CAT and PIRC, the Public Interest Research Centre based in Machynlleth
v. a scientist stated the need to take an integrated ecosystem approach, including the whole Dyfi catchment out to the Irish Sea at the Dyfi Platform event.

To emphasise this, the EVO should not assume that local people are solely interested in local issues. Everyone is a local somewhere, and research indicates that potential end-users are interested in all scales, from the local to the global, and the EVO should accommodate this feedback. Further insights from the workshops in Machynlleth include:

- Universal agreement with the EVO aim, i.e. to solve environmental issues;
- No sign-up procedure wanted. This was identified as an unnecessary obstacle. EVO should prompt sign-up only when a user needs to save EVO output to an account;
- Definitely requires functionality for users to immediately search tools, data holdings, etc., upon arrival so that end-users can quickly discern whether EVO meets their user needs;
- Near universal appreciation for jigsaw pieces as a communication tool to convey the EVO's integrative approach;
- Universal agreement that tool options should be made fully available and not dictated by assumed needs, i.e. non-technical users can judge for themselves whether they can or cannot use a tool;
- Mixed feelings were recorded for whether or not a scale should be used to communicate level of difficulty for each tool. To avoid offence, alternatives should be investigated;
- "Learn more" tabs should be universally available and lead to a page that uses both text, visuals and case studies as well as external links to provide ample information to make an informed choice;
- When using a tool, a progress bar should be shown to communicate how many steps are involved to reach the end of their particular enquiry;
- Many communicated the need for a 3D visualisation tool that would use GIS functionality to drape data layers over. This need was identified by both experts and non-experts; and
- Participants appreciated the use of a familiar mapping interface, e.g. Google Earth.

5.10.3 Development Meetings in the Eden

The first meeting focused on the challenges of farming and water quality management in the Eden catchment. Interest was expressed by the farmers in the access to live data being collected as part of the Eden Demonstration Test Catchments project, particularly in relation to water quality and rainfall data. A number of farmers also expressed an interest in hosting monitoring of other environmental variables such as soil moisture and soil temperature that would
also assist them with their farming practices. Issues raised about water-related more to water resources and its cost, as flooding was not perceived to be an issue affecting them directly. Technological ways to improve the efficiency of farming and reduce costs were of interest, such as optimising fertilizer application times. Measures suggested to alter diffuse pollution and water runoff should be cost neutral and allow the farmers to continue to produce food.

The second meeting focused more on the exploration of data, understanding of water processes in the landscape, and the initial development of model scenarios. A discussion of flooding in Morland village using the EA’s flood inundation predictions highlighted that the local knowledge of the residents could be used to ‘ground truth’ these model predictions and help to improve the way the model is set up to run.

A lot of interest was expressed in the ability to look at ‘live’ data from the local stream, with a number of questions raised as a result (see Section 5.10.8). In addition, it was suggested that measurements of soil moisture and rainfall could be helpful and used to provide flood predictions. Interest in alternatives to a web-based platform such as the use of Apps was suggested for when people are away from their computers. Among the attendees, the understanding of rainfall and runoff processes and when to expect flooding in the local area was relatively good. Discussion of scenarios for model development centred around the need for ‘realistic’ representation of current farming practices, ensuring that runoff management measures were proportionate to the area and that low intensity farming or woodland conversion were unpopular due to the adverse economic and social impacts on the rural economy. Increasing woodland in certain areas was a more acceptable alternative. Some scepticism was expressed by some attendees of the usefulness of the availability of the data for them personally:

- What was the use of water quality information for residents?
- If I want to know what the weather is doing I just look out of the window.”

Further environmental questions raised during these meetings are included in Section 5.10.8.

5.10.4 Evaluation Meetings

The results from four evaluation sessions of the local EVOp demo are reported. A wide range of different stakeholders attended the sessions including scientists, representatives from government agencies and charities, land managers, local residents and farmers. After being demonstrated or using the local EVOp demo, attendees took part in a discussion and were asked to fill in a brief questionnaire to gain their feedback. The feedback from all sessions is reported collectively, firstly in terms of the more quantitative questionnaire responses, followed by the main themes and specific issues emerging from the free text responses and broader discussion.

5.10.5 Quantitative Feedback

Figure 5.11 summarises responses to the main questions on the likely usage, ease of use and appearance of the local EVOp demo.

The results from the questionnaire data suggest that the respondents have a mixed perception of the local EVOp demo. Although the total number of responses does not represent a large sample size, there are a greater number of positive than negative responses to questions about interest in using the demo and its appearance. The large number of neutral responses perhaps reflects that the demonstrator, as shown, does not currently meet the needs of those users, which as a pilot might be expected. The potential use of the local EVOp demo was seen more for work as opposed to home purposes, indicating how stakeholders currently view its likely utility.

5.10.6 Qualitative Feedback

A number of very interesting and helpful discussions were held during the evaluation sessions, yielding a
A whole range of suggestions were made for broader enhancements of the local EVOp demo. In particular, it was felt the tools needed a clearer focus and applicability to land management scale decision making, be that a farm scale tool or clearer implications of the impacts of decisions made at the farm level in terms of economic cost or practical changes needed e.g. what is the cost of the topsoil lost per year? How much woodland and where?

The availability of tools specific to land management actions were also suggested, using automated data collection such as sensors for soil moisture to inform a farming activity such as when traversing the land in vehicles would not cause damage.

The concept of bringing together different data sources was widely welcomed, although extension of this was needed to provide for the interdisciplinary data needs of different users and linkages between existing projects to provide evidence for the modelled changes in land management practice. For flooding, examples of case studies suggested are the National Trust Holnicote flood management project, and the Eden Rivers Trust's ALFA project. The ability to utilise historical data to understand the context of current predictions was also suggested as a way to extend the current range of tools. It was indicated that a better understanding of the underlying risks posed by the environment is required in farm business planning. An example was given of being able to demonstrate an increase in frequency of high-intensity rainfall events, relative to the last 50 years. The risks associated with this were not only the ‘end of pipe’ problems of flooding or diffuse pollution risk but also those in medium- to long-term farm planning, such as decisions on crop grown and infrastructure investment, which can ultimately affect environmental outcomes. There is clearly an enthusiasm for the potential offered by the local EVOp demo; however this requires further refinement to translate it into a true decision support tool.

5.10.7 Questions raised by residents

Questions raised by residents include:

- What species were in this area historically?
- Why can't the rivers be dug out like they used to be?
- Why are there restrictions on managing the river?
- Why is there more flooding now?
- Can I get home if the river floods?
- What was the local drainage project in the village for?
- What is being done in the local area?
- What are people in this area concerned about?
- What lives in the river?
- What animals live around here?
- What plant/ animals are in trouble?
- Why aren't the rivers cleared?
- What wildlife is in the Beck?
- Why are there algae in the stream?
- Is there an economic case for wind farms?
- Is our waste really getting recycled? Is landfill a sin?
- Why are they cutting the trees down next to the Beck?
- Why have the starlings been disappearing?
- Will I get flooded?
- Does recycling go to landfill?
- What's the point of recycling?
- Does the salt from the roads affect the fish in the rivers - is it killing them?
- Why are onshore windfarms used?
- Environmental projects - what is going on in my local area?

5.10.8 Questions raised during workshops with residents and farmers

Questions raised by residents and farmers include:
- How high are the nutrient values in Morland Beck?
- How do they compare to other locations?
- Are what we are seeing in the stream legacy effects from farming practices years ago?
- How much N, P, K are we losing?
- What are the monetary values of those losses?
- Can we do something about the manure being washed off the land?
- Do these results depend on what season it is?
- How long does it take for the water to get into the stream after a storm?
- Are there historical water quality data available for any sites in the local area?
- How has the water quality changed since 2000?
- Are we actually in a much improved environment compared to years ago?
- Do we actually need to improve water quality?
- What are the options for controlling the flow of water off farmland?
- What affect does vegetation on the river banks and bed have on the flow of water?

5.10.9 Potential for the future

Overall, there was universal agreement that EVOp has the potential to provide a tool that holds both educational and scientific value. Results clearly demonstrate demand for the EVO at a local scale. The workshop attendees in particular identified the huge benefits from using a ‘cloud’ platform, e.g. accessing data that is not normally available to them, as well as using tools that they do not usually have on their own desktops. Above all, stakeholders saw EVOp as an effective means to taking a whole systems approach to solving environmental issues and would like to see it made available as soon as feasibly possible.

There is a great deal of potential to further develop the local EVOp demo and incorporate some of the additional features illustrated by the storyboard. In particular, to make the outputs from modelling more tangible and potentially useful, the results from the hydrological model need to be fed into a hydraulic model set up for a particular community. This would enable the effects of different land use and land management scenarios to be tested in terms of predicted inundation maps. By linking these maps to socioeconomic data, assessments of the costs and benefits of options could be made, providing the community with information with which to make decisions. It is essential that additional functionality within EVOp is matched by the careful development of supporting material and help features to empower and educate users in how to carry out analysis in a considered way.

At a simpler level, the addition of more data and sensors from within the study catchments or across more locations would expand the geographical range of EVOp, while expansion into other issues such as diffuse pollution would provide more information on specific localities, highlighted by the local community workshops.

In terms of tools, the ability to import and manipulate data, rather than stream an image, would allow more options for how the user can view data at sites and compare data between sites. Creating a greater sense of ownership of EVOp by the wider community is important for its continuation and future success; this may partly be achieved by the development of crowd source tools to enable a wide range of people to contribute to tackling science problems.

5.10.10 Specific opportunity to link sensors and models

Environmental models are essential for understanding processes and creating predictions in the natural environment. However, models usually require a wide range of data in order to generate results. Recent technological advances which allow the potential to capture, transfer and visualise field measurements, are growing rapidly, but, there are many fundamental hydrological and environmental issues to resolve; e.g. scale issues, resolution, data formats and process function.

Models are often built, calibrated and validated with synthetic, incomplete or simplified datasets. The establishment of environmental and virtual observatories is helping to inform us of the past, present and possible future state of watersheds and will supply the tools to quantify and assess the impacts of past and future management through data sensing and visualisation.

There are many different types of environmental data which can be used in models. For example, these data can be quantitative or qualitative, they can be one point measurement or a gridded map; instantaneous or time series based; and data can be a real measurement or a spatially interpreted synthetic map. A vast array of historic environmental data exists in a range of different formats. Traditionally, the most common way to collect data was to physically go out and measure it or have some sort of remote recording device which needs human intervention to download it. In the last century, telemetering environmental sensors started to evolve. For example, in the 1920s the first environmental telemetered data was collected from weather balloons for weather forecasting. The concept of remotely connecting to a sensor and acquiring real time data was starting to grow. However, early forms of telemetry used telephone lines and basic radio communication. With the development of GSM mobile networks, it is now possible to telemeter more
environmental sensors. And, the speed of these networks is also growing, GSM has been superseded by GPRS and GPRS has been superseded by 3G. This is not a trend that will slow down. 4G technology is starting to be rolled out further and our mobile network signal footprint is growing fast globally. Where we cannot access a mobile network, new communication methods and new wireless protocols can be used.

Being able to now access this superfast mobile network allows us to connect to more sensors, download large files faster and access sensors in real time. With the development of newer faster communication methods it will soon be possible to collect larger files at faster speeds from further away.

It is not just communications which are advancing, so too are sensors. For example, over the past decade, the technology behind in-situ water measurements has become more robust and the data is more accurate. It is now possible to gather real time water quality data from local catchments and advise on the status of the channel. However, the advancement of this technology does not necessarily lead to fully automated systems. Sensors will still always need to be calibrated by humans.

New sophisticated sensor networks, which gather more data and transmit it more quickly means that the volume of data collected will be greater. Thus, the amount of data collected is growing and it needs to be archived in meaningful ways. This was highlighted by Google CEO Eric Schmidt when he stated in a speech in 2010 that every two days the amount of information generated is equal to everything that was gathered from the dawn of time until 2003.

It is information that is needed rather than simply data. Therefore the role of the EVO is to inform on what data we have, what it can be used for and how, when linked to EVO tools, it can be used for science or to inform decision making.

There are many applications where environmental sensors are currently linked to forecasting models. For example weather radars are linked to weather forecasting models, and gauging station and rain gauge networks are linked to flood forecasting models. Sensors can be used in real time to help reduce the uncertainty of short term predictions. Obtaining reliable data is vital, but reliable data is expensive to collect.

![Schematic of the EVOp local work package exemplar.](image-url)
For example, not every river in the UK is monitored for flow or level. Therefore some settlements close to unmonitored rivers are not connected to a flood warning system. This is linked to the cost of monitoring these rivers and to the accuracy of model approximating to the local area.

Flow and level measurements are vital for understanding flood characteristics of a river, but also the severity of a flood. However, it is just as important to convey the accuracy of the data and the implication of uncertainty on the results. Equally as important are qualitative forms of data from floods. The concept of ‘crowd sourcing’ using mobile devices is starting to change the way environmental data is collected. Whether it is collecting georeferenced photos of a flood on a mobile device or recording the location of pollution breaches on a blog, this new data source from mobile technology gives a new level of data that can be used. For example, pictures of flood extents can help to calibrate a hydraulic model and therefore reduce uncertainties associated with predictions.

Figure 5.13 highlights a schematic of how the local EVO exemplar functions by bringing together cloud based databases and models along with catchment knowledge (Figure 5.13 - layer 1). Layer 1 exploits existing cloud based resources, tools and models. In the EVO pilot it was shown, using Google Maps, how local communities can gain access to live environmental sensors in their catchment (Figure 5.13 - layer 2). Data from these catchments has been used in cloud modelling allowing stakeholders to better understand future scenarios in their catchment (Figure 5.13 - layer 3). The bulk of the effort is driven by the need to integrate datasets within a common referencing system in forms that make the use of the data clear to the end-user. Computing on the cloud also creates its own range of technological challenges. However, each step forward seems to open up a vast array of potential to link spatial and temporal maps with novel sensor and qualitative data.

The technology behind environmental sensors is still advancing. More sophisticated sensors are being developed that will allow measurement of new environmental parameters in situ (e.g. Phosphate measurement directly being measured in the field more quickly and accurately). The cost of producing sensors is rapidly decreasing as new technologies advance (e.g. a raingauge disdrometer can now be produced for £10) and new low cost telemetry options are becoming available (e.g. 4G network and zigbee wifi communication). With these new developments it will be possible to create low cost dense networks of sensors that produce more accurate environmental data. With this, a new array of database technologies will arise allowing the user to directly connect to the right data source more quickly. Connecting these new data sources directly to models using cloud technology will reduce uncertainty around environmental predictions.
The EU Water Framework Directive has enacted a legislative imperative to ensure all European waters bodies reach ‘good ecological status’ by 2015. Nationally this requires improvements to modelling hydrological quantity and quality in all water bodies and water resources in a more integrated manner and at the same time assess the uncertainties in these predictions. Assessment of uncertainty will be especially important when conducting scenario testing for quantifying likely environmental change (Cloke et al. 2012). Examples of current models that can be run at national scales include G2G (e.g. Bell et al., 2007a and 2007b), which is being used as the basis for national flood forecasting (e.g. Price et al., 2012) and mass balance mixing models of flow and water quality based on monitoring evidence such as SimCAT (Crabtree et al., 2009). However what these models do not allow for is understanding and testing where competing conceptual structures of processes best-predict stream discharge and quality and if this can be related to catchment characteristics.

The EVO project produced national exemplars for both hydrology and biogeochemistry to explore the ways in which cloud-computing could support the development of an integrated modelling framework to deliver ensemble predictions of hydrological and biogeochemical behaviour in catchments for the whole of the UK, and estimate the uncertainties associated with these predictions.

6.1 Hydrological National Exemplar

The national hydrological modelling conducted for the EVOp project is the first of its kind to test competing models of rainfall-runoff structures nationally, and in a comprehensive uncertainty analysis procedure to quantify predictive uncertainties. With regard to the modelling methodology, the model structural exploratory scheme (FUSE) developed by Clark (e.g. Clark et al., 2008) was used. FUSE is to date the most comprehensive tool available to researchers in the hydrological sciences for the exploration and assessment of both model structural and parameter uncertainties in the manner attempted here.

With regard to the geographical scope of the work, FUSE has been applied at catchment scale with almost complete national coverage; that is to say, nearly all of the regularly monitored catchments brought within the NRFA stream gauging network have been included. This extends the modelling assessment far beyond what has been attempted in previous studies for the U.K (e.g. Bell et al., 2007a and b; Arnell, 2011) and reflect the first national scale benchmarking of predictive capability. Taking these points into account, the research is therefore able to demonstrate results not only for individual catchments but also the patterns of model structural performance and parameter uncertainty that emerge across the whole landmass of mainland Great Britain, with the exception of those near-coastal catchments and adjacent areas for which no stream data were made available.

Key questions of interest are:

- What happens when we join up data nationally?
- What happens when we join up modelling nationally?
- What can this deliver in terms of national capability?

The modelling has therefore been aimed at achieving a national picture of the ability to predict streamflow, with the broadest feasible range - so far as this is possible within the National River Flow Archive (NRFA) gauging network of catchment sizes, locations and characteristics. The catchments exhibit differences in flow control and management, such that some are almost wholly natural, whereas others may be highly modified for regulation (for example, by flow controls during floods, or by abstractions for irrigation). In the UK, many catchments will lie somewhere between these two extremes; they are neither wholly natural nor wholly managed. The list drawn from NRFA records comprises 1,454 stream gauge stations in the UK (Figure 6.1), of which 1,403 are in Great Britain and another 51 in Northern Ireland. Catchment sizes range from ~1 km$^2$ to 104 km$^2$, and some catchments are located on offshore islands (the Hebrides, Orkneys and Shetlands).

By including such a wide range of geologies, there is also clear inclusion of the influence of different groundwater and base flow conditions. Thus, many catchments in areas overlying the chalk and other potentially aquiferous rocks will exhibit high base flow
indices (BFI) which define the potential contributions of groundwater; similarly, some catchments in these locations may also exhibit major losses to groundwater, such that runoff is much lower than would otherwise be expected from consideration alone of mean annual rainfall and evaporation from surface topographic features.

In addition to achieving the national coverage outlined above, the modelling seeks to achieve the finest spatial and temporal resolutions - with respect to inputs and outputs - commensurate with the time and resources available. A daily time step has thus been applied in all the calibration work, such that rainfall and evaporation inputs, the stream flow data and the model hydrographic outputs, are all expressed in daily intervals. With respect to the spatial resolution of the input data, rainfall and evaporation are sourced from daily values at 1 km² resolution and then aggregated for each catchment according to the area cut.

Two further aims in the modelling are related to dealing with calibration and prediction uncertainty. In particular, the research seeks to demonstrate the influence and effect of both by specifically including multiple model structures in the calibrations. In this way, not only are the best (and worst) performing model calibrations derived for each catchment according to particular metrics or combinations thereof and through the application of dense sampling in the parameter space, but these calibrations are achieved using a selection of different hydrological model structures. In this way, the best performing structures can also be identified for each catchment and metric, or metric combination. The research therefore highlights how model structural differences affect
model calibration; it also shows how model structural performance varies across space and by catchment.

### 6.1.1 Chosen modelling methodology: conception

FUSE has been developed as a tool to aid identification of the most appropriate model structure to use for a particular problem (Clark et al., 2008; Kavetski and Clark, 2010). The scheme as presently coded applies to a set of lumped catchment models.

An important research question in hydrology is to be able to understand what level of complexity is needed in a conceptual model of rainfall runoff processes to provide useful predictions, given imperfect data and knowledge of catchment behaviour. There is no doubt this will vary depending on the questions being asked of a particular modelling application, and so different types and complexities of models may be needed for different purposes. The work focused on identifying the broader patterns of model prediction capability, and hence benchmarking national capability, whilst recognising that model structures are not perfect and where the catchments themselves may be highly modified and lack critical details that might inform why model deficiencies do or do not occur. Hence, the method embraces the potential for model structural error; and this in turn is likely to vary from place to place (Beven, 2000, 2002, 2007). In this respect, a poor calibration may be caused by major incongruities between the physical properties of the system - the catchment being modelled - and the model being applied to simulate it. There also may be situations where a calibration appears to be good even though the underlying structure is a poor representation of the reality. This may provide "the right answer for the wrong reasons". In addition, there may be many ways in which an acceptable answer may be obtained as defined by good predictive capability, so that the model demonstrates a significant degree of model equifinality (Beven, 2006; Beven and Freer, 2001). The aim of the method, within a comprehensive uncertainty analysis procedure is to aid diagnosis of these possible modelling outcomes, and thereby contribute to understanding of the most appropriate structure or structures to use for a particular application. Moreover, a preliminary study using FUSE to evaluate model structures in an uncertainty analysis framework reveals that individual model performance is different in different regions and no single structure is likely to be 'best' across all catchments (Coxon, 2011). The need to assess for multiple model structures is thus clearly warranted from both theoretical and evidential standpoints.

### 6.1.2 Chosen modelling methodology

The FUSE scheme uses four primary source model structures, all of which have been applied widely and are well respected, these include TOPMODEL, VIC, PRMS and SAC (Clark et al., 2008) (see Figure 6.2). These are all broadly similar in that they incorporate state variables for soil water - in one or more stores - with fluxes which allow the movement of water through the system according to particular process laws. The equations of state and the parameters which are used in them govern the flux rates at any time-step in each model. Solution of the fluxes and updating of state variable quantities is carried out using an implicit Euler scheme, which is considered and demonstrated to be more conceptually and mathematically correct than other schemes typically employed in hydrological modelling (Kavetski and Clark, 2010).

An important feature of FUSE is that the sophistication of the code allows new model structures, here called 'variants', to be formed out of any component of any of the four source models. Thus one variant may comprise components of PRMS and TOPMODEL only, whereas another may use components of TOPMODEL, VIC and SAC, and so on. The mixing of the models' features in this way is not entirely without limit and there are conceptually feasible variants which are not practical to include due to their complexity and the awkward structure of the code needed to run them. Nevertheless, FUSE permits over 1,000 variants to be tested and explored, each with a parameter and equation set controlling fluxes and states in the manner described. One of the most important considerations here is to be able to simulate more than 1,100 catchments for a range of model types and within an uncertainty analysis procedure that allows understanding of the limits of the predictive capability, and to express the uncertainties in the predictions.

### 6.1.3 Acquisition and preparation of data

In order to conduct the calibrations, the main inputs of rainfall and evaporation need to be prepared for each catchment and calibration time period of interest. Likewise the stream flow data from the NRFA records need preparation, and in particular to be examined for gaps or errors in any record which might make it unsuitable for use. A general rule applied initially in the work conducted - the "80-10 rule" - was that in any calibration period, the stream flow record should be at least 80% complete, and the length of any single, contiguous gap in the record no longer than 10% of the total calibration period, excluding the initial warm up. The application of this rule meant that —150 of the stream flow records were unusable.

Rainfall and evaporation input data were provided in mm per day. With respect to the rainfall data provided, this is the daily 1k m² resolution record prepared by the EA and the Met Office. The methodology for the preparation of which is reported in Keller et al., 2006. To use in FUSE, the daily rainfall for each square kilometre cell is first compiled into a time series for that cell, covering the period from 1st January, 1961 to 31st December, 2008, which is the entire data record period provided. The total for each day for a particular catchment is then summed by selecting the source cells (or part thereof where appropriate) relating to the catchment cut area and aggregating all of each day's total for those cells, and then repeating this for the next day, and then the next, and so on, thus forming an equivalent daily time series for the catchment as a whole.
A similar method is applied to the evaporation product, sourced from the UK MORECS records (Hough and Jones, 1997). However, the MORECS data are first provided at 40 km resolution (thus 1600 km² per cell), so the daily time series are first divided into single square kilometres, and these are then aggregated for each cut catchment area in the same way as for the rainfall. It should be noted that throughout the potential evaporation product ("PET") was used from the MORECS data rather than actual evaporation product. The reason being that within each model structure in the FUSE scheme a calculation is made for actual evaporation losses.

Regarding the cut catchments, it was not possible to obtain a product to use (based on the NRFA catchment outlines dataset), so the areas and outlines were calculated from a 50m resolution DEM of Great Britain, resampled from the 5m NextMap data available from NEODC data sources; a similar DEM was obtained latterly for use to cut out the catchments in Northern Ireland. Of 1,403 catchments aimed to be cut in Great Britain, over 1,250 were cut so as to produce areas within +/- 5% of those on the NRFA database, and a further 100 or so to within +/- 10%. Generally, the areas cut and the shapes obtained were judged as acceptable, and the overall extent of catchment coverage - even after removal of those not usable in the first calibrations because of gaps in the streamflow record - was considered more than adequate to satisfy the project’s aim of achieving national hydrological modelling (Figure 6.3).

Regarding the streamflow data, these were all provided in units of mean flow discharge per day, expressed in cubic metres per second. These data were converted to equivalent mm per day, using the areas cut for each catchment, before being used in the FUSE calibrations.

6.1.4 Sampling, model evaluation and model performance metrics

The approach to each set of model simulations follows the same path, namely to begin with a review of the streamflow data to establish the most suitable calibration period. A further restriction made on the calibrations conducted so far is that the usable calibration period should be 10 years long, plus a one year start up period, and should end on or after 31st December, 1998. Thus, the most recent possible calibration period would cover from 1st January, 1999, to 31st December, 2008, with a warm up period from 1st January, 1998; similarly, the oldest acceptable period, based on the same selection method, would cover from 1st January 1989, running to 31st December 1998, with 1997 as the warm up year. These latter requirements were applied so as to ensure the initial set of calibrations conducted extend over comparatively recent periods which may still be considered broadly equivalent with the present in terms of climate, land use, hydrographical response and catchment flow management

Once the streamflow period had been chosen, the rainfall and evaporation data for the same period are also selected from the catchment aggregated datasets.
in order to begin running the FUSE calibration. Further choices required are which model structural variants to apply in the calibration, and how many points to sample in the model parameter space.

For every catchment's results reported, the decision was made after some preliminary testing and exploration to conduct the first set of calibrations using 2,000 sample points per catchment per model. The total number of sample points per catchment is then simply a multiple of the number for each model structure. Also, the sampling scheme is a space-filling SOBOL scheme, similar to a Latin-Hypercube method, and incorporated in FUSE's general program structure; the use of SOBOL is explained in more detail by Clark et al., 2008.

With respect to the model structures of interest, a core aim within EVOp was to demonstrate the effects of evaluating multiple model structural simulations and uncertainty. This has never been demonstrated before in the UK and is only really possible with more powerful cloud computing type resources.

During the model evaluation of each catchment and each of the four model structures, the predicted discharge was compared with the observed. A set of calibration performance metrics were then calculated and were related to each sampled point in the multi-dimensional parameter space.

With respect to calibration there is a wide range of possible metrics that might be used to quantify the calibration adequacy, and these metrics may in turn be split up in different ways, for example by season (Figure 6.7), to provide more discrimination between one performance metric and another, or one catchment and another. The only metrics commented on within this report are the Nash Sutcliffe index ("NS"), the sum of absolute errors ("SAE"), and the Nash-Sutcliffe index of the logarithm of flows ("NSlog"). The method of calculation of the NS and NSlog indices is shown in the online Annex.

These particular metrics have been chosen because they can be used to indicate how well a model has been calibrated, not only to the overall flow record, but...
also with an emphasis on certain flow magnitudes. Thus, the NS index is often found to be particularly good at calibrating for the higher flood flow peaks, whereas the NSlog score is better for evaluating model structures that perform well for low flow periods; the SAE score appears to be a useful measure for assessing general model simulations for the whole period.

With respect to the running of the FUSE scheme, this has been conducted on a high performance computing (HPC) cluster, which is, for the purposes reported here, a closed cloud computing resource. Jobs submitted permit many different catchments to be run at once. In the first main calibration exercise reported here, the run comprised some 8.8 million simulations, and took eight working days to complete on the HPC cluster.

The abstracted output requires further analysis and processing before the data can be presented as usable results for inclusion in scientific literature. Dealing with the SAE metric, the top 5% of results for each model and catchment are considered usable. Although this appears on the face of it to be an arbitrary cut off, it can be considered in an equivalent way to the standard of accepting as significant a probability of 0.05 (i.e. 5%) or lower in a statistical test such as a Student's 't' test. In the same way, the best 5% of NS and NSlog scores are also treated as usable, with the proviso that all such scores must be greater than zero. A feature of NS and NSlog is that the maximum possible score is 1, denoting perfect agreement between the modelled and observed output. Similarly, a score of zero denotes a calibration result that is no better than using the mean flow (or mean of the log flow) for the whole series, which would be of no value in this work. It follows that only scores above zero are used, and these in turn must be within the top 5% of the results (Figure 6.4).

6.1.5 Initial results: examples of spatial presentation and analysis

The procedure of catchment selection and calibration was conducted for all of the catchments satisfying the requirements of the most recent 10 year period selection and after application of the 80-10 rule. The abstracted results were analysed, and can then be plotted to begin to benchmark the national picture of predictive capability for all catchments analysed. Figure 6.4 provides a useful overview of the sorts of results the national hydrological modelling has generated. The results plotted here are from 1,103 catchments, this being the number that satisfied the first calibration period, and the 80-10 rule. Figure 6.5 shows the best NS score for each catchment and model structure from the Monte Carlo simulations, as explained above. The results clearly

(a) all NS output data across the four models. Most of these calibrations must be discarded because any NS score <0 represents a calibration worse than simply using the mean flow.

Figure 4, (a) and (b) Example of FUSE output, the calibration data here being the Nash-Sutcliffe index ("NS") achieved by each of the four main source models - TOPMODEL, VIC, PRMS and SAC - for the catchment of the River Thames at Kingston, stream gauge no. 39001. To aid comparison between the models, the sample points are plotted cumulatively on the x-axis, 2000 points sampled per model structure. See figure text by (a) and (b) for detail.

(b) the same data as in (a) but only showing the acceptable NS score (>0). The calibrations actually used for EVOp purposes are then a subset of these. Note also how performance differences between models are evident.
indicate differences between the best model simulations achieved with each model. It is striking how in closer analysis, the poor performance of some of the models can be related almost immediately to geology or land use characteristics. For example, both TOPMODEL and PRMS do poorly on areas dominated by chalk. More detailed analysis also shows that in many areas a NS score of 0.8 or higher has been calculated. Given that the inputs of rainfall and evaporation have been lumped, sometimes over quite large areas (up to 104 km$^2$ in the case of the Thames at Kingston), and the inputs and outputs are also aggregated to daily periods, such high calibrations scores are considered a very promising start; it will be of great interest to see to what extent these results can be improved upon with further work, for example by trialling other model variants.

The NS score is particularly good for calibrating for the higher flows, so it is of interest to compare results where the calibration metric better-matches the lower flows, using the NSlog score. Rather than showing this for each model individually, the results can also be viewed across the whole model ensemble, showing the best result for each catchment regardless of the model structure used (Figure 6.6).

Likewise, inter-seasonal comparisons are also made possible on the same basis, using the ensemble best result for reach catchment (Figure 6.7).

6.1.6 Single objective versus multiple objective calibration performance criteria

In the example results, only one metric at a time has been considered. However, a broader calibration parameter set for each catchment may be provided by considering multiple performance criteria i.e. using metrics in combination to calculate a more generally applicable set of calibrations across the different metrics or models. For example, it is evident from the contrast between high and low flow performance, in Figure 6.6, and the seasonal differences, in Figure 6.7, that trying to obtain an overall best fit for all seasons and flow conditions will require a degree of compromise. Similarly, when including additional metrics (for example NS, NSlog and SAE in combination) the best parameter values generating the best results for each metric individually may not be those that generate an equivalent best value for the other two metrics.

6.1.7 Other considerations and calibration issues

One aspect of the work conducted to date is that no allowance has been made for catchments departing fundamentally from the conceptual structures shown in the FUSE scheme. In particular, although the four main model structures used in FUSE are immediately applicable to a wide range of soils, geologies and climates, there are difficulties when these are applied to catchments where the flows are strongly affected by groundwater, in particular high base flow indices, losses to groundwater or from abstractions to extra-catchment areas. Abstractions and irrigation are likely to affect overall water balance. If severe this is difficult if not impossible to compensate for by parameter value adjustments alone. Similarly, a catchment may gain water from sources beyond its topographic watershed. For example for industrial discharges or domestic outflows sourced from reservoirs well outside the catchment area. In future work, it would be of great interest to see whether model calibration performance can be improved in the catchments most subject to these factors, for example by trying to take into account recorded abstraction and discharge data where these are available. This of course would be greatly simplified in a full EVOp where such data and models were more directly coupled in a more sophisticated framework than can be achieved in this demo pilot.

Another aspect to consider is the reliability of the flow gauge data itself, irrespective of whether there are groundwater or abstraction factors to account for. The modelling here demonstrates clearly that for many

![Figure 6.5 Best NS scores for each catchment and model structure; results shown for 1,103 catchments, 2,000 sample points per model structure. A score of 1 is a perfect simulation, scores below 0.6 would not be normally classified as good simulations of high flood flow behaviour.](image-url)
catchments, there is no uniquely 'best' model to use for national hydrological modelling; rather the model structure most appropriate for one catchment appears to differ from that most appropriate for another. However, the veracity of this finding may need to be tempered by assessing the value of the calibration datasets. For many of the stream gauges, the data are likely to be at their most reliable when the flows are within bank. However, once the stream or river is in flood, the discharge becomes more speculative, and during large flood events, where the water is well over bankfull, the stream discharges may be seriously in error (either over- or under-estimated). Work is in hand to undertake a review of stage-discharge relationships at various gauges in the UK, to see how consideration of the uncertainties in the stream gauging may affect overall calibration and model structural uncertainties. This work is beyond the scope of the EVOp, but presents an important and potentially valuable opportunity for further scientific research, and one that would also benefit the usefulness of the EVOp.

6.1.8 Northern Ireland

Although stream flow data were provided for 51 catchments in NI, there is no rainfall or evaporation product, equivalent to those for GB that can be used as inputs for the FUSE modelling. This point aside, the catchment cuts have been prepared for Northern Ireland and these can assist with the biogeochemistry national exemplar. Also, if suitable rainfall and evaporation products become available, calibrations using FUSE could be conducted quickly to augment the national hydrological modelling already completed for Great Britain.

6.1.9 Unique science and demonstrations of the hydrological national exemplar

- The first ever full exploration of the national hydrological modelling capability for greater than 1,100 catchments.
- The first ever national assessment of multiple model structures in a closed cloud computing resource.
- The first ever national comprehensive assessment of model uncertainty analysis to understand parameter and model structure uncertainty and predictive capability.
- The first ever national multi-criteria assessment of model simulation performance that explicitly assesses if models are fit for purposes for high flows, low flows and seasonal responses.
- Improvements to the hydrological modelling predictive capability by using a grand ensemble of model structures.
- Ability to extract model structures and parameter sets that are 'behavioural' for simulating 'tailored'

Figure 6: best NS scores contrasted with best NSlog scores, for the entire combined multi-model ensemble and each catchment. These metrics indicate extra detail in the calibration performance, NS being most indicative of a good match of the modelled output with high flows and NSlog of a good match of the model with low flows.
Figure 6.7 Best NS scores for the entire model ensemble for each catchment, contrasting summer with winter performance. The poorer calibrations in the summer in the south, particularly in areas dominated by the chalk, will be noted; similarly the poorer calibrations in winter in Scotland, over the northern highlands, are striking, and are possibly due to snow melt.

- Identify linkages between model structures and parameters to catchment characteristics than can aid regionalisation and predictions in 'ungauged' catchments.

6.1.10 Potential 'near possible' opportunities due to this research

- More explicit coupled linkages between discharge fluxes and the biogeochemistry components to understand the monthly and seasonal dynamics of water quantify and quality fluxes.
- Improve the diagnostics (i.e. understanding model deficiencies to build better models) of model streamflow predictions by explicitly taking into account the uncertainties in the observed data products.
- Develop the first national flood inundation simulation framework that explicitly included the uncertainties in the predicted upstream boundary conditions. This will allow the inundation uncertainties in given flood return periods to be explicitly quantified
- Further increase the spatial complexity of model structures used in analysis to understand the limits of the predictive capability
- Enhance the understanding of highly modified river systems by including the national EA abstractions licence and time series information for the UK (some 22,000 licence agreements) and improve the predictive capability in these areas and lead towards an improved national water resources model of the UK to assess water security issues
- The ability to improve the assessments of environmental change scenarios on water quality and through the biogeochemistry modelling component the associated water quality.

6.1.11 Barriers

- The project has identified the current difficulty in the UK to bring together all the required observational and catchment characteristics to make this modelling possible. This was a considerable time sync and we now have a framework to make any additional simulations relatively easily to achieve
- Although we have been able to demonstrate a multi-model ensemble that includes a comprehensive assessment of uncertainty for >1,100 catchments without a fully implemented cloud computing resource we are still limited in the demonstration we have conducted.
Within a fully functioning cloud computing resource it would have been possible to -

i. Analyse a range of model spatial complexities rather than just 'lumped' conceptual structures;

ii. Run models for sub-daily input-output simulations and therefore better able to capture more convective storm responses;

iii. Run simulations for greater than 10 years to understand multi-decadal model behaviour and trends;

iv. Simulate multiple scenarios of input rainfall uncertainties and thus improve model diagnostics.

6.1.12 References


Kavetski D and Clark MP. 2010. Title: Ancient numerical daemons of conceptual hydrological modeling: 2. Impact of time stepping schemes on model analysis and prediction. Water Resources Research, 46, article number W10511, DOI: 10.1029/2009WR008896


6.2 Biogeochemistry National Exemplar

Nutrient enrichment of water bodies is the single biggest source of water pollution in the UK, generating adverse impacts on the chemical quality and ecological status of headwater streams, lowland rivers, lakes, estuaries and the coastal zone. In order to address the challenge, integrated management is needed of all of the sources which contribute to this flux, and the pathways linking sources within the landscape to the receiving water body. However, development of integrated catchment management strategies in practical terms is limited by the availability of science understanding and knowledge which is transferable between scales and catchments, from data-rich to data-poor areas of the UK.

This exemplar was developed to determine the extent to which cloud computing infrastructure could support the development of national capability in integrated catchment management.

6.2.1 The challenge

Observational data informing process understanding is often generated at relatively small experimental scales, and is not necessarily directly scalable for application at the whole catchment scale without the development of a modelling solution, bespoke for the system under investigation and the data available to drive that model. Policy makers and environmental managers seeking to develop management and mitigation options for impacted systems have had to either

i. fund the development of bespoke modelling and monitoring programmes for each catchment or interest,

ii. use knowledge acquired from inadequate, low resolution catchment monitoring in the catchment of interest or neighbouring catchment, or

iii. use knowledge acquired from high resolution studies in systems which might not be directly comparable with the catchment of interest.

In order to deliver effective understanding of catchment function under environmental change for all UK catchments there is, therefore, an urgent need to develop better mechanisms for the transfer of knowledge and science understanding between data-rich and data-poor systems. The National Biogeochemical Modelling Framework developed under EVO, and supported by cloud computing infrastructure provides an opportunity to address this need.

6.2.2 Limitations of existing modelling approaches

Dynamic modelling approaches, such as the INCA modelling suite for N, P, C and sediment (Whitehead et al. 1998; Wade et al., 2005; Lazar et al., 2010), provide the opportunity to capture the science understanding generated by high resolution research on catchment behaviours at a range of scales, but expert knowledge and high concomitant costs are associated with the calibration of the model(s) to local conditions in each application.

Simpler correlative statistical modelling approaches, such as the Global News model (Seitzinger et al., 2010), can generate visually attractive simulations of catchment behaviour at regional to global scale, but lack a physical basis (or representation of the specific physical conditions controlling functional behaviour in differing environments) and are frequently highly inaccurate and necessarily uncertain, generating a high risk when used to support operational management and policy development (Greene et al., in review).

There is, therefore, a need to develop physically-based modelling approaches that can be run without the need to expert involvement for all areas of the UK, including both data-rich and data-poor or unmonitored catchments that can accurately simulate the likely flux of nutrients to waters within complex landscapes of differing environmental character, and their likely response to mitigation and management under realistic policy scenarios.

6.2.3 The barriers

The national scale biogeochemistry exemplar developed under EVOp directly addressed this challenge, exploring the use of cloud computing to provide a physically-based modelling framework to support ensemble biogeochemical modelling across the whole of the UK to provide predictive capability to quantify nutrient (nitrogen, N, and phosphorus, P) fluxes to inland and coastal waters in the UK, at geographic scales ranging from 4 km² grid to catchment, river basin and UK national scale.

The objective for this exemplar was to demonstrate the benefits of modelling major nutrient cycles, together with uncertainty and scenario analysis for predicting impacts of nutrient mitigation strategies (e.g. land fertilisation intensity and stocking densities), on nutrient flux behaviours to UK waters, within a cloud computing environment. This has delivered cloud-enabled national biogeochemical modelling capability, demonstrating potential to capitalise on extensive national investment in the development of science understanding, data sets and modelling tools to support integrated catchment management, allowing knowledge transfer from data rich to data poor regions. The approach involved (1) the development of a physically-based biogeochemical modelling framework to represent the major geoclimatic regions of the UK, and (2) bringing together, for the first time, national data sets, models and uncertainty analysis into a cloud computing environment, allowing exploration and benchmarking of current predictive capability for national scale biogeochemical modelling.

The sections that follow provide a description of the national biogeochemistry storyboard, proposed user profile, and the methods and analysis undertaken to enable the storyboard in a cloud computing environment, making it accessible to users via the EVOp portal. Visualisation of the outputs and unique features of the work carried out are highlighted, in

Environmental Virtual Observatory

www.evo-uk.org
addition to an account of the user help systems embedded in the portal. Finally, the potential for future cloud-enabled biogeochemical modelling within a future EVO framework, together with the opportunities and barriers to further development, are outlined.

6.2.4 Storyboard and stakeholders
The outline of the storyboard for the national biogeochemistry exemplar is provided in Annex 1. The storyboard was designed to illustrate an example of how and why users may interact with this component of the EVOp. Users identified include Government departments and agencies such as Defra, EA, SEPA, WAG and NIEA who need to know the percentage reductions in N and P flux to waters that are possible using existing policy instruments to address issues such as WFD (EU Water Framework Directive) compliance and OSPAR (Oslo and Paris Convention for the Protection of the Marine Environment of the North-East Atlantic) reporting. In such cases, the user in search of evidence would enter the EVOp portal and chose to explore the ‘Diffuse Pollution’ topic.

A map interface directs the users to select the scale at which they require N and P outputs (e.g. River Catchment, WFD River Basin District, Country, Coastal Drainage Unit, OSPAR or UK). Once the scale has been selected the user moves on to help-enabled web pages that provide options and advice for model and data selection, scenario generation opportunities, and output format until the desired result is achieved (e.g. a map showing N and P flux at a 4 km² resolution across the UK, pie charts showing the percentage composition of sources of N and P flux in a river catchment, or bar charts showing the load of N and P exported to UK waters from each landscape type).

6.2.5 Steps taken in implementation of biogeochemistry national exemplar storyboard
The biogeochemistry storyboard is currently available as a web-based cloud-enabled exemplar in the EVOp portal (reference WP2). Implementation of the storyboard in this form comprised a series of key steps in the pilot: (i) development of a cloud-enabled and interrogable database for the nutrient flux model selected for the exemplar, (ii) implementation of the modelling structure in the cloud and (iii) visualisation of the storyboard as a web interface in the EVOp.

6.2.6 Development of database for macronutrient model application

6.2.6.1 Outline of nutrient model chosen for exemplar in the pilot
The Export Coefficient Model (ECM) (Johnes, 1996) was used in this exemplar to provide initial demonstration of the national capabilities of N and P flux modelling within the EVOp portal (Greene et al., in review). The ECM takes a semi-distributed approach, calculating mean annual total N and total P loads delivered to a water body (freshwater or marine) as the sum of the nutrient loads exported from each nutrient source in its surface topographic catchment. Sources of N and P include diffuse export from differing land cover classes, fertiliser use by crop type, livestock wastes by livestock type and management system, human waste discharges via point sources and atmospheric deposition to land and water within each catchment. The model equation is as follows:

\[ L = \sum_{i=1}^{n} E_i \left( A_i \left( I_i \right) \right) + p \]

where:

- \( L \) = Load of nutrients (N or P)
- \( E \) = Export coefficient for nutrient source \( i \)
- \( A \) = Area of river basin occupied by land use type \( i \), or number of livestock type \( i \), or people
- \( I \) = Input of nutrients to source \( i \)
- \( p \) = Input of nutrients from precipitation/deposition

The ECM approach has been adopted and applied for modelling nutrient pollution worldwide (European Commission, 2002; Matias and Johnes, 2012; Nasr et al., 2012) owing to its relative simplicity and limited data requirements, which are easily accessible from readily available datasets. Although the ECM does not directly incorporate the complex processes involved in simulating nutrient pollution flux (including groundwater pathways for nutrient transport) and requires significantly less data input than process based models, it has good prediction accuracy (Johnes & Butterfield, 2002; Johnes et al., 2007) and is especially suitable for areas where few observed data are available. Therefore, the model tends to meet the needs for long-term nutrient assessment in catchments and nutrient management plans, by providing accurate source apportionment which is scalable from grid to national scale, and transferable from data-rich to data-poor environments (see Section 3a (i)). For these reasons, plus model ownership, the ECM was considered applicable for the EVOp.

The unique parameter values (input and export coefficients) for the ECM were originally developed using field-scale data on land use and management, together with detailed information on sewage waste management and discharges, and rigorously tested against water quality data in two UK river catchments (Johnes, 1996; Johnes and Heathwaite, 1997). That model generated predictions within ± 5% of observed N and P loadings. However, for modelling nutrient flux in multiple catchment types across the UK, and to support national scale policy development, a national biogeochemical modelling framework (geoclimatic region) for the ECM was later developed (Johnes et al., 1996; Johnes and Butterfield, 2002; Johnes et al., 2007). Coefficients for the input and export of sources of N and P were generated for six main geoclimatic regions across England and Wales (Figure 6.8a).

The sub-models represent N and P flux from major geoclimatic units in England and Wales that comprise broadly similar climate, geology, soil type, topography
and natural vegetation cover. These landscape units, therefore, display broadly similar ranges of N and P export/retention potential as a function of hydrologic flow volume, velocity, timing and routing from land to water. The coefficient sets of both N and P have been tested by rigorous multi-catchment application and historical curve fitting to long term water quality records for at least three catchments within each of the six geoclimatic regions, each with a minimum of 10 years of observed N and P data, and a total of 75 catchments across England and Wales (Figure 6.8b). Predictions have given an r² of 0.98 when correlated with observed N and P data. An example of model validation for one site with long-term observational data for TP is given in Figure 6.9 (after Bennion et al. 2005).

![Figure 6.8 Calibration and validation of the Geoclimatic Regions framework for England and Wales (after Johnes et al., 1997; 2007; Johnes and Butterfield, 2002).](image)

![Figure 6.9 Example of model validation. Parameter sets calibrated and validated for Windermere South Basin (a) were applied to input data for Esthwaite Water (b). Model estimates of mean annual TP concentration in inflowing streams, converted to mean annual lake TP concentrations using the OECD (1982) equations linking lake and inflow TP concentrations are compared with observed TP concentrations in each lake (after Bennion et al., 2005).](image)
6.2.6.2 Developing National Biogeochemical Modelling capability through delivery of the revised geoclimatic regions modelling framework, updated and extended to include Scotland and Northern Ireland

The first UK-wide biogeochemical modelling framework (based on geoclimatic regions) was developed for sub-model implementation of the ECM in the EVOp portal, enabling demonstration of national biogeochemical modelling capability within a cloud computing environment. The original geoclimatic region structure, comprising six landscape units in England and Wales (Figure 6.8), was refined during the pilot and extended to comprise nine distinct landscape units across Scotland, England, Wales and Northern Ireland; each geoclimatic region was assigned input and export coefficients for N and P flux from source to water, based on the earlier work of Johnes and colleagues on the source-transfer-delivery pathway for each source type, by geoclimatic region in England and Wales. The distribution and description of the nine revised regions across the UK are provided in Figure 6.10.

6.2.6.3 Methods for delineating the revised geoclimatic regions modelling framework for the UK

Delineation of the nine revised regions involved the first comprehensive use of the British Geological Survey (BGS) Parent Material Model (PMM) data, which was provided by the BGS at a spatial resolution of 50m (Lawley, 2011). These data gave digitised information on the basic foundations of soils, their structure, drainage and geochemistry across the UK. Metrics of slope gradients extracted from a high resolution DEM and gridded runoff data generated from the hydrology National Exemplar (Section 2d (ii)), both at 50 m spatial resolution, were also used for classification. A rule-based methodology was developed to separate out nine distinct geoclimatic units (Table 1 in Annex 1). These rules were based on the characteristics of the three sets of data used, in terms of capacity for N and P export/retention, building on and proving greater clarity to the classification of the original six regions.

First, the characteristics of the original six regions (pink, green, blue, brown, yellow and red) were re-examined and explicit rules for separation better defined (e.g. unambiguous geology, slope and runoff thresholds). A further three regions (olive, orange and purple) were identified as key landscape units, and these were similarly delineated using distinctive features of their landscape and biogeochemical function.

A presumption in the ECM is that the area outlined in the yellow geoclimatic region (Figure 6.10) represents a geoclimatic region in the UK that has the highest potential rates of N and P flux from land to water due to steep slopes, high rainfall and low base flow index. They have the lowest actual (realised) rates of export, however, as these upland moorland peat areas (> 300 m amsl) mainly support low intensity sheep production, and to a lesser extent cattle grazing and are therefore used relatively extensively. This means that despite the high degree of slope, abundance of rainfall generating runoff averaging 1200-2000 mm per year, together with the relatively high proportion of overland flow and near-surface lateral quickflow as a function of thin soils and scarce vegetation that overlie impermeable pre-Cambrian bedrock, the high nutrient export potential of these landscapes is not translated into high nutrient flux rates.

The regions assigned as purple also have high N and P export potential, similar to the coefficients of the yellow regions. However, these landscape units are typically hilly lowland (< 300 m amsl) peat systems overlying impermeable Palaeogene rock that have developed in areas such as estuaries, valleys and other topographic depressions. Poor drainage leads to the area becoming water-logged. Owing to their relative accessibility compared to upland peat areas, the purple regions are subjected to increased agricultural intensity. However, relatively low nutrient export rates occur owing to nutrient retention within the developing peat layers and the tight cycling of any available nutrients within the system. Likewise, the coefficients for the orange regions represent high export potential, but low actual nutrient export rates as a result of peat soils overlying Eocene bedrock in the non-intensive agricultural regions.

Low to moderate N and P flux potential is represented in the coefficients for the flat dry regions of the UK, classified here as brown, despite intensive arable production with associated high rates of fertiliser N and P applications to crops and grass. This reflects the fact that despite a high rate of N and P input to this landscape, the flatness of the topography, the low rates of runoff (< 150 mm per year) and permeable soils generate a low actual rate of nutrient export. In comparison, the model presumes the sensitivity to N and P export is greater in the lowland hilly blue region, which is underlain by permeable bedrock (Chalk, Jurassic Limestone), because of the high rate of N and P input, combined with the higher rate of nutrient export potential generated by steeper slopes, and higher rainfall intensity.

The geoclimatic regions coloured pink have a somewhat similar geographic distribution to the yellow regions, but occur on moderately elevated (< 300 m amsl) acidic soils underlain by impermeable metamorphic bedrock (e.g. Old Red Sandstone). Differences between both regions also include greater export rates for N and P due to the greater intensity of crop and grassland production and higher livestock densities commonly supported in these regions. The accumulation of N and P inputs here are likely to generate a substantial pool of N and P which has potential for export to adjacent waters in wet conditions. Finally, the highest rates of N and P export are predicted for the green and olive regions, representing flat lowland areas with heavy clay soils (green), river alluvium and flat coastal plains underlain by marine or estuarine sediments (olive). These flat, wet, low permeability landscapes are subjected to the highest rates of grassland fertiliser application in the UK, together with the highest stocking densities for
dairy and beef cattle production, which collectively lead to a combination of high N and P input rates and export potential. These regions are most sensitive to the loss of N and P than other regions because of the erodibility and hydrological flow routing traits of heavy clay soils.

6.2.6.4 Preliminary testing of the revised geoclimatic regions modelling framework with external data

The nine revised geoclimatic regions were fully tested using base flow index (BFI) values and catchment descriptions of hydrological catchments monitored in the national river flow archive (NRFA). Catchment boundaries, representative of all nine regions, were overlaid on the geoclimatic regions and the assigned BFI values (ranging from 0-1) were examined for consistency with the newly classified geoclimatic regions. For example, the blue regions coincided with a BFI of > 0.8 and the green regions had a BFI of < 0.3 (where 1.0 is a theoretical 100% baseflow contribution). In addition, BFI values and hydrologic classification data at a 1 km² spatial resolution (data: hydrology of soil types (HOST)) were also used in a similar way for intra-catchment testing of the regions when catchment-based data was not suitable.

However, further testing of the model extension to Scotland and Northern Ireland, through model calibration and validation against long-term and multiple catchment observed N and P data in each geoclimatic region type is still needed, to confirm the suitability of the coefficient ranges for these regions. The ECM also doesn’t take account of groundwater pathways for nutrient transport; these may be important for long-term nutrient assessments, and consequently may need to be accounted for in future iterations of the model. Modelling output from this new framework, as presented for Scotland and Northern Ireland should therefore be viewed as preliminary until validation has been undertaken.

Figure 6.10 Revised geoclimatic region framework, extended to include Scotland and Northern Ireland; the first biogeochemical modelling framework for the UK.
6.2.7 Data for ECM application

The year 2000 was selected for demonstration of the ECM in the EVOp portal. The digital data required for model application were acquired from source, manipulated off-line in ArcGIS v 10 and transferred to a geospatial database for subsequent integration into the EVOp portal infrastructure (see section 3.1.4).

Data for land use and livestock (total number of cattle, pigs, sheep and poultry) in Britain (England, Wales and Scotland) were taken from the Annual Agricultural Census Returns for 2000 at a spatial resolution of 4 km$^2$ grid. The data comprised the area of land used for cereal crops, other arable crops, bare fallow land, permanent grassland, temporary (ley or rotational) grassland, the area of rough grazing land (unfertilised), and the area of woodland/orchards. Corresponding data for Northern Ireland were sourced from the Northern Ireland Agricultural Census 2000. The total number of humans in Britain and Northern Ireland were obtained from respective 2001 census of human population. Atmospheric N deposition across the UK data was sourced from Defra at a spatial resolution of 5 km$^2$. Owing to a deficiency of distributed P deposition data, a predefined value (Johnes, 1996) was adopted.

Additional information (input coefficients) to accompany the input data included values for the average amount of N and P produced per human/livestock unit annually, the nature and extent of sewage treatment facilities/livestock manure handling, fertiliser applications rates to crops and grassland and N fixation (taken from the Survey of Fertiliser Practice), using coefficient ranges previously reported by Johnes et al (2007) and Johnes and Butterfield (2002). In a fully realised application of the model, there would be scope for refinement of these values using spatially distributed data from public utility and Government department data resources, incorporated within the cloud-enabled geospatial database.

6.2.8 Development of a cloud-enabled integrated and interrogable database

The ECM model database was developed at a grid-based spatial scale of 4 km$^2$ across the UK, comprising 63,241 independent grids. Each 4 km$^2$ grid was given a unique identification number and converted to an ArcGIS shapefile. Input parameters (e.g. permanent grass, urban area) were given a unique codename and parameter information was extracted per grid by intersection of the data shapefiles with the 4 km$^2$ grid shapefile. After data population, a shapefile describing the model database and 4 km$^2$ grid boundaries was then overlaid on a shapefile containing the revised geoclimatic region framework (example shown in Figure 6.11). The proportion of each geoclimatic region in each 4 km$^2$ grid was extracted and a percentage composition assigned per grid. The shapefile (model database plus 4 km$^2$ grid boundaries) was then intersected with shapefiles representing the geographic boundaries of various reporting unit (river catchment, WFD RBD, CDU, OSPAR, country). Further columns were created in the model database to indicate the spatial location of each 4 km$^2$ grid with respect to the various reporting units.

Figure 6.11 Example of the 4 km$^2$ gridded dataset overlaying the revised geoclimatic region model framework.
6.2.9 Model implementation in the cloud

Model implementation within the cloud is described in Section (WP2).

Incorporate the new geoclimatic regions typology and the extension of the framework to include both Scotland and Northern Ireland. Scenarios tested represent conditions appropriate under (1) Good Agricultural Practice policy guidance, (2) mitigation measures appropriate to the delivery of reduced diffuse N and P fluxes to support WFD compliance, in addition to those tested under (1), and (3) addition of measures to ensure compliance with the standards required under the EU Urban Wastewaters Treatment Directive (UWwTD) to all sewage sources in the UK. At present UWwTD compliance is only required for larger wastewater treatment works (WwTW) serving a population equivalent greater than or equal to 10,000 persons. The scenario testing suggests that even with all measures in place, a maximum of 58% reduction in P export and 30% reduction in N export would be possible, with the greatest rates of reduction in P export occurring in major urban centres, while the greatest rates of N export reduction occur in rural areas.

Figure 6.12 Examples of the EVO interface - a) Map page - scale selection, b) Model selection, c) Scenario selection, and d) Output selection.

6.2.10 Examples of outputs

Examples of the model output at all scales for N and for P are presented in Figures 6.13 - 6.20. Figures 6.13, 6.14, and 6.15 show model outputs for TP export, TP export from diffuse sources, and and TP export from point sources to inland and coastal waters (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones. Figures 6.16, 6.17 and 6.18 show comparable model outputs for TN, demonstrating the dominance of diffuse sources in the N flux signal nationally. This contrasts with the signal for TP which is more evenly split between diffuse and point sources nationally, but shows significant hotspots associated with urban centres when viewed at 4 km$^2$ grid scale where point sources clearly dominate the TP signal.

Figures 6.19 and 6.20 show the national biogeochemical modelling capability delivered by the cloud-enabled modelling structure for P, and N. This uses the model to run simultaneous, multiple geoclimatic region scale, distributed scenario testing. Scenarios tested are based on those previously reported by Johnes et al. (2007) but extended to incorporate the new geoclimatic regions typology and the extension of the framework to include both Scotland and Northern Ireland. Scenarios tested represent conditions appropriate under (1) Good Agricultural Practice policy guidance, (2) mitigation measures appropriate to the delivery of reduced diffuse N and P fluxes to support WFD compliance, in addition to those tested under (1), and (3) addition of measures to ensure compliance with the standards required under the EU Urban Wastewaters Treatment Directive (UWwTD) to all sewage sources in the UK. At present UWwTD compliance is only required for larger wastewater treatment works (WwTW) serving a population equivalent greater than or equal to 10,000 persons. The scenario testing suggests that even with all measures in place, a maximum of 58% reduction in P export and 30% reduction in N export would be possible, with the greatest rates of reduction in P export occurring in major urban centres, while the greatest rates of N export reduction occur in rural areas.
Figure 6.13 Modelling outputs for TP loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.

Figure 6.14 Modelling outputs for diffuse source TP loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.

Figure 6.15 Modelling outputs for point source TP loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.
Figure 6.16 Modelling outputs for TN loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.

Figure 6.17 Modelling outputs for diffuse-sourced TN loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.

Figure 6.18 Modelling outputs for point-sourced TN loads (kg / ha) across the UK using data for the year 2000. Outputs are shown in order of increasing spatial area, ranging from 4 km$^2$ grids up to OSPAR zones.
Figure 6.19 Modelling outputs for TP loads (kg / ha) based on nutrient management scenarios across the UK using data for the year 2000.

Figure 6.20 Modelling outputs for TN loads (kg / ha) based on nutrient management scenarios across the UK using data for the year 2000.
6.2.11 Unique design features of the biogeochemistry national exemplar

The unique features of the biogeochemistry national exemplar are -

- Revised and tested national biogeochemical modelling framework - novel, developed using high resolution data and for full UK (extended to include Scotland and Northern Ireland)
- Gridded model runs - using % of each geoclimatic region
- Accumulation of gridded outputs to generate output at any scale
- Including Northern Ireland in model runs
- Scenario option - extra feature
- Scenario per geoclimatic region - useful for management purposes
- Combining N and P load with runoff generated from hydrological component of the National Exemplar to generate concentrations
- Pie charts offer source apportionment of load estimates at any scale from 4 km² grid scale to OSPAR reporting unit scale
- Cloud-based computing allows generation of outputs very efficiently, with multiple-scale, multiple-source manipulation available at the touch of a button
- A range of visualisation options are possible, and the structure is designed to accept multiple model types and structures, facilitating the development of national biogeochemical ensemble modelling capability (see below), and fully-coupled hydrological-biogeochemical modelling capability for dynamic modelling of N and P cycling dynamics at sub-annual scale.

6.2.12 Opportunities

A criticism of current ways of working in catchment science and management is that model calibrations are fixed in time, and new data is not used to refine model calibrations, as it is collected. By using the computational power and data-source interconnections that the cloud computing model provides, there is the opportunity to rapidly and continuously re-assess model parameter performance and associated predictive uncertainty. As data-poor areas become richer with targeted monitoring, this new information could be put to rapid use in understanding the system, improving parameterisation of models operating within the framework, and detecting when ‘sufficient’ data has been collected to improve model fit to observed behaviours and reduce the associated uncertainties.

By enabling ensemble modelling of biogeochemical behaviours within the cloud computing environment offered within EVO it will be possible to operate the models within an uncertainty framework, to provide guidance on those priority areas, particularly in data-poor regions, where collection of additional observational data is needed to reduce predictive (and management) uncertainty. This ensures that the measurements that are made have the maximum potential information content for minimal cost.

The large computational resources provided to users through cloud computing create further opportunities for models to be used in innovative ways. For example, the type of modelling approach explored and developed in EVO is typically used as a management decision support tool to predict the likely effectiveness of mitigation measures, and then to develop a catchment restoration plan based on the optimal predicted combination of measures for that catchment. Currently, the number of possible options that can be explored by the user is limited by both model computational time and the user’s perception of which individual or combinations of options will be likely to work for a given site. Through the adoption of Monte Carlo modelling methods, coupled with the computational power available in the cloud, it would be possible to calculate a broad ensemble of complex mitigation scenarios using this and other similarly structured modelling approaches. This ensemble approach has a number of advantages:

- Each mitigation scenario can be ranked against a range of metrics including costs and effectiveness;
- Combinations of actions that may not have been considered can be included in the analysis;
- It is possible to limit the amount of environmental improvement that is feasible without significant alterations to the landscape and system of food production, allowing the user to make choices which improve water quality while also protecting food security; and
- When working with stakeholders, it is possible to show the range of options that have been considered and set stakeholder-suggested options in context with all other potential mitigation approaches, weighing the benefits of each proposed scheme against the costs in terms of water quality and food security.

In the biogeochemistry exemplar the export coefficient model is one possible model suitable for this scale of application, which can capitalise on the enhanced functionality provided by the cloud infrastructure underpinning EVO. It provides the capacity to simulate annual total N and total P export to any catchment outlet, or at 4 km² grid scale for any area of the UK, regardless of relative observational N or P flux data availability. It also provides the capability to apportion sources according to sectoral contributions (point source discharges from sewage treatment works, septic tanks; diffuse source loading from dairy vs beef cattle production, cereal vs other arable crop production, permanent vs temporary grassland). However, it is not the only model which has this capacity. Another opportunity for the development of the EVO National Biogeochemical Modelling Framework is to take the information from the national scale modelling and geoclimatic region modelling framework and use it to inform the parameterisation of spatially detailed models, such as SCIMAP (Reaney et al. 2011, Milledge et al. 2012). SCIMAP is normally applied on a 25 m² grid to catchments and represents the hydrological dynamics at sub-annual scale.

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connectivity and potential nutrient or sediment export. The approach has been successfully tested against both ecological (Reaney et al. 2011) and water chemistry data (Milledge et al. 2012) and is used by both the EA and Rivers Trusts to support the development of integrated catchment management.

The model is normally applied by fitting the pattern of land cover coefficients to an observed spatial pattern of the determinand of interest. Milledge et al. (2012) showed that there are significant differences in the effective land cover parameter in different parts of the UK. These differences could be linked to the national scale models and hence enable a transfer of knowledge to the finer spatial scale. The incorporation of SCIMAP into the portal would create a tool focused on a different set of questions, at a different spatial scale / resolution for a different set of users, and providing an alternative range of functionality and model output capability to the export coefficient model explored within EVO.

6.2.13 International opportunities

Other models developed by teams from Alterra, The Netherlands (de Vries and colleagues), and from the EU JRC (Leip and colleagues) in Ispra, have developed similar types of approaches, with slightly different foci or functionality, for C, N and in one case for P. An example of one of these pre-existing model outputs for N is presented in Figure 6.21, alongside the export coefficient model output for N generated in this programme. While these have been developed for application across the EU-27, and not calibrated to observed data, at least for the UK, they provide an alternative conceptualisation of the rates, and apportionment of C, N and P flux across complex landscapes, typically running at 5 km² grid scale resolution. They also provide enhanced and/or alternative capability options, including simultaneous simulation of both gaseous and aqueous C and N fluxes, together with C and N sequestration under current and future scenarios of land use, land management and climate change.

There is, therefore, a clear opportunity to bring these and other physically-based models into the cloud-enabled National Biogeochemical Modelling Framework to provide increased functionality and ensemble modelling capability. Given the enhanced capacity offered by this cloud-enabled platform, a statistical comparison, and uncertainty analysis function could also be developed, providing the user with the opportunity to derive a comprehensive assessment of:

i. the potential sources of nutrient flux,
ii. the process controls on nutrient flux behaviours in complex landscapes,
iii. the likely range of future behaviours under changing environmental conditions,
iv. a statistical assessment of the areas of agreement and disagreement within the model ensemble, and
v. an estimate of the uncertainties associated with each simulation and the areas (geographically, or in terms of process controls) of greatest disagreement and therefore uncertainty in current conceptual models of C, N and P flux at grid to landscape scale. This opportunity would provide a major step forward in knowledge transfer to the end-user community, and in coupled phase (gaseous, terrestrial, aqueous) understanding of the major biogeochemical cycles to the science, policy and science research communities.

All of these approaches work at an annual time step, averaging ‘typical’ behaviours either in a physical rules-based system to take explicit account of variation in the natural biogeochemical function of differing landscape typologies, or transferring observational data on specific fluxes from each environmental compartment from data-rich to data-poor environments using a rules-based approach.

Another type of approach which, with some adjustment, could be brought into EVO is physically-based dynamic nutrient flux modelling, operating for individual nutrient fractions, and at a sub-annual, typically daily time step. Examples of this type of modelling include the INCA modelling suite developed by Whitehead and Wade (see, for example Whitehead et al., 1998; Wade et al., 2005; Lazar et al., 2010). At present, while this approach has been developed and tested across a wide range of European catchments, each application requires expert knowledge and high resolution observational water quality data to calibrate the model to local conditions. As such, this type of approach has been restricted to application in data-rich systems. However, recent advances in statistical modelling under the USGS SPARROW Modelling programme (SPAtially Referenced Regressions On Watershed attributes) provide an opportunity to bring dynamic biogeochemical modelling capability into EVO.

SPARROW is a mass-balance catchment modelling approach which relates observed water quality to catchment nutrient inputs and other catchment attributes. SPARROW tracks the transport of nutrients from inland waters to the coastal zone, explaining spatial patterns in stream water-quality conditions in relation to human activities and natural processes. From this approach, the model generates parameter values for a range of processes, and produces predictions of long-term average loads, concentrations, and flux rates from each parameter with associated error estimates for all stream reaches within the modelled catchments. Examples of typical model output currently generated for the conterminous USA (a, b) and a major global watershed (the Mississippi; c, d) are presented in Figure 6.22.

If the model were to be constrained to run at geoclimatic region scale in the UK, it could be used to generate optimal parameter ranges from data-rich areas which could be used within the National Biogeochemical Modelling Framework to run dynamic, daily time-step models in data-poor areas, enhancing biogeochemical modelling capability to provide daily time-step ensemble modelling capability for a range of nutrient fractions, within an uncertainty framework. If the model were to be constrained to run at geoclimatic region scale in the UK, it could be used to generate optimal parameter ranges from data-rich areas which
could be used within the National Biogeochemical Modelling Framework to run dynamic, daily time-step models in data-poor areas, enhancing biogeochemical modelling capability to provide daily time-step ensemble modelling capability for a range of nutrient fractions, within an uncertainty framework.

Work to adapt the EVOp National Biogeochemical Modelling Framework approach for application across the conterminous USA would also provide a significant step forward in developing an international exemplar of the extension of physically-based biogeochemical modelling capability internationally. This would allow a wider range of geoclimatic regional sub-models to be developed and tested in another data-rich region, and provide the platform from which to upscale this regional modelling framework approach to provide physically-based nutrient flux modelling in both data-rich and data-poor regions globally. The models are ready to move to this next level, but are currently running on different platforms which are not presently aligned. There is also the clear potential to extend this initially to modelling nutrient fluxes across the EU-27, and to develop a much wider range of functionality within physically-based nutrient flux modelling by comparison and alignment with the pre-existing suite of European nutrient flux models developed by the Alterra and JRC groups. The cloud-enabled modelling framework developed in EVOp provides the necessary infrastructure to support this development.

Figure 6.21 Simulation of N flux to aquatic systems using physically-based regionalised modelling approaches (a) UK national export coefficient model for the year 2000 (this project), and (b) IDEA and INTEGRATOR combined models for EU27, for the year 2002 (Leip et al., 2011).

6.2.14 The barriers

The only significant barrier to the realisation of these opportunities is time and funding to support development of the ensemble modelling capability and, ultimately, for data collection where model parameterisation is limited in data-poor regions. The various groups who own the IP for these models are keen to progress this aspect of the biogeochemical modelling function and have worked on a suite of prior programmes including the European N Assessment (Sutton et al., 2011) and UN SCOPE Global N Cycling programmes (see for example (Alexander et al., 2002; Boyer et al, 2002; Howarth et al., 2012; Johnes and Butterfield; 2002). The European and USA N cycling communities, in particular, are ready to move to the next stage to generate physically-based modelling of N flux from land to inland and coastal waters, from grid to major catchment scale, and within the development of a cloud-enabled platform to enhance the data handling and storage capacity. The only barriers to realising this potential is sufficient funding.

There is the potential to extend this capability to global scale, and the barriers there, in addition to funding, are data availability and access, issues associated with data security, and the engagement of a wider range of international groups. The latter would be developed under the umbrella of the International Nitrogen Initiative. The greater barrier would be associated with data access and security. However, a number of global datasets already exist and are readily available. Progress to overcome this barrier could be made by the adjustment of existing modelling approaches to accommodate specific data availability at Global scale.
6.2.15 References


An exemplar which demonstrated the potential value of the EVO approach to a global-scale science and policy question was developed. It addressed the sensitivity of carbon, water and energy fluxes to current uncertainty in climate projections from the 22 GCMs used in the 4th IPCC Assessment. The IT problems being tackled related to:

- increased accessibility to a large climate change impact model by the terrestrial climate change impacts community;
- increased speed of computing;
- elasticity and auto-scalability.

This global exemplar was intended to develop a third approach to that being developed for the local and national exemplars thus providing an independent exploration of possible futures for EVO. It demonstrates the potential benefits of exploiting developments in other scientific communities (i.e. bioinformatics) and addresses particular challenges in cloud-enabling large, complex models and managing the associated costs.

### 7.1 Science background

General Circulation Models (GCMs) have been the main tool to address issues of climate change. The complexity of these come with two penalties. First, even with the fastest computers, it remains only possible to make a few very selected simulations to investigate a given problem, thus restricting the number of global emissions scenarios that can be tested, and accessibility by the impacts community. Second, there remains a great deal of uncertainty surrounding climate projections. This is in part due to their complexity which needs to be explored and communicated by the impacts community. This is a particular concern for modelling land surface response, given its dual role as a fundamental component of the climate-carbon cycle system, and its direct link to food and water security. For this reason, an intermediate methodology was developed which:

1. emulates climate models,
2. captures the full complexity of land surface models.

This system provides an ability to assess terrestrial ecosystem changes that might be expected in a warming world and of great value to the climate change impacts community. More specifically the “pattern-scaling” methodology is utilised, with the concept being that changes in surface climate, for each month and at each geographical position, are linearly proportional to the amount of average warming over land. In addition, a global thermal energy balance model was built which maps from different pathways in atmospheric greenhouse concentrations to mean global temperature increase over land, which allows scaling of the patterns. This structure is called the “GCM analogue model”, (Huntingford and Cox, 2000) where “analogue” means replication (of the GCM). The analogue model system was developed for Version 3 of the Met Office Hadley Centre GCM (HadCM3; Gordon et al., 2000) linked to the Met Office Surface Exchange Scheme (MOSES; Cox et al., 1998) and the Dynamic Global Vegetation Model (DGVM), called TRIFFID (e.g. Clark et al., 2011; Huntingford et al., 2000). The full scheme was called IMOGEN (“Integrated Model Of Global Effects of climatic aNomalies”) (Huntingford et al., 2010). This system operates relatively quickly, and a full transient simulation between modelled years of 1860 (for pre-industrial times) and year 2100, and for all “land points”, can be undertaken in around 24 hours on the latest processors. However, to sample full climate uncertainty, this work needed to be repeated for climate patterns derived from the full 22 GCMs that contributed to the 4th IPCC assessment and using the enhanced land-atmosphere model which will contribute to the next Unified Model of the UK, namely JULES.

The science aims of the EVOp global exemplar were:

- To deliver a version of IMOGEN-JULES framework with inputs/outputs that are in a format that could be easily operated from a web interface, and driving its operation in a compute “cloud” environment.
- To define a set of scalable climate patterns representing the 22 GCM simulations that contributed to the 4th IPCC assessment, all on a common grid of 2.5°x3.75° spatial resolutions.
To develop a working prototype applying this IMOGEN-JULES framework, within the cloud, to explore the uncertainty bounds of current GCM predictions on change in soil carbon stocks in soil (but with outputs for a wide range of other carbon and water fluxes).

7.2 Steps taken in implementation

7.2.1 Step 1
The first step as in all exemplars concerned the identification of potential end-users to ensure a clear focus to the work carried out within the EVO Pilot. A storyboard was created (see online Annex) to ensure a logical structure to the problem would be completed which addressed a specific need. Two end-users were chosen;

i. A NERC climate change impact scientist interested in the impact of climate projects on carbon fluxes to and from the atmosphere and the implications of uncertainty in climate projections spatially at a global scale

ii. A government department (e.g. DECC) interested in exploring methods of communicating uncertainty in climate projections.

The navigation route they take to explore these questions were identified as being essentially the same.

7.2.2 Step 2
Translation of the storyboard navigation path into EVOp is currently accessed through a "Global" button within "Explore by Location". Eventually, other pathways from the portal home page would be activated (a "Climate Change" option within "Explore by Topic", "Show me the Data" and "Show me the Resources").

This takes the user to a welcome page which provides some information on the model (Figure 7.2):

7.2.3 Step 3
The end-users define an emission scenario through a web portal (Figure 7.3). Options include:

- Ecosystem Variables
  - Carbon: Soil Carbon, Vegetation Carbon, Net Primary Productivity
  - Water: Evaporation, Soil moisture, Runoff
  - Vegetation: Fractional cover of plant functional types (PFTs)

- Dates for model run
  - Absolute 2020, 2050 and/or 2100
  - Relative to pre-industrial 1860

- Output type
  - Data
  - Maps

If the emission scenario has already been run before, the user would be able to access maps held in the model library at no charge. Due to the large amount of data, data is not stored (Figure 7.4).

Currently, years are restricted to 2020, 2050 and 2100 due to resource limitations. A full implementation of the model would enable any year to be requested. After 3-5 days, an email is sent with the information requested demonstrating ~85-90% reduction in computing time which would be required without an EVO cloud solution (each one of the 22 GCM analogue models normally requires 3 days computing time = 66 days).

Figure 7.1 Schematic of accessing IMOGEN runs library or cloud resources using global exemplar. (See folder for original flowchart).
Figure 7.2 Portal welcome page.

Figure 7.3 Select options.
7.2.4 Step 4
Unlike the other EVO exemplars, for this exemplar the emission scenarios to be selected by the users sit on an Amazon EC2 compute node initialised via the ‘Biocloud Central’ web server. The benefits of this are that the amount of continual logging steps and authentication steps are significantly reduced relative to stepping through the Amazon EC2 console. This significant reduction in computing time was made possible through the implementation of Steps 5 - 8.

7.2.5 Step 5
Developing a set of scalable climate patterns representing the 22 GCM simulations that contributed to the 4th IPCC assessment, all on a common grid of 2.5°x3.75° spatial resolutions. This was a major piece of work as all GCMs do not use a common grid and there are many complexities e.g. resolving issues relating to coastal grid squares.

7.2.6 Step 6
These patterns together with JULES and IMOGEN modelling systems were ported to a custom virtual image, CBL-Imogen, based on the CloudBioLinux virtual image. The Amazon EC2 platform was selected as the biggest supporter of open source software. There are costs associated with the use of the Amazon cloud but the computer usage would have exceeded those provided for academic use and there is a cost verse time trade-off. Benefits relative to the use of HPC is greater accessibility and flexibility. CloudBioLinux was used to enable the efficient utilisation of the Amazon cloud resources and exploit the extensive experience from the bioinformatics community using this cloud-managing interface. CloudBioLinux incorporates CloudMan, allowing it to be deployed as clusters of compute nodes. The benefits are an accessible and reproducible cloud environment that enables decentralisation of services and realises a scalable model. A fully functional computer cluster is created on demand that can be scaled depending on the requirements defined by the user (fast but expensive or slow and cheaper). Computers are run in parallel thus increasing speed. Once the model runs are complete, the cluster created terminates and the instances are stopped automatically.

All code is open-course and available in github:
- Imogen Infrastructure Portal: https://github.com/afgane/imogen
- GCM analogue portal: https://github.com/afgane/ghem
- CloudBioLinux: https://github.com/chapmanb/cloudbiolinux

7.2.7 Step 7
Unlike the other EVO exemplars, a free and open source post-processing tool called GrADS to create maps from model output was used in the cloud. This is important for cloud computing as licensing may restrict this kind of deployment. This is also a major step for the climate change modelling scientists who have traditionally used expensive proprietary software approaches. Unfortunately, resources were not available to fully implement this in a dynamic way but the principal has been demonstrated.

Figure 7.4 Access data (for demonstration purposes data is currently provided from the library).
Figure 7.5 Mean soil carbon estimate (kgC/m²), the standard deviation from the ensemble of the 22 GCM analogue models, the minimum and the maximum. Maps indicate the impact of uncertainty in climate projections for soil carbon across the Amazon, Central and West Africa and SE Asia.

Figure 7.6 Mean net primary productivity (kgC/m²/year), the standard deviation from the ensemble of the 22 GCM analogue models, the minimum and the maximum. Again, maps indicate the impact of uncertainty in climate projections lie primarily in the Amazon, Central and West Africa and SE Asia.
7.2.8 Step 8
A series of output maps for emailing to users were designed. This is a cost-effective way of delivering results as maps and parameters are saved, but not the data. This is because storing large datasets in cloud and direct download off the cloud incur an ongoing cost but dispatching over e-mail is free (Figure 7.5).

7.3 Unique selling points of the global exemplar
The following aspects have been tested / explored in the EVOp Global exemplar:

- Cloud-enabling of a large, complicated model to increase accessibility and flexibility in use of computer resources with major reductions in run time from 66 days to 3 days.
- Demonstration of value of use of more commercial cloud providers. Usage would have exceeded public/academic resources and greater flexibility and accessibility than HPC solution.
- Cloud-based web portal using a solution which minimised authentication and verification needs, being the closest to our ideal user scenario.
- Cloud-based post-processing, non-proprietary map visualisation tool.
- Autoscable use of computing resources for cost efficient use of computing time.
- The benefits of using Open source solutions with all code developed for the project available online.

7.4 Future funding / next steps.
Funding to cloud-enable the JULES model under the NERC Big Data initiative has been secured. This builds on the interest raised through the success of this EVO global exemplar. Once completed, this new project will provide greater accessibility to this important model beyond its primary land-atmosphere community.

7.5 References
The Pilot Environmental Virtual Observatory, EVOp, was a proof of concept project to develop new cloud-based applications for accessing, interrogating, modelling and visualising environmental data, by developing local and national scale exemplars. EVOp has demonstrated how cloud technologies can make environmental monitoring and decision making more efficient, effective and transparent to the whole community.

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