BioVeL – Biodiversity Virtual e-Laboratory

Deliverable Report D2.1

State-of-the-art & trends review on biospheric carbon sequestration, ecosystem functioning and valuation, and invasive species management

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Table of Contents

State-of-the-art & trends review on biospheric carbon sequestration, ecosystem functioning and valuation, and invasive species management

Publishable summary

This report reviews the state-of-the-art and research trends for each the three science areas selected for the BioVeL project. The three science areas are: a) biospheric carbon sequestration; b) ecosystem functioning and valuation; and c) invasive species management. For each science area the report addresses: i) the science-policy context; ii) the main scientific questions being addressed in the area; iii) the most relevant research groups, networks and projects; iv) the existing models and methods; v) data source requirements; vi) the typical and most challenging workflows; and vii) web service requirements.

The report concludes that the needs of biodiversity and ecology sciences for new leading-edge integrative IT tools are growing rapidly, while existing, reliable and open web services and workflow management services to fulfill these needs are still scarce. The planned and on-going developments of the BioVeL project, demonstrating the success of the virtual laboratory approach will go a long way towards meeting this need, and will open new perspectives for biodiversity analysis. However several gaps will remain unbridged and there are some constraints as well.

1 Introduction

„The aim of the Biodiversity Virtual e-Laboratory (BioVeL) project is to provide a seamlessly connected environment that makes it easier for biodiversity scientists to carry out in-silico analysis of relevant biodiversity data and to pursue in-silico experimentation based on composing and executing sequences of complex digital data manipulations and modelling tasks. In BioVeL scientists and technologists will work together to meet the needs and demands for in-silico or ‘e-Science’ and to create a production-quality infrastructure to enable pipelining of data and analysis into efficient integrated workflows.” … „Web services, from which workflows can be constructed, are increasingly available, providing access to data of relevance to biodiversity science and analytical software ...” (DoW 2011)

The aim of this report to provide detailed reviews for the three science areas selected for the project.

2 The three science areas identified

„Scientists are pressed to provide convincing evidence of changes to contemporary biodiversity, to identify factors causing decline in biodiversity and to predict the impact, and to suggest ways of combating biodiversity loss. Altered species distributions, the changing nature of ecosystems and increased risks of extinction all have an impact in important areas of societal concern, such as ecosystems services, CO2 sequestration and invasive species management.” (DoW 2011)

The following chapters cover the above mentioned three areas from the cross-sectional viewpoint of science and web service, workflow technology.

2.1 ECOSYSTEM FUNCTIONING & VALUATION

by
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Pelin Yilmaz

2.1.1 Science-policy context

As it is stated in the Millennium Ecosystem Assessment published in 2005 (MEA 2005a) *„Over the past 50 years, humans have changed ecosystems more rapidly and extensively than in any comparable period of time in human history, largely to meet rapidly growing demands for food, fresh water, timber, fiber, and fuel. This has resulted in a substantial and largely irreversible loss in the diversity of life on Earth".* These statements are still as relevant as ever in spite of economy problems. The extensive exploitation of ecosystems has contributed to substantial net gains in economic development (Fig. 2.1-1), but these gains have been achieved at growing costs in the form of biodiversity loss, the degradation of many ecosystems and their human health and well-being related services, and the exacerbation of poverty for considerable groups of people (MEA 2005a, 2005b). As it has been prognosticated by MEA, the accelerated biodiversity loss and degradation of ecosystems can grow significantly worse during the first half of this century due to habitat change, habitat transformation, climate change, invasive alien species, overexploitation and pollution. The challenge of halting biodiversity loss and reversing the degradation of ecosystems while meeting increasing human demands for their services can be partially met under some optimistic scenarios, but these require significant changes in policies, institutions, and practices (MEA 2005a). Others strongly emphasize the necessity to change the way of decision-making surrounding environmental issues, by understanding the importance of biodiversity and ecosystem services, and by making clear the ways that our policy and management choices affect the variety of the goods and services we receive from different ecosystems (Linthurst et al. 2008, Cowling at al. 2008). Considering it from a more global viewpoint, the anthropogenic pressures and growing trends on the Earth's biogeochemical system have reached a scale where safe living of humanity can not be safeguarded in some regions and even at the global scale (Rockström et al. 2009). Far beyond the growing risk of human-induced environmental disasters, there is another emerging threat: the slowly rising shortage of cheap fossil energy and other natural resources, which can enforce a transition process from today's oil-addicted growth economy to a smaller, and more sustainable world economy, which must have to be more cooperative with the Earth's ecosystems (Czúcz et al. 2010). As Global Footprint Network stated recently „… humanity now demands over 50 percent more than what the planet can regenerate. We have entered a global auction, with more people bidding for fewer resources. In this world, managing our use of natural capital — and not overusing it — is the recipe for economic success" (GFN 2011).

The MEA analysis pointed out that „science can help ensure that decisions are made with the best available information, but ultimately the future of biodiversity will be determined by society" (MEA 2005b). At the same time science is required to develop and improve effective tools and sound scientific methods for ecosystem classification, monitoring, diagnostics, valuation, modeling, predicting and ecosystem management technologies, as well as to assess a variety of restoration and trade-off analysis between management options and ecosystem services at even finer (landscape level) spatially explicit resolution (Cowling et al. 2008, Linhurst 2008, Haines-Young & Potschin 2010, Haines-Young et al. 2012). A desired move to sustainable development will require an appropriate mixture of regulations, technology, financial investment, new scientific approach and education, as well as changes in individual and societal behaviour and adoption of a more integrated, rather than conventional sectoral approach to ecosystem management (Palmer et al. 2005, TEEB 2010).

The concept of ecosystem services provides a robust and operative tool for observing, analyzing and communicating the interactions between ecosystems and society. Since the seminal works of de Groot (1992), Daily (1997) and Costanza et al. (1997), the importance of ecosystem services has gained wide recognition and become a mainstream concept in environmental planning and policy arenas including biodiversity conservation, sustainable land and water use, climate change mitigation, ecosystem restoration and the design of green infrastructure. Appropriate understanding of ecosystem services can also inform agricultural, fisheries and forestry policies as well as efforts to address resource efficiency. Ecosystem services can be understood as a key component in the "societal domain → disturbance → environmental domain → ecosystem services → societal domain" feedback cycle, and they are suitable to illustrate narratives and to highlight strategic research directions (Carpenter et al. 2006, Collins et al. 2009, Carpenter et al. 2009, Potschin and Haines-Young, 2011).

As a response to the increasing recognition of the ecosystem service concept, in 2002 the Conference of Parties of the Convention on Biological Diversity (CBD) have agreed to set global targets to achieve a significant reduction in the current rate of biodiversity loss by 2010 (CBD 2002). These targets involved the goal of maintaining the "capacity of ecosystems to deliver goods and services and support livelihoods". Despite considerable efforts and consistent communication there has been only a limited success in achieving CBD's 2010 targets (CBD 2010a, 2010b). After that the tenth meeting of the Conference of the Parties to the Convention on Biological Diversity, held in October 2010, in Nagoya have adopted a revised and updated Strategic Plan for Biodiversity, with its Aichi Targets (CBD 2010b). This inspired the EU to launch a more operative biodiversity strategy to 2020 (EC 2011), which contains 6 mutually supportive targets in support of the headline objective to halt the loss of biodiversity and the degradation of ecosystem services by 2020. Target 2 in particular requires that by 2020, ecosystems and their services are maintained and enhanced by establishing green infrastructure and restoring at least 15% of degraded ecosystems. Recognising the need to improve knowledge of ecosystems and their services in the EU, Member States are expected to map and assess the state of ecosystems and their services in their national territory by 2014. Their activity will be supported by the Commission by initiating research on operationalizing the concept of ecosystem services, their evaluation and mapping[1], and establishing a scienctific

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[1] See EU-FP7 projects: **OPERAS** – *Operational Potential of Ecosystem Research Applications* and **OpenNESS** – *Operationalisation of Natural Capital and Ecosystem Services: From Concepts to real-world Applications*

working group and policy interface on the Mapping and Assessment of Ecosystem Services (MAES).

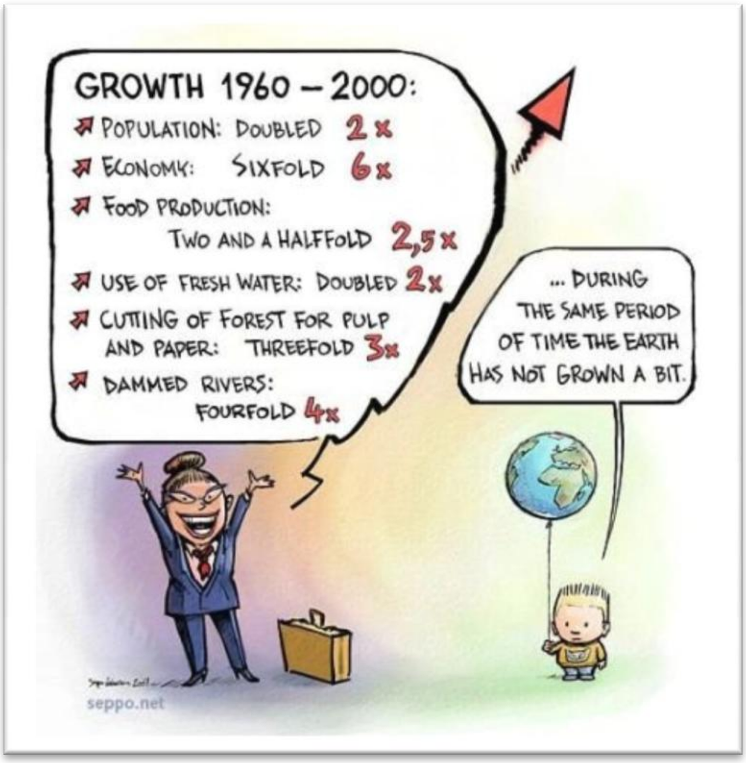


Figure 2.1-1 A cartoon from Seppo Leinonen, Finland (www.seppo.net)

2.1.2 Review on the main scientific questions

There are several schools of ecology which closely influence our current thinking of ecosystems and their services, including: systems ecology (Odum 1983, De Angelis 1992, de Ruiter et al. 2005), landscape ecology (including classification and mapping – Tansley 1935, Whittaker 1970, Grabherr & Kojima 1993, Turner et al. 2004, Cohen et al. 2004), functional ecology (Grime 1977, Grime 2001, Bonan et al. 2002, Lavorel and Garnier 2002, Díaz et al. 2004, Kattge et al. 2011 – plant and vegetation oriented, while Fierer et al. 2007, Simon & Daniel 2009, Fuhrman 2009, Barberán et al. 2012 – are microbiological examples for functional classification and diversity of taxonomic groups difficult to identify as taxonomic species), and the role of biodiversity in ecosystem functioning (Loreau et al. 2001, Hooper et al. 2005, Constanza et al. 2007, Watson et al. 2011, Naeem et al. 2012). Nevertheless, despite a detailed knowledge on several aspects of ecosystem functioning, operative approaches on evaluating ecosystem services and opening them for policy contexts are markedly missing. Notably, the most important scientific challenge is to further deepen our understanding of the links between ecosystem state and human wellbeing, filling the knowledge gaps for all major ecosystems and service types (Fig. 2.1-2). This requires intensive research activity in the development of scientifically sound and easy to measure metrics, modeling frameworks and policy relevant indicators for all major steps of this framework.

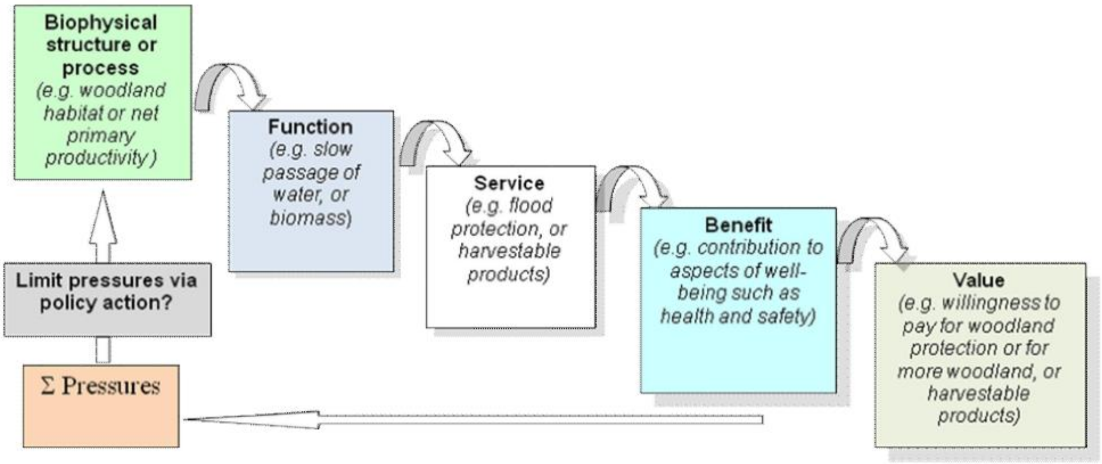


Figure 2.1-2 The ecosystem service cascade framework (Potschin & Haines-Young 2011) applied in numerous global and national ecosystem service assessments, including TEEB (2011)

Considering the current and expected trends of ecosystem science, the main scientific questions can be summarized as follows:

- *What are the trade-offs among different ecosystem functions and services in various ecosystems? How do different management regimes influence these trade-offs and affect ecosystem service supply?*

  The capacity of ecosystems to supply different services is not universal, excessive delivery of a specific service (e.g. firewood) can result in decrease in the supply of other services from the same ecosystem (e.g. habitat provision or erosion control). Human management activities can significantly influence the "service profile" of an ecosystem. Agricultural ecosystems, for example, are managed to maximize supplies of certain provisioning services at the expense of all other services. Pristine ecosystems, on the other hand, generally maximize regulating and supporting services. Most human land management activities can be regarded as optimalizing the supply of certain services at the cost of inputs from external energy (e.g. fossil fuels) and material flows (e.g. fertilizers, pesticides). Nevertheless, all services cannot be maximized at the same time. There are several important trade-offs between the availability of the different ecosystem services (Seidl et al. 2007, Braat & Ten Brink 2008, Cesaro et al. 2008, Haines-Young et al. 2012). Such trade-offs might be obvious at the endpoints of the human disturbance range (i.e. in case of pristine sites and urban/industrial areas), but they are also present and should be expressly considered in any human land use decision. This requires comparable metrics (indicators) for each ecosystem service, to evaluate and optimize land use decisions at any given scale, so that are optimal combinations of land uses could be identified.

- *What kind of direct or proxy indicators can be used to evaluate ecosystem service supply?*

  As with many processes of economic importance, some of the ecosystem service flows can be directly estimated using money as a universal measurement unit (cf. TEEB 2010, Maes et al. 2011). Even though this approach is obviously favourable for policymakers, most ecosystem services (including all regulating and cultural services) do not offer any straightforward and feasible way for monetization. Biophysical indicators of service provisioning capacity and/or socio-economic indicators of the actual use of these services may offer a solution in these cases (OECD 2004, MEA 2005, TEEB 2010). Biogeochemical process models in particular can provide sophisticated quantitative bio-physical indicators which can meaningfully contribute to ecosystem service assessments in data deficient situations (Boyd & Banzhaf 2007, Layke 2009, Mapende 2009, TEEB 2010). Developing appropriate indicators supported by reliable underlying models and data sources are one of the major challenges in ecosystem service assessments.

- *What is the contribution of ecosystem state (including biodiversity and natural capital stocks) to ecosystem service flows?*

  This is one of the major underlying questions which needs to be addressed in order to be able to optimize ecosystem management for ecosystem services. The relationship between biodiversity and ecosystem functioning within environmental constraints has emerged as a central issue in ecology during the last two decades (Loreau et al 2001, Hooper et al. 2005, Naeem et al. 2012). There is no real understanding of the relationships between biodiversity, ecosystem structure, function, and services, even though the contribution of biodiversity to the delivery of services is generally acknowledged (Luck et al., 2009; de Bello et al., 2010). Biodiversity deeply determines several services (e.g. pollination or pest control), whereas other services seem to be less sensitive to biodiversity and depend more on the presence of a small group of species or functional groups (e.g. agricultural products, erosion control, etc). Relationships between variables describing ecosystem status and the capacity of ecosystems to deliver a specific service may be deeply nonlinear. Threshold-type relationships have been demonstrated for some situations (e.g. Scheffer, 2009), but to verify the existence of similar thresholds in more general contexts further research is needed (Groffman et al., 2006). Characterizing ecosystem status with relevant descriptor variables which can either be measured or modeled using available data is also a challenging task. Nevertheless, if we can find such variables and relying on them we can measure/model changes in ecosystem status, then based on an operative understanding of the links between ecosystem status (including biodiversity, internal stocks, thresholds, etc) and ecosystem service flows it will be possible to predict ecosystem service supply for a wide range of scenarios and management options.

- *How large are the variability, dynamic and spatio-temporal variations of the productivity and internal/marginal material stocks & flows of different natural or semi-natural terrestrial ecosystems simulated by a model under various ecological conditions and different management regimes?*

  This is the basic explorative question-complex on which ecosystem field researchers, modellers and related users are working. Most research has focused on net primary production and/or carbon cycle (i.e. Kimball et al. 2000, Churkina et al. 2003, Hasenauer et al. 2005, Schmid et al. 2006, Turner et al. 2007, Ueyama et al. 2010, Chiesi et al. 2011, Hasenauer et al. 2012). Some efforts tried to incorporate different management options (i.e. Merganičová et al. 2005, Tatarinov & Cienciala 2006, Pretzsch et al. 2008) or successional change (Bond-Lamberty et al. 2005). An increasing number of papers apply model simulations to predict effects of climate change on ecosystem functions (Boisvenue & Running 2010).

- *Are there appropriate spatially-explicit methods (models) available for investigating the effects of multiple drivers on ecosystem service supply? Are the existing ecosystem models applied in various local and regional settings sound and reliable?*

  There are a range of spatially-explicit methods of varying complexity which can be utilised for analysing the effects of multiple drivers on ecosystem service supply. These methods range from simple spreadsheet-type approaches, to complex statistical and process-based models (Table 2.1-1). Nevertheless, an operative application of these models in ecosystem service assessments still requires significant research efforts in most cases. There are different methodological approaches to identify the benefits and limitations (including uncertainty) of each method (Beven & Binley 1992, Thornton et al. 2000, Beven & Freer 2001, Ratto et al. 2001, Prihodko et al. 2008, Wang et al. 2009, Hidy et al. 2012). In regional studies the available experimental data are scarce and mostly come from heterogenous sources, so multi-site comparison of different models could provide us valuable knowledge about model constraints (Hanson et al. 2004, Wattenbach et al. 2010).

Table 2.1-1 Models and methods proposed for spatially-explicit assessment of ecosystem service supply within the OpenNESS project

Model	**References**
IMAGE (Integrated Model to Assess the Global Environment)	Bouwman et al. (2006)
GLOBIO (Global Biodiversity Model)	Alkemade et al. (2009)
CLIMSAVE Integrated Assessment Platform (integrated European models covering over 20 ES)	Holman & Cojocaru (2010); Holman & Harrison (2011)
ESTIMAP ES Mapping Tool for the European scale (a suite of ES sub-models for pollination, coastal protection, recreation and water purification)	Maes et al. (2011)
Biome-BGC (a terrestrial ecosystem model which quantifies several key indicators for ES, e.g. carbon sequestration, water retention, etc)	Thornton et al. (2002)
InVEST2.1 (Integrated Valuation of Environmental Services and Tradeoffs)	Tallis et al. (2011)
ARIES v1.0 beta (Artificial Intelligence for Ecosystem Services)	Bagstad et al. (2011)
Methodology for spatial mapping of ES using CORINE, biotope data (SutiGIS), EUNIS habitat classification data, and biodiversity databases	Vihervaara et al. (2011)
EEA Land and Ecosystem Accounting Framework and its extension using expert-based mapping	EEA (2006); Kienast et al. (2009)
Bayesian Belief Networks (BBNs)	Aitkenhead & Aalders (2009); Barton et al. (2008)
State-and-transition models (STMs)	Quétier & Lavorel (2009); Bestelmeyer et al. (2011)
WOFOST (WOrld FOod Studies; A process-based model for the quantitative analysis of the growth and production of annual field crops); FSSIM (a bio-economic farm model for simulating the response of EU farming systems to agricultural and environmental policies)	Boogaard et al. (1998); Diepen et al. (1989); Janssen et al. (2011); Louhichi et al. (2010)
CAPSIS (a platform of several forest models, including Fagacae (even-aged oak forests); Samsarra (mixed uneven-aged mountain forests); Oak-Pine (mixed Sessile oak-Scots pine forests); Sylvestris (even-aged Scots pine forests)	De Coligny et al. (2003); Pérot et al. (2010); Courbaud et al. (2001); Vallet et al. (2009)
SUMO2 (dynamic vegetation succession and carbon sequestration model)	Wamelink et al. (2009)
Yasso07 / GAYA (dynamic soil carbon models); SMART2 (dynamic soil model of the nutrient cycle); GREEN (Geospatial Regression Equation for European Nutrient losses; terrestrial and aquatic retention of nutrients and its monetary valuation)	Liski et al. (2005); Repo et al. (2011); Raymer et al. (2009); Grizzetti et al. (2008); Grizzetti et al. (2005)
SPECIES (broadscale and landscape species suitability, distribution and vulnerability); PROPS (statistical chance of occurrence of plant species and vegetation types)	Pearson et al. (2002); Harrison et al. (2006); Wamelink et al. (2005; 2011).
METAPHOR shaking windows (metapopulation analysis under climate change)	Schippers et al. (2011)
DIMO (dynamic plant species dispersal model); Species dispersal model (landscape probability for dispersal for species dependent on climate and land use)	Greft-van Rossum et al. (2008); del Barrio et al. (2006)
SMALLSTEPS, Maxent Landscape Habitat distribution, Conefor Sensinode 2.2 and GUIDOS (habitat connectivity models and landscape level indicators of structure)	Rooij et al. (2008); Saura & Rubio (2010); Vogt et al. (2007); Philips & Dudik (2008)
LARCH, ECI Plan-it and Stacking tool (models/tools for assessing ES in relation to Green Infrastructure)	Steingröver & Van Rooij (2010)
BioScore (cost-effective assessment of policy impact on biodiversity using species sensitivity scores)	Louette et al. (2010)

2.1.3 Most relevant research groups, networks or projects

Numerical Terradynamic Simulation Group

There are several groups conducting research in global biochemical cycles/global change/ecosystem studies that deserve mentioning. The NTSG (Numerical Terradynamic Simulation Group) at the University of Montana is highlighted here, because in spite of being a US-based research group, their activity has a strong impact on the worldwide scientific community in the field of carbon cycle research. The primary goal of the group is the modelling and monitoring of ecosystem function on multiple scales which include model development as well as providing global, remote sensing based databases. One of their well known projects is the Biome-BGC project, which is the development of a state of the art model to simulate carbon, nitrogen, energy and water storage and fluxes in the ecosystem. They are also involved in the NACP (North American Carbon Program) that is a contribution to the GCP (Global Carbon Project). Besides other remote sensing based global products, the research group focuses on the retrieval and validation of MODIS (Moderate Resolution Imaging Spectroradiometer) land products such as the MODIS Gross Primary Production/Net Primary Production (GPP/NPP) Project (MOD17) which provides global estimates of GPP and NPP for different vegetation types (www.ntsg.umt.edu).

Global Earth Observation System of Systems (GEOSS) and the Group on Earth Observations (GEO)

The goal of GEOSS is to provide decision makers with scientific information that can advance societal benefit areas including human health, ecosystems, climate change and air and water quality. The GEOSS architecture integrates environmental observation, monitoring data and measurements with modeling (www.epa.gov/geoss).

GEO is a voluntary partnership of governments and international organizations. It provides a framework within which these partners can develop new projects and coordinate their strategies and investments. As of March 2012, GEO’s Members include 88 Governments and the European Commission. In addition, 64 intergovernmental, international, and regional organizations with a mandate in Earth observation or related issues have been recognized as Participating Organizations. GEO is constructing GEOSS on the basis of a 10-Year Implementation Plan for the period 2005 to 2015 (www.earthobservations.org/about_geo.shtml).

ALTER-Net – A Long-Term Biodiversity, Ecosystem and Awareness Research Network

ALTER-Net brings together 26 leading institutes from 18 European countries. They share the goal of integrating their research capability to: assess changes in biodiversity, analyse the effect of those changes on ecosystem services and inform the public and policy makers about this at a European scale (www.alter-net.info/about-alter-net)

TEEB - The Economics of Ecosystems and Biodiversity

The TEEB Study is a major international initiative to draw attention to the global economic benefits of biodiversity, to highlight the growing costs of biodiversity loss and ecosystem degradation, and to draw together expertise from the fields of science, economics and policy to enable practical actions moving forward. It produces reports regularly for ecologists and economists, for policy makers, for local and regional policy, for business and for citizens.

The main aims are to synthesize and present the latest ecological and economic knowledge to structure the evaluation of ecosystem services under different scenarios, and to recommend appropriate valuation methodologies for different contexts. It also aims to develop guidance for policy makers at all levels in order to foster sustainable development and better conservation of ecosystems and biodiversity. It enables easy access to leading information and tools for improved biodiversity-related business practice and to raise public awareness of the contribution of ecosystem services and biodiversity towards human welfare, of an individual's impact on biodiversity and ecosystems, as well as identifying areas where individual action can make a positive difference (www.teebweb.org).

UK NEA – UK National Ecosystem Assessment

The UK National Ecosystem Assessment (UK NEA, 2009-2011) was the first analysis of the UK's natural environment in terms of the benefits it provides to society and continuing economic prosperity. The UK NEA has provided new information on the changing natural environment in terms of ecosystems and the range of services that ecosystems provide to people (http://uknea.unep-wcmc.org). It addressed 10 key questions, which are summarised in the Synthesis of Key Findings

- What are the status and trends of the UK's ecosystems and the services they provide to society?
- What are the drivers causing change in the UK's ecosystems and their services?
- How do the ecosystem services affect human well-being, who and where are the beneficiaries, and how does this affect how they are valued and managed?
- Which vital UK provisioning services are not provided by UK ecosystems?
- What is the current public understanding of ecosystem services and the benefits they provide?
- Why should we incorporate the economic value of ecosystem services into decision-making?
- How might ecosystems and their services change in the UK under plausible future scenarios?
- What are the economic implications of different plausible futures?
- How can we secure and improve the continued delivery of ecosystem services?
- How have we advanced our understanding of the influence of ecosystem services on human well-being and what are the knowledge constraints on more informed decision-making?

ARIES – Artificial Intelligence for Ecosystem Services

ARIES is a flexible, integrative modeling platform, which purpose is to make environmental decision making easier and more effective. It capable to incorporates probability models as well as ecological process models, and turns to ad hoc models where appropriate models do not exist or are inadequate for local contexts. It maps the potential provision of ecosystem services (sources), their users (use), and biophysical features that can deplete service flows (sinks) using spatial Bayesian conditional probability models or other existing ecological models (www.ariesonline.org). Actually, the main ecosystem service modeling components are: carbon sequestration and storage (rather simple probabilistic models for source, use, sink and flow); aesthetic viewshed and proximity; flood regulation; coastal flood regulation; subsistence fishery; sediment regulation; water supply and recreation. The recent version of the ARIES platform provides various regionalized models through case studies for five US sites, Dominican Republic and Madagascar (Bagstad et al. 2011).

OpenNESS – Operationalisation of Natural Capital and EcoSystem Services: From Concepts to Real-world Applications; and OPERAs – Operational Potential of Ecosystem Research Applications (upcoming FP7 projects)

Openness and OPERAs are upcoming European collaborative projects under the call FP7 ENV.2012.6.2-1 (“Exploration of the operational potential of the concepts of ecosystem services and natural capital to systematically inform sustainable land, water and urban management”). These proposals are currently (07/2012) in the negotiation phase, and will probably start in late 2012 or early 2013.

The main goal of OpenNESS is to deliver innovative and practical ways of applying the concepts of natural capital and ecosystem services in land, water and urban management in Europe and to examine how they link to, and support, wider EU economic, social and environmental policy initiatives. To this end OpenNESS will develop and refine approaches for mapping and modelling the biophysical control of ecosystem services, and test these methods in concrete, place-based case studies in a range of social-ecological systems throughout Europe and in other parts of the world.

The main goal of OPERAs is to explore, demonstrate and validate mechanisms, instruments and best practices that will serve to maintain and enhance a sustainable flow of a broad range of services from ecosystems. This goal involves developing spatially and temporally explicit metrics and methods to provide operative links between ecosystem function, biodiversity and service provision including biophysical models, quantitative analysis methods of functional biodiversity, and land use change models.

As both OpenNESS ans OPERAs focus on issues that can be potentially addressed with the "ecosystem services" toolkit currently developed in BioVeL, they can be potential users for these BioVeL products.

MAES – EU Working Group on Mapping and Assessment of Ecosystem Services

MAES is an EU working group initiated by the Comission to provide a science-policy interface in support of Target 2 of the EU Biodiversity strategy to 2020. Accomplishing this target requires significant efforts from the member states including mapping and assessing the state of ecosystems and their services in their national territory by 2014. In order to ensure a coherent and successful outcome in all of these activities MAES has the following core tasks and responsibilities: (1) to streamline reporting activities, (2) to perform a scoping study on the available resources, and (3) to provide methodological guidance. MAES activities are not research activities per se but will benefit from ongoing and future related research projects funded by EU and MS including OpenNESS and OPERAs. Nevertheless, the mapping and assessment activities of the EU member states coordinated by MAES may be seen as important potential users of the BioVeL applications.

Metagenomics and the main projects addressed to the microbial domain of ecosystems

The field of metagenomics addresses the function and composition of microbial communities (Handelsman et al., 1998). The main distinguishing feature between metagenomics and genomics, is that metagenomics is concerned with the analysis of DNA from whole communities while genomics is concerned with the analysis of DNA from a single cell or organism.

The field of metagenomics can be broadly subdivided into two distinct categories: 1) whole genome shotgun sequencing (Chen and Patcher 2005), and; 2) single gene surveys (typically directed studies of ribosomal RNA gene).

Using a combination of these techniques, one can gain an overview of the relative abundances of microbial taxa, identifying for example the most dominant species of a complex community in a particular habitat. Furthermore, identifying gene families and placing them within individual pathways can also provide insights into the functional capacity of a community, whilst spatiotemporal approaches to such analyses can provide a complex picture as to the fundamental biogeochemical and metabolic processes being carried out by a particular community. The ultimate goal of metagenomics will be to provide predictive models of microbial ecosystems and the ecosystem services they provide.

A number of studies have involved the comparison of multiple metagenomes from different environments (Tringe et al., 2005; Dinsdale et al., 2008; Delmont et al., 2011). Dinsdale et al. (2008) demonstrated that the prevalence of different functional groups could be used to predict the environmental conditions of each ecosystem. A more recent study by Iverson et al. (2012), demonstrated how ecosystems are shaped by complex communties of unculturable microbes, by reconstructing genomes from mate-paired short-read metagenomes, including an uncultured marine group II Euryarchaeote genome. This represents an important advance as their method allowed for assigning functional ecosystem role to individuals within a community directly from the assembled genomic sequences. Coupled to other techniques that can elucidate active metabolic processes, such as metatranscriptomics (Helbling et al. 2012), we can begin to establish a link between the genotypic traits of an organism and their functional roles. Thus we can begin to connect composition, function and environmental characteristics both at the local and global level making metagenomics indispensible for the future study of ecosystem functioning.

The following projects are relevant:

MicroB3 – Biodiversity, Bioinformatics, Biotechnology

The EU 7FP project Micro B3 (www.microb3.eu) is developing innovative bioinformatic approaches and a legal framework to make large-scale data on marine viral, bacterial, archaeal and protists genomes and metagenomes accessible for marine ecosystems biology and to define new targets for biotechnological applications.

CAMERA – Community Cyberinfrastructure for Advanced Microbial Ecology Research and Analysis

The aim of this project (http://camera.calit2.net) is to serve the needs of the microbial ecology research community, and other scientists using metagenomics data, by creating a rich, distinctive data repository and a bioinformatics tools resource that will address many of the unique challenges of metagenomic analysis. The Project was initiated by the Gordon and Betty Moore Foundation, beginning in Jan 2006.

MG-Rast – The Metagenomics analysis server

MG-RAST server is an automated analysis platform for metagenomes providing quantitative insights into microbial populations based on sequence data (http://metagenomics.anl.gov).

EBI Metagenomics service

The EBI Metagenomics service (www.ebi.ac.uk/metagenomics) is an automated pipeline for the analysis and archiving of metagenomic data that aims to provide insights into the functional and metabolic potential of a sample.

SILVA – Comprehensive ribosomal RNA database

SILVA is a comprehensive on-line resource for quality checked and aligned ribosomal RNA sequence data (www.arb-silva.de).

Megx.net – Marine ecological genomics

Megx.net allows access to integrated environmental and (meta)genomic data intended for use in marine microbial ecology (www.megx.net).

2.1.4 Evaluation of existing models and methods

There is a high number of sound ecosystem models running on stand alone systems, i.e. CASMOFOR (Somogyi 2002-2011), EFIMOD (Komarov et al. 2003), CO2FIX (Schelhaas et al. 2004) as empirical regression-based simulators; SORTIE (Pacala et al. 1993), Biome-BGC (Running & Hunt 1993), BALANCE (Grote & Pretzsch 2002) as ecophysiology based process models; CENTURY Soil Organic Matter agroecosystem model (Parton et al. 1987); LPJ Dynamic Global Vegetation Model (Sitch et al. 2003, Gerten et al. 2004) and many others. According to our present knowledge, nothing of these ecosystem process models have been implemented yet into service oriented architecture (SOA), while few of others mainly focused on estimating some ecosystem service features coupling ecological and economical valuation compartments (Feng et al 2011, Bagstad et al. 2011).

One example of SOA-based model is a prototype web application for dynamic wetland ecosystem service simulation using the Open Geospatial Consortium Web Processing Services standard (OGC WPS). This wetland ecosystem application involves and integrates five submodels for land terrain, evapotranspiration, water surface extent, wetland water table level and waterfowl population density simulations (Feng et al. 2011). The OGC WPS specification (Schut 2007) is a relatively new technology, which is spreading fast in the environmental domain (Čepický & Becchi 2007, Baranski 2008, Brauner 2008, Fenoy et al. 2012). It seems, that ARIES, Artificial Intelligence for Ecosystem Services – one of the most interesting projects – apply OGC WPS standard also (Bagstad et al. 2011). The recently emerged idea of 'Model Web' – models as web services (Geller 2008) also apply OGC WPS standard (Dubois et al. 2009, Jodha 2009, Maué 2010, Duboi et al. 2011). The Web Service Description Language (WSDL) based services coupled to workflow management system is also proving to be a very powerful modeling solution in general (Gil et al. 2007, Collins et al 2009, Ludäscher et al. 2009, Schade et al. 2012).

Due to the science-policy context, the scientific questions selected earlier, and the need of web service implementation of matured and powerful terrestrial biogeochemical model, we concluded to select the Biome-BGC model to build and implement as core for web services, because of its wide acceptance, having great potential and flexibility, open source, good documentation and subject of continuous development.

Biome-BGC

Biome-BGC is a process-based, mechanistic biogeochemical model that can be used to simulate carbon, nitrogen and water fluxes of different terrestrial ecosystems, including evergreen and deciduous forests, grasslands and shrubs (Running and Hunt 1993; White et al. 2000; Churkina et al. 2003; Vetter et al. 2008; Trusilova et al. 2009).

Similarly to other process-based biogeochemical models, Biome-BGC was constructed to simulate plant growth and related biogeochemical processes in environmental conditions that can differ from the past and present circumstances (Kramer and Mohren 2011). Biome-BGC uses state-of-the-art representation of key physiological and biogeochemical processes like initiation and cessation of growing season, photosynthesis, allocation, autotrophic respiration (including growth and maintenance respiration), soil organic matter decomposition, evapotranspiration, nitrogen availability and allocation, and stomatal conductance limitations due to environmental stress factors (Running and Coughlan 1988; Running and Gower 1991; Wang et al. 2005; Vetter et al. 2008; Trusilova et al. 2009). The model explicitly handles the nitrogen cycle which is essential considering the well recognized importance of nitrogen availability in forest growth (Magnani et al. 2007; Ciais et al. 2008; De Vries et al. 2009; Hlásny et al. 2011).

Most recently Biome-BGC was extended to include disturbance and to provide a more detailed description of soil processes, plant phenology and mortality (Di Vittorio et al., 2010; Hidy et al., 2012) and agricultural practices (Ma et al., 2011).

MTCLIM – Mountain climate simulator

The mountain climate simulator is a kind of pre-processing model of Biome-BGC in areas where no meteorological measurements have been taken. It addresses the problems of estimating daily near-surface meteorological parameters from nearby observations (even from several tens of kilometres distant). It is designed to handle the special problems encountered in mountainous terrain, but it is applicable in flat terrain as well. An important advantage is that the output format generated by MT-CLIM fit to the input meterological data requirements of Biome-BGC, so it is easy to build a data processing chain.

The home page of the model at the site of Numerical Terradynamic Simulation Group is www.ntsg.umt.edu/project/mtclim, where one can download version 4.3 and can find the reference publications (Bristow et al. 1984, Glassy & Running 1994, Kimball et al. 1997, Running et al. 1987, Thornton & Running 1999). A further important publication reports on in depth testing of the model over the complex terrain of the Austrian Alps (Thornton et al. 2000).

InVEST - Integrated Valuation of Ecosystem Services and Tradeoffs

InVEST is a family of script tools in the ArcGIS ArcToolBox environment to map and value the goods and services from nature which are essential for sustaining and fulfilling human life. InVEST models are spatially-explicit, using maps as information sources and producing maps as outputs. InVEST returns results in either biophysical terms or economic terms. InVEST models are based on production functions that define how an ecosystem's structure and function affect the flows and values of environmental services. The models account for both service supply and the location and activities of people who benefit from services.

Since data are often scarce, the initial versions of InVEST offer relatively simple models with few input requirements. These models are best suited for identifying patterns in the provision and value of environmental services. With validation, these models can also provide useful estimates of the magnitude and value of services provided (www.naturalcapitalproject.org/InVEST.html).

Measuring (microbial) diversity and functionality

Metagenomic approaches which assess the diversity and composition of organismal assemblages in ecosystems (Amaral-Zettler et al. 2009) are supported by an increasing number of analytical protocols able to break down the genetic profiles of environmental samples into ecologically effective units, i.e. taxonomic clades that correspond to species (Schloss & Handelsman 2005; Caron et al. 2009), as well as to define diversity measures based on genetic information alone (Lozupone et al 2007). Although today the majority of environmental sequencing surveys are still concerned with the composition of biological diversity in a single habitat, comparative studies are becoming increasingly popular (Nold et al. 2010; Lauber et al. 2009, Stoeck et al. 2009). In these cases clustering approaches such as UniFrac (Lozupone and Knight 2005) are typically employed algorithms to assess between-community similarity, also known as beta-diversity. Along with newly developed analytical software such as MEGAN (Mitra et al. 2009), GenGIS (Parks et al. 2009), SONS and and TreeClimber (Schloss and Handelsman 2006a; 2006b), researchers are now able to compare the community structures of habitats across environmental gradients, over geographic distances, or between different habitats (Schloss and Handelsman 2008).

Considering microbial functionality, the community ecology in a given habitat can be described genetically by breaking down the diversity of genes in a metagenome according to their function. In other words, the state of the environment can be inferred from the active genes in a community, i.e. genes involved in dealing with acidification, oxygen depletion (Jayakumar et al. 2009), detoxification (Lavik et al. 2009), heat shock response (Pearson et al. 2010), nitrogen acquisition (Frias-Lopez et al. 2008), and many other processes characteristic for a certain ecological condition. Similar to diversity assessments, ecological assessments also begin to compare the metabolic activities between communities across environmental gradients, over geographic distances, or between different habitats. Exemplary studies are those of DeLong et al. (2006) who demonstrated a gradient of taxonomic composition and metabolic capabilities in a 3000-m range of ocean depths, while Tringe et al. (2005) used environmental genome tags to show the difference in functions encoded by communities of microorganisms in soil, marine, acid mine drainage, and whale fall habitats. These approaches were recently extended to show significant functional distinctions in the microbial and viral communities sampled from nine different habitat types (Dinsdale et al. 2008).

2.1.5 Evaluation of data source requirements for a biogeochemical process model represented by Biome-BGC

Biome-BGC requires three groups of information: geomorphologic and site characteristics, vegetation eco-physiological parameters, and meteorological data.

Geomorphologic and site characteristics include site elevation and latitude, shortwave albedo, total atmospheric deposition of Nitrogen, total biological fixation of Nitrogen, effective soil depth, soil physical characteristics, and atmospheric CO_2 mixing ratio. Those input data can be acquired from specific databases but there are not too many data sources available, and there is no generalizable solution to provide these characterstics. Here we simply refer to Vetter et al. (2008) for a typical example on the estimation of site characteristics.

Similarly, there is no universal solution for the ecophysiological parameterization of Biome-BGC. White et al. (2000) provides default parameter values for typical terrestrial ecosystems (deciduous and evergreen forests, grasslands, shrubs). However, as it is proposed by the developers of the model, the ecophysiological parameters should always be provided by the users of the model for local applications. Some of the parameters can be measured on the field (allocation, carbon/nitrogen ratio of plant compartments, etc.), but there are many situations when direct measurement of the parameters are not possible. The parameters can also be estimated using model-data synthesis (or in other words, model-data fusion, or calibration) using mathematical methods (see e.g. Trusilova et al., 2009; Wang et al., 2009; Hidy et al., 2012). Model-data synthesis has many associated problems (see Hidy et al., 2012) but in many cases there is no alternative to using this method. We note that in some cases development of the model logic (structural improvement) is crucial to get meaningful parameter estimations (Hidy et al., 2012).

Considering the meteorological data requirement of the model, there are a large number of possible data sources that can be used. As the availability of meteorological data is crucial for the estimation of the past and future evolution of the carbon balance, species composition, invasive species distribution and many other issues that are related to the BioVeL project and biodiversity in general, here we provide a detailed description of the possible data sources of past, present and future meteorology. We do it so because there is no similar documentation available on data availability for the public. The description might be useful for the ecological niche modelling performed within BioVeL as well.

2.1.5.1 Past and present weather

Data from national meteorological services

Standard meteorological measurements are routinely performed worldwide by the national meteorological and hydrological services. The measurement network provides the highest possible quality meteorological data based on regularly calibrated, professional equipment (thermometers, rain gauges, humidity sensors, etc.). In some regions of the World the measured data are freely available to the public, but in some regions (e.g. in Europe), the data is (generally) not available for the research community. Meteorological measurements typically provide information about air temperature at 2 m height, wind speed at 10 m height, atmospheric pressure at surface level, precipitation amount from 6 UTC to 6 UTC in the consecutive day, and relative humidity at 2 m height. Biome-BGC mainly uses temperature and precipitation data, which are the most common parameters.

National meteorological services might further process the measured data to provide homogenized time series for selected meteorological parameters (homogenization means accounting for instrument change, dislocation of the meteorological station and other effects). National meteorological services might implement sophisticated methods for data interpolation (Lakatos et al. 2008).

Data availability changes from country to country, so no further description is given here about the specific national meteorological and hydrological services.

Point data from international data sources

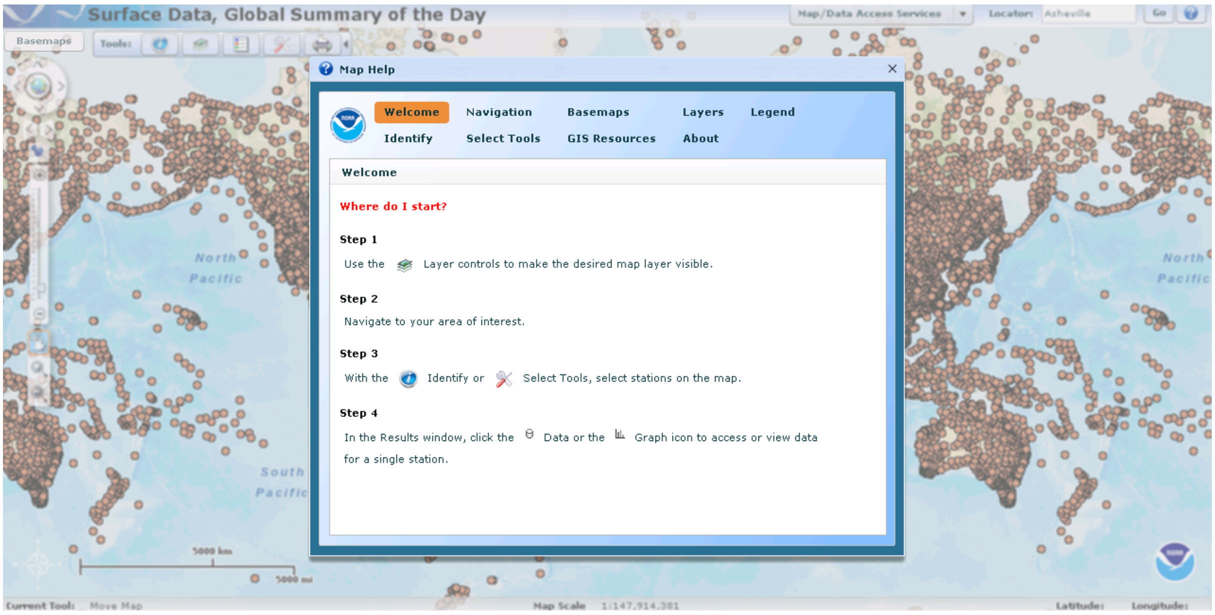
In several countries meteorological activities are coordinated by the World Meteorological Organization (www.wmo.int/pages/about/documents/WMO990.pdf). WMO organizes worldwide data dissemination as numerical weather prediction heavily relies on measurements made in separate countries. According to WMO Resolution 40 (www.wmo.int/pages/about/Resolution40.html) some specific data measured by the national meteorological and hydrological services are freely available to the research community (for non-profit purposes). Those data are available for the public at the website of the National Oceanic and Atmospheric Administration (NOAA), National Environmental Satellite, Data, and Information Service (DESDIS) National Climatic Data Center (NCDC), as part of the Global Surface Summary of Day (GSOD) database (www.ncdc.noaa.gov/cgi-bin/res40.pl?page=gsod.html).

Users that accept the conditions of WMO Resolution 40 can have quick access to meteorological measurements made by several weather stations worldwide.

According to the documentation at the NOAA NESDIS NCDC website, GSOD provides the following meteorological parameters (with units and numerical precision; www.ncdc.noaa.gov/cgi-bin/res40.pl):

- Mean temperature (0.1 Fahrenheit)
- Mean dew point (0.1 Fahrenheit)
- Mean sea level pressure (0.1 millibar)
- Mean station pressure (0.1 millibar)
- Mean visibility (0.1 miles)
- Mean wind speed (0.1 knots)
- Maximum sustained wind speed (0.1 knots)
- Maximum wind gust (0.1 knots)
- Maximum temperature (0.1 Fahrenheit)
- Minimum temperature (0.1 Fahrenheit)
- Precipitation amount (0.01 inches)
- Snow depth (0.1 inches)
- Indicator for occurrence of Fog, Rain or Drizzle, Snow or Ice Pellets, Hail, Thunder, Tornado/Funnel Cloud

NOAA NESDIS NCDC also provides a GIS-based data selection tool for GSOD: http://gis.ncdc.noaa.gov/map/gsod/. Using the GIS tool users can easily extract data for their locations of interest. The figures below demonstrate the data selection mechanism (Fig. 2.1-3 and 2.1-4).



Welcome

Where do I start?

Step 1

Use the Layer controls to make the desired map layer visible.

Step 2

Navigate to your area of interest.

Step 3

With the Identify or Select Tools, select stations on the map.

Step 4

In the Results window, click the Data or the Graph icon to access or view data for a single station.

Figure 2.1-3 Start page for the GIS-based data selection at GSOD

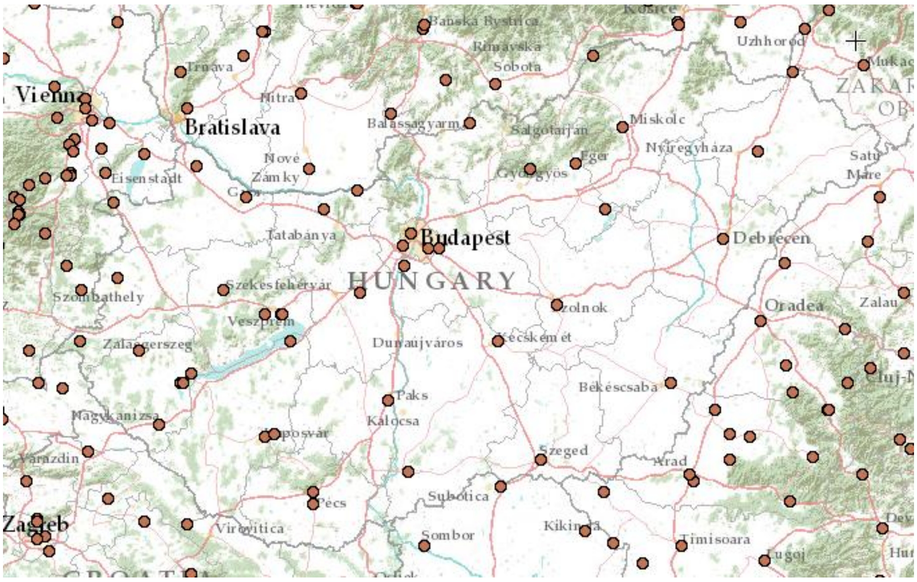
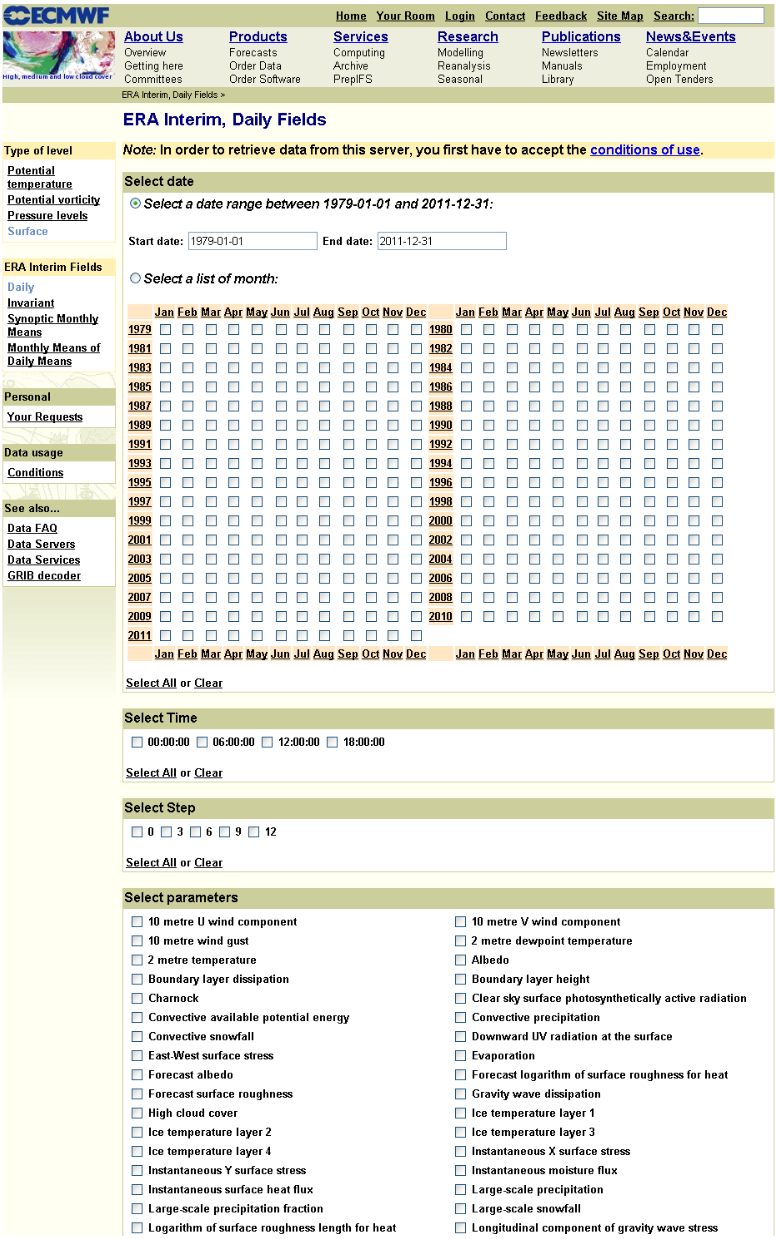


Figure 2.1-4 Map of the stations in Hungary that provide or provided data to GSOD

Daily maximum and minimum temperature and precipitation amounts are generally available from GSOD for many stations. It means that after unit conversion those data can be used as input to Biome-BGC. The files are available in ASCII format.

Data from meteorological reanalyses

In meteorological terminology *analysis* means the reconstruction of the state of the atmosphere in 3 dimensions (at the surface, and also vertically) at a given time (including temperature, wind speed, atmospheric pressure, moisture content, cloud coverage and many other meteorological parameters). Meteorological analysis is an important step in numerical weather prediction (and in general, in weather forecast). Analysis is based on measurement data (surface measurements, upper air soundings by radiosondes, satellite readings, etc.) and background information from previous simulations made by numerical weather prediction models (Dee et al., 2011).



ERA Interim, Daily Fields

Note: In order to retrieve data from this server, you first have to accept the conditions of use.

Select date

● *Select a date range between 1979-01-01 and 2011-12-31:*

Start date: 1979-01-01 **End date:** 2011-12-31

○ *Select a list of month:*

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1979	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1980	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1981	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1982	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1983	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1984	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1985	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1986	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1987	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1988	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1989	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1990	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1991	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1992	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1993	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1994	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1995	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1996	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1997	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	1998	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
1999	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2000	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2001	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2002	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2003	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2004	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2005	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2006	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2007	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2008	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2009	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	2010	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
2011	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐													
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec

Select All or Clear

Select Time

☐ 00:00:00 ☐ 06:00:00 ☐ 12:00:00 ☐ 18:00:00

Select All or Clear

Select Step

☐ 0 ☐ 3 ☐ 6 ☐ 9 ☐ 12

Select All or Clear

Select parameters

☐ 10 metre U wind component	☐ 10 metre V wind component
☐ 10 metre wind gust	☐ 2 metre dewpoint temperature
☐ 2 metre temperature	☐ Albedo
☐ Boundary layer dissipation	☐ Boundary layer height
☐ Charnock	☐ Clear sky surface photosynthetically active radiation
☐ Convective available potential energy	☐ Convective precipitation
☐ Convective snowfall	☐ Downward UV radiation at the surface
☐ East-West surface stress	☐ Evaporation
☐ Forecast albedo	☐ Forecast logarithm of surface roughness for heat
☐ Forecast surface roughness	☐ Gravity wave dissipation
☐ High cloud cover	☐ Ice temperature layer 1
☐ Ice temperature layer 2	☐ Ice temperature layer 3
☐ Ice temperature layer 4	☐ Instantaneous X surface stress
☐ Instantaneous Y surface stress	☐ Instantaneous moisture flux
☐ Instantaneous surface heat flux	☐ Large-scale precipitation
☐ Large-scale precipitation fraction	☐ Large-scale snowfall
☐ Logarithm of surface roughness length for heat	☐ Longitudinal component of gravity wave stress

Figure 2.1-5 Web interface for data download from the ERA Interim database (http://data-portal.ecmwf.int/data/d/interim_daily)

Analysis fields represent the state of the atmosphere in a physically consistent manner and are the results of an optimization procedure (called data assimilation). During the years the mathematical methods used for meteorological analysis improved substantially (Dee et al., 2011). In the same time computer resources increased significantly, which enabled the application of more sophisticated data assimilation techniques. These developments led to the need to re-analyze the archive meteorological measurements in a unified way using the most up-to-date methodology. In this sense meteorological reanalysis is a database about the state of the atmosphere for a long time period (typically several years or decades).

There are a number of reanalysis projects that can be used for scientific purposes. A good summary can be found at the website of Reanalysis Intercomparison and Observations (www.reanalyses.org). Well-known reanalysis projects are the NCAR/NCEP reanalysis (Kalnay et al., 1996), the ERA-40 reanalysis (Uppala et al., 2005), and the ERA-Interim reanalysis (Dee et al., 2011) (Fig. 2.1-5).

Some of the reanalysis projects have coarse spatial resolution (e.g. NCAR/NCEP reanalysis have 2.5×2.5 degree resolution) which means that they are not suitable to estimate meteorological parameters of small regions. Most recent reanalysis projects like ERA Interim might provide suitable input data for Biome-BGC. The open access web-interface of ERA Interim (http://data-portal.ecmwf.int/data/d/interim_daily; Fig. 2.2-5) only provides data at a relatively coarse resolution (1.5×1.5 degrees), but finer resolution (~0.5×0.5 degrees) data can be accessed via national meteorological services (if they are member states or cooperating states of the European Centre for Medium-Range Weather Forecasts (ECMWF; http://ecmwf.int). Reanalysis data might be used to get improved estimations of daily minimum/maximum temperature, global radiation or vapour pressure deficit for larger regions. Precipitation estimations can be retrieved from the reanalysis databases, but they are generally based on short range weather forecasts, and are not based on direct precipitation observations. It means that the quality of precipitation data from reanalysis projects is questionable. Biome-BGC users might consider choosing alternative precipitation data sources for the simulations (see below).

Note that meteorological data provided by short range weather forecasts (provided e.g. by ECMWF) can also be used as meteorological input to the model, but they suffer from the same, precipitation related problem as described above. The advantage of the short term weather forecast data is its higher spatial resolution (see e.g. www.ecmwf.int/publications/cms/get/ecmwfnews/1264512002630).

The reanalysis data is available in GRIB (GRIdded Binary) format, which is a common data standard used by meteorologists and oceanographers. Alternatively, the data can be retrieved as NetCDF (Network Common Data Format) files.

Gridded meteorological data (WorldClim, CRU, E-OBS)

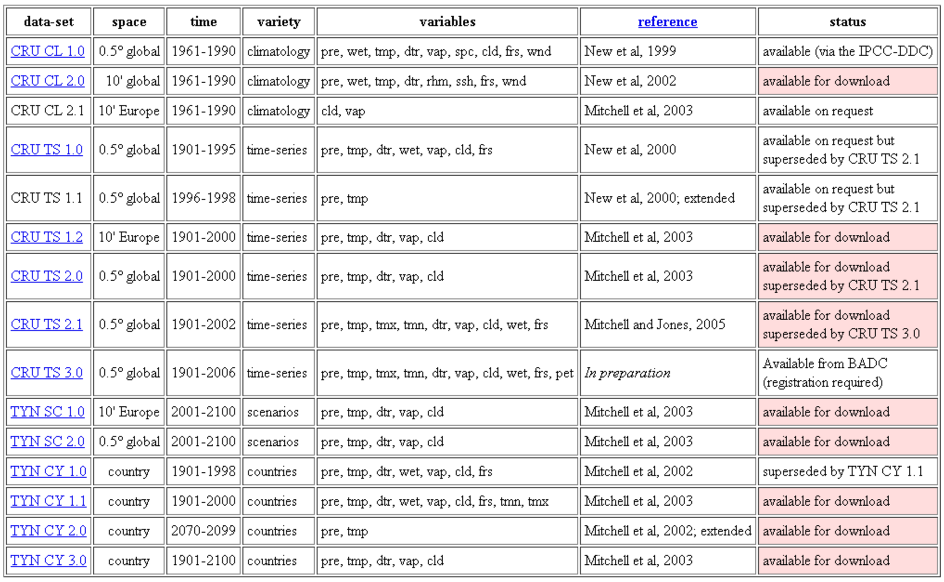
Point measurements (see above) are only available at selected locations with (generally) limited spatial representativeness. Limited spatial representativeness means that it is not trivial to get information for other locations that can have different climate characteristics due to topography or atmospheric circulation patterns. Spatially representative datasets overcome the problem posed by the point measurements. Reanalysis provides data in a regular geographical grid where the data is meant to represent average conditions for the entire grid cell. It means that reanalysis data has larger spatial representativeness. However, as we shown above, reanalysis data can not be considered as measured data since it is derived from the joint use of models and measurements. Another disadvantage of reanalysis data is the relatively coarse spatial resolution, and the poor performance of precipitation estimations.

There is a need to use datasets that are derived directly from measurements, and have fine spatial resolution. This need is especially emphasized in case of precipitation which exhibit large spatial variability. Meteorological stations are located irregularly at the surface, which means that sophisticated mathematical methods are needed to create easy-to-use gridded datasets (see e.g. Haylock et al., 2008).

The increasing number of freely available, high resolution gridded datasets reveals the great interest about climate change and meteorology in general. Here we describe three important datasets, keeping in mind that other datasets also exist but they are out of scope of the BioVeL project.

WorldClim is one of the datasets that contains monthly averages of selected meteorological parameters (Hijmans et al. 2005; www.worldclim.org) for the 1950-2000 period. Available parameters include monthly mean, maximum and minimum temperature, monthly precipitation plus 19 derived bioclimatic variables. The spatial resolution of the dataset is 1 km^2. Note that WorldClim also publishes past climate reconstruction datasets and also climate scenarios.

The Climatic Research Unit (**CRU**) of University of East Anglia disseminates high resolution gridded datasets at the CRU website (www.cru.uea.ac.uk/cru/data/hrg/; Fig. 2.2-6). CRU also publishes climate scenarios. CRU data contains monthly averages for selected meteorological parameters at variable spatial resolution.



data-set	space	time	variety	variables	reference	status
CRU CL 1.0	0.5° global	1961-1990	climatology	pre, wet, tmp, dtr, vap, spc, cld, frs, wnd	New et al, 1999	available (via the IPCC-DDC)
CRU CL 2.0	10' global	1961-1990	climatology	pre, wet, tmp, dtr, rhm, ssh, frs, wnd	New et al, 2002	available for download
CRU CL 2.1	10' Europe	1961-1990	climatology	cld, vap	Mitchell et al, 2003	available on request
CRU TS 1.0	0.5° global	1901-1995	time-series	pre, tmp, dtr, wet, vap, cld, frs	New et al, 2000	available on request but superseded by CRU TS 2.1
CRU TS 1.1	0.5° global	1996-1998	time-series	pre, tmp	New et al, 2000; extended	available on request but superseded by CRU TS 2.1
CRU TS 1.2	10' Europe	1901-2000	time-series	pre, tmp, dtr, vap, cld	Mitchell et al, 2003	available for download
CRU TS 2.0	0.5° global	1901-2000	time-series	pre, tmp, dtr, vap, cld	Mitchell et al, 2003	available for download superseded by CRU TS 2.1
CRU TS 2.1	0.5° global	1901-2002	time-series	pre, tmp, tmx, tmn, dtr, vap, cld, wet, frs	Mitchell and Jones, 2005	available for download superseded by CRU TS 3.0
CRU TS 3.0	0.5° global	1901-2006	time-series	pre, tmp, tmx, tmn, dtr, vap, cld, wet, frs, pet	*In preparation*	Available from BADC (registration required)
TYN SC 1.0	10' Europe	2001-2100	scenarios	pre, tmp, dtr, vap, cld	Mitchell et al, 2003	available for download
TYN SC 2.0	0.5° global	2001-2100	scenarios	pre, tmp, dtr, vap, cld	Mitchell et al, 2003	available for download
TYN CY 1.0	country	1901-1998	countries	pre, tmp, dtr, wet, vap, cld, frs	Mitchell et al, 2002	superseded by TYN CY 1.1
TYN CY 1.1	country	1901-2000	countries	pre, tmp, dtr, wet, vap, cld, frs, tmn, tmx	Mitchell et al, 2003	available for download
TYN CY 2.0	country	2070-2099	countries	pre, tmp	Mitchell et al, 2002; extended	available for download
TYN CY 3.0	country	1901-2100	countries	pre, tmp, dtr, vap, cld	Mitchell et al, 2003	available for download

Figure 2.1-6 List of high resolution datasets that are published by CRU (www.cru.uea.ac.uk/cru/data/hrg/)

CRU TS 2.1 and CRU TS 1.2 datasets are frequently used for different purposes including data source for spin-up simulations with Biome-BGC (Hidy et al., 2012). The datasets cover the time period of 1901-2002 (CRU TS 2.1) and 1901-2000 (CRU TS 1.2). CRU TS 2.1 provides data for the land are globally, at 0.5×0.5 degree resolution. CR TS 1.2 only provides data for the European land area, but in a finer spatial resolution (1/6×1/6 degree). CRU TS 1.2 is of particular interest for the European users (Mitchell et al., 2004). CRU TS 1.2 contains average temperature and diurnal temperature range, as well as monthly precipitation amount data (plus two other parameters related to humidity and cloud cover). Though the quality of CRU TS 1.2 was found to be poor when applied to single points in heterogeneous terrain (Eastaugh et al., 2010), experience shows that it performs well in typical homogeneous terrain (e.g. in the lowlands of Hungary).

As WorldClim and CRU datasets provide monthly means, weather generator must be adapted to create virtual meteorological time series in daily time step (needed by Biome-BGC). There are several stochastic weather generators available for this purpose. An example is the C2W statistical weather generator (Bürger, 1997).

In the frame of the European Union funded ENSEMBLES project (www.ensembles-eu.org) a new, interpolated, high resolution gridded dataset was created based on station measurements and sophisticated interpolation techniques (Haylock et al., 2008; Fig. 2.1-7). This so-called **E-OBS** dataset contains daily data for selected meteorological parameters in 0.25×0.25 degree regular (or 0.22×0.22 degree rotated) grid for Europe (http://eca.knmi.nl/download/ensembles/download.php). This dataset is available from 1950 to present day and it is continuously updated. Daily maximum and minimum temperatures, plus daily precipitation amounts are available from E-OBS, and this data can directly be used together with Biome-BGC.

The high resolution gridded datasets are available in different file formats. WorldClim data is available in ESRI grid (raster) format, GeoTIFF format, and generic grid format. CRU data is available as ASCII text (note that some of the CRU datasets are also available as NetCDF files from other sources). E-OBS data is available in NetCDF format.

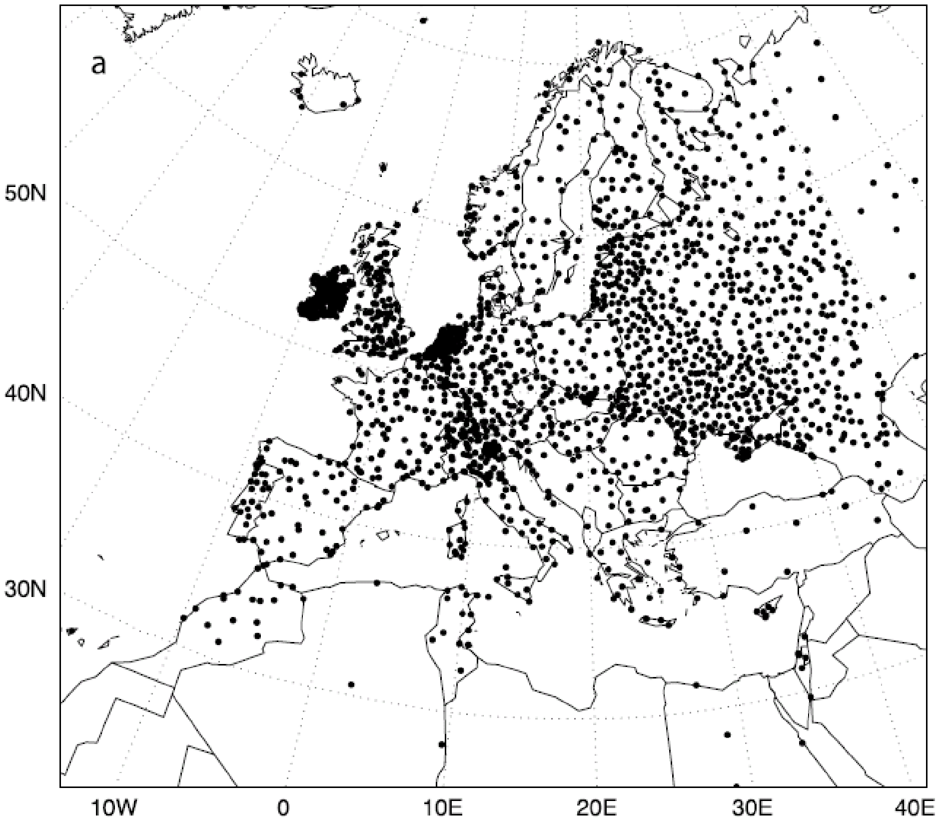


Figure 2.1-7 Map of the meteorological stations that were used to create the precipitation data of E-OBS (Haylock et al., 2008; their Fig. 1a)

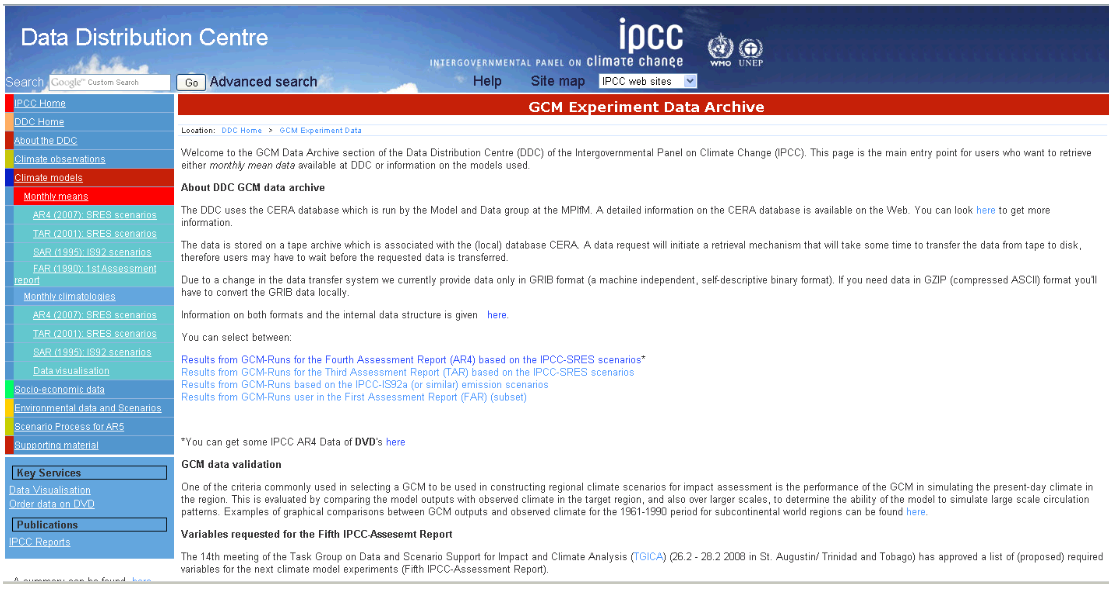
2.1.5.2. Weather scenarios

In order to design climate change related impact studies with Biome-BGC (or with other models), the user has to choose an appropriate meteorological data source (typically results from climate models are needed). This task is not simple given the large number of available simulation results and the problems associated with the climate data (incorrect representation of amount and frequency of precipitation, inadequate representation of fine scale topography, etc.). Below we provide a brief overview about the most important climate change related data sources, and we also describe the correction procedure that is needed to provide realistic input data for Biome-BGC (and other models).

Availability of Global Climate Model (GCM) results

The Intergovernmental Panel on Climate Change (IPCC) is the leading international organization for the assessment of climate change. IPCC does not only issue assessment reports on the current understanding of climate change (the latest report is IPCC Fourth Assessment Report that was published in 2007; IPCC, 2007a), but it also disseminates climate change related data to the public.

The IPCC Data Distribution Centre (DDC) recommended by the IPCC Task Group on Data and Scenario Support for Impact and Climate Analysis (TGICA) was established in 1998. The DDC provides climate, socio-economic and environmental data, both from the past and also in the form of scenarios projected into the future. The DDC is primarily designed for climate change researchers, but materials contained on the site may also be of interest to educators, governmental and non-governmental organizations, and the general public. At the DDC website users can select between the results from GCM-Runs used by the four IPCC assessment reports that were published so far, and the user can download monthly means, decadal and 30-year means (climatologies) based on global climate model simulations (Fig. 2.1-8).



Welcome to the GCM Data Archive section of the Data Distribution Centre (DDC) of the Intergovernmental Panel on Climate Change (IPCC). This page is the main entry point for users who want to retrieve either *monthly mean data* available at DDC or information on the models used.

About DDC GCM data archive

The DDC uses the CERA database which is run by the Model and Data group at the MPIfM. A detailed information on the CERA database is available on the Web. You can look here to get more information.

The data is stored on a tape archive which is associated with the (local) database CERA. A data request will initiate a retrieval mechanism that will take some time to transfer the data from tape to disk, therefore users may have to wait before the requested data is transferred.

Due to a change in the data transfer system we currently provide data only in GRIB format (a machine independent, self-descriptive binary format). If you need data in GZIP (compressed ASCII) format you'll have to convert the GRIB data locally.

Information on both formats and the internal data structure is given here.

You can select between:

Results from GCM-Runs for the Fourth Assessment Report (AR4) based on the IPCC-SRES scenarios*
Results from GCM-Runs for the Third Assessment Report (TAR) based on the IPCC-SRES scenarios
Results from GCM-Runs based on the IPCC-IS92a (or similar) emission scenarios
Results from GCM-Runs user in the First Assessment Report (FAR) (subset)

*You can get some IPCC AR4 Data of **DVD**'s here

GCM data validation

One of the criteria commonly used in selecting a GCM to be used in constructing regional climate scenarios for impact assessment is the performance of the GCM in simulating the present-day climate in the region. This is evaluated by comparing the model outputs with observed climate in the target region, and also over larger scales, to determine the ability of the model to simulate large scale circulation patterns. Examples of graphical comparisons between GCM outputs and observed climate for the 1961-1990 period for subcontinental world regions can be found here.

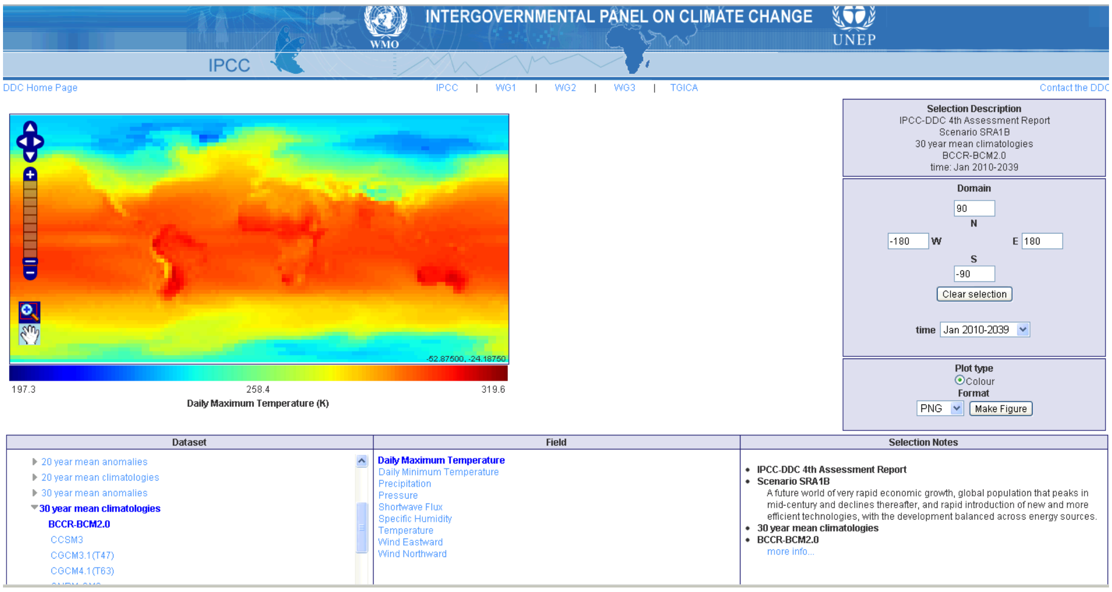
Variables requested for the Fifth IPCC-Assesemt Report

The 14th meeting of the Task Group on Data and Scenario Support for Impact and Climate Analysis (TGICA) (26.2 - 28.2 2008 in St. Augustin/ Trinidad and Tobago) has approved a list of (proposed) required variables for the next climate model experiments (Fifth IPCC-Assessment Report).

Figure 2.1-8 IPCC DDC web interface where GCM results can be downloaded (www.ipcc-data.org/gcm/monthly/ddc_gcmdata.html)

The Fourth Assessment Report (IPCC, 2007a) is based on six greenhouse-gas emission scenarios: A1B, A1FI, A1T, A2, B1 and B2 (these are the so-called SRES scenarios; Nakicenovic and Swart, 2000). The detailed meaning and the assumptions of the emission scenarios can be seen at www.ipcc.ch/pdf/special-reports/spm/sres-en.pdf. 19 climate modeling centers run different global climate models to simulate the climate in the future. The climatologies of the climate model projections can also be viewed through the DDC visualization service (www.ipcc-data.org/maps/) (Fig. 2.1-9).

Note that due to the coarse spatial resolution of the current GCMs, the output meteorological fields are generally not suitable for application with Biome-BGC. So-called downscaling techniques are needed to obtain meteorological data on finer spatial resolution (e.g. on a grid with 10-50 km horizontal resolution).



Selection Description
IPCC-DDC 4th Assessment Report
Scenario SRA1B
30 year mean climatologies
BCCR-BCM2.0
time: Jan 2010-2039

Domain
N 90
W -180
E 180
S -90

time Jan 2010-2039

Plot type
● Colour
Format
PNG

- **IPCC-DDC 4th Assessment Report**
- **Scenario SRA1B**
  A future world of very rapid economic growth, global population that peaks in mid-century and declines thereafter, and rapid introduction of new and more efficient technologies, with the development balanced across energy sources.
- **30 year mean climatologies**
- **BCCR-BCM2.0**

Figure 2.1-9 DDC visualization centre (www.ipcc-data.org/maps)

Availability of RCM results

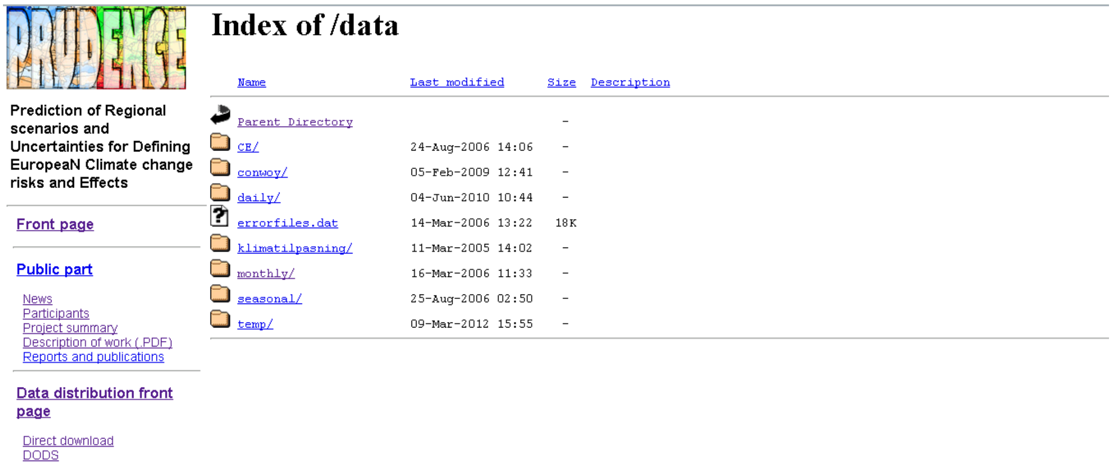
Interpolation of GCM-scale changes to a finer resolution is the simplest way of adding spatial details to GCM-based climate change scenarios. To improve the representation of the meteorological data in the finer resolution grid cells, observed climate information could be used. This may be achieved using high resolution observed monthly climatologies or can be done simply by perturbing an observed monthly or daily time series by the GCM changes interpolated to the site in question. This approach is sometimes termed 'unintelligent' downscaling because no additional meteorological insight is added in the interpolation process that goes beyond the GCM-based changes; the basic spatial patterns of present climate are assumed to remain largely unchanged in the future. This very simple downscaling method is easy to apply and allows impact assessment models to use climate scenarios at a resolution that would otherwise be difficult or costly to obtain.

Another downscaling option is to use a higher resolution limited-area model (known as Regional Climate Model - RCM) to generate climate change scenarios at the required, finer spatial resolution (see also: climateprediction.net/content/regional-climate-models). Such regional climate models typically cover an area the size of Europe, have a spatial resolution of about 10-50 km and are driven by boundary conditions taken from the GCM for one particular period in the present and one in the future (Déqué, 2007; Bartholy et al., 2007, 2008; Pongrácz et al., 2011).

The IPCC DDC does not currently contain any results from RCM experiments. Several modeling centers around the world developed their own RCMs and those centers frequently participate in research projects dealing with climate change. Some of these project results could be downloaded from specific web pages. In the followings a few downloadable regional climate model results are going to be presented.

PRUDENCE

PRUDENCE was a European-scale investigation (EU 5th Framework Programme) which ended in 2004. The main objective of the project was to provide high resolution climate change scenarios for Europe at the end of the twenty-first century by means of dynamical downscaling (regional climate modeling) of global climate simulations. The main aim was to quantify the uncertainties in predictions of future climate and its impacts, using several climate models and impact models. 21 European research institutes and universities took apart in the PRUDENCE project and simulated the future climate according to A2 and B2 SRES scenario. The results of the RCMs are available at the homepage of the project (http://prudence.dmi.dk; Fig. 2.2-10). The simulations have been run for two 30 years periods in the future (2021-2050, 2071-2100) and one for the past called reference period (1961-1990). The adaptation of these RCM results in Hungary was performed by the Department of Meteorology, Eötvös Loránd University and the expected temperature and precipitation changes for the future already investigated and presented for Central Europe (Bartholy et al., 2007, 2008).



Prediction of Regional scenarios and Uncertainties for Defining EuropeaN Climate change risks and Effects

Front page

Public part

News
Participants
Project summary
Description of work (.PDF)
Reports and publications

Data distribution front page

Direct download
DODS

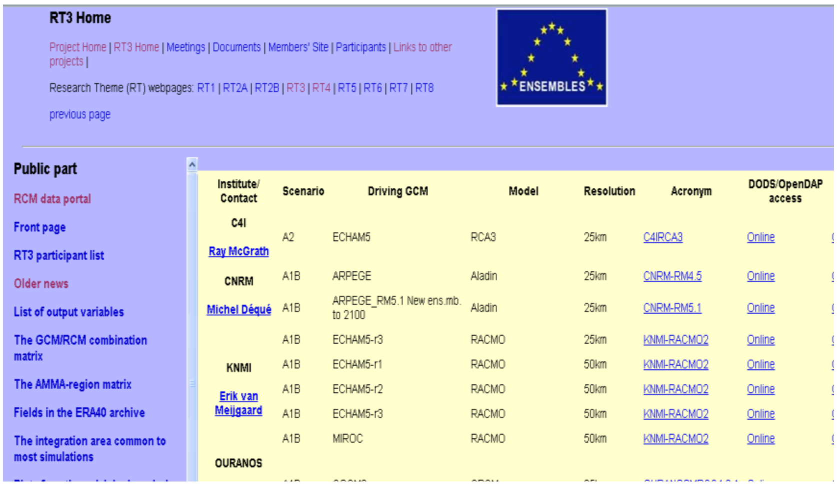
Index of /data

Name	Last modified	Size	Description
Parent Directory		-	
CE/	24-Aug-2006 14:06	-	
conwoy/	05-Feb-2009 12:41	-	
daily/	04-Jun-2010 10:44	-	
errorfiles.dat	14-Mar-2006 13:22	18K	
klimatilpasning/	11-Mar-2005 14:02	-	
monthly/	16-Mar-2006 11:33	-	
seasonal/	25-Aug-2006 02:50	-	
temp/	09-Mar-2012 15:55	-	

Figure 2.1-10 Web interface for downloading PRUDENCE data (http://prudence.dmi.dk/)

ENSEMBLES

The next EU-financed major effort in regional climate modeling was the ENSEMBLES project (van der Linden and Mitchell, 2009), financed under Framework Programme 6. A major archive of data in 25 km resolution covering the transient periods 1951-2100 or 1951-2050 according to the SRES A1B scenario is available at the Danish Meteorological Institute (DMI). In order to execute a climate change related impact study (for example, modeling crop growth or using Biome-BGC), continuous time series are required. At the webpage of the ENSEMBLES, by choosing the third research theme (RT3) a lot of RCM results are available for download in NetCDF format (Fig. 2.1-11).



RT3 Home

Project Home | RT3 Home | Meetings | Documents | Members' Site | Participants | Links to other projects |

Research Theme (RT) webpages: RT1 | RT2A | RT2B | RT3 | RT4 | RT5 | RT6 | RT7 | RT8

previous page

Public part

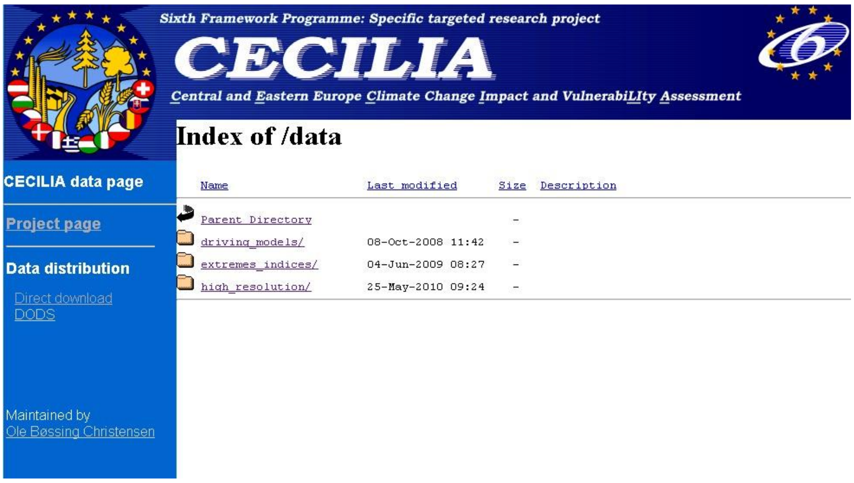
- RCM data portal
- Front page
- RT3 participant list
- Older news
- List of output variables
- The GCM/RCM combination matrix
- The AMMA-region matrix
- Fields in the ERA40 archive
- The integration area common to most simulations

Institute/ Contact	Scenario	Driving GCM	Model	Resolution	Acronym	DODS/OpenDAP access
C4I Ray McGrath	A2	ECHAM5	RCA3	25km	C4IRCA3	Online
CNRM Michel Déqué	A1B	ARPEGE	Aladin	25km	CNRM-RM4.5	Online
	A1B	ARPEGE_RM5.1 New ens.mb. to 2100	Aladin	25km	CNRM-RM5.1	Online
KNMI Erik van Meijgaard	A1B	ECHAM5-r3	RACMO	25km	KNMI-RACMO2	Online
	A1B	ECHAM5-r1	RACMO	50km	KNMI-RACMO2	Online
	A1B	ECHAM5-r2	RACMO	50km	KNMI-RACMO2	Online
	A1B	ECHAM5-r3	RACMO	50km	KNMI-RACMO2	Online
	A1B	MIROC	RACMO	50km	KNMI-RACMO2	Online
OURANOS						

Figure 2.1-11 Web interface for downloading ENSEMBLES data (www.ensembles-eu.org)

CECILIA

The CECILIA (Central and Eastern Europe Climate Change Impact and Vulnerability Assessment) project started in 2006 with the participation of 16 institutions from 12 European countries (financed under Framework Programme 6 of the European Union). The main objectivity was to improve the understanding of local climate change in Central and Eastern Europe. The project constructed very high resolution (10 km) climate projections, and conducted impact studies of hydrology, water quality, and water management, air quality issues in urban areas, agriculture and forestry. The final report of CECILIA accessible at www.cecilia-eu.org. The publications related to the project could be found at the CECILIA website (www.cecilia-eu.org/publications.php) and the datasets are available at http://cecilia.dmi.dk with username and password (Fig. 2.1-12).



Sixth Framework Programme: Specific targeted research project

CECILIA

Central and Eastern Europe Climate Change Impact and VulnerabiLIty Assessment

Index of /data

```
Name                 Last modified      Size  Description
Parent Directory                         -
driving_models/      08-Oct-2008 11:42   -
extremes_indices/    04-Jun-2009 08:27   -
high_resolution/     25-May-2010 09:24   -
```

CECILIA data page

Project page

Data distribution

Direct download
DODS

Maintained by
Ole Bøssing Christensen

Figure 2.1-12 Web interface for downloading CECILIA datasets (http://cecilia.dmi.dk). Username and password are required

CLIMATE PREDICTION NET

It is worth mentioning one other interesting project which is called Climateprediction.net (http://climateprediction.net).

Although Climateprediction.net does not provide climate scenarios for the public, the project is a good example for the application of the Berkeley Open Infrastructure for Network Computing (BOINC) technology which will be used within the frame of the BioVeL project by the Hungarian group.

Climateprediction.net is a global computing project to produce predictions of the Earth's climate up to 2100 and to test the accuracy of climate models. People around the world could offer processor time of their computers (when they are switched on, but are not using them in full capacity) to connect them to a global system. ClimatePrediction.net uses those computers to run climate models. Using this technique Climateprediction.net could collect a great deal of computing capacity. Participants of the project use the BOINC technology.

Though the datasets are not available for download at the Climateprediction.net website, if somobody participates in this project he/she gets a software called ’weather at home’ which provide informations about the expected climate change associated with the country where the participant lives.

Bias correction of RCM data

When climate researchers try to predict the climate and weather conditions in the future they always calculate expected changes (for example, the climate will be *x* degrees warmer then at the present or precipitation will decrease/increase during the summer periods). These values are calculated by comparing the climate model results simulated for the future and the climate model result simulated for the past. However, every climate model results have systematic errors (Déqué, 2007; Hlásny et al., 2011). These errors could be quantified during the validation progress, which is an essential step in every case when we work with RCM results.

If the climate model results are used in climate change related impact studies, these systematic errors generally cause problems, and in some cases the impact models fail to provide realistic results due to the inaccurate representation of e.g. precipitation frequency and amount (Fig. 2.2-13). We can only perform reliable simulations if the systematic errors inherently present in the RCM data are eliminated (Déqué, 2007).

Bias correction is the procedure which removes the systematic error from the model results and creates reliable values for the future. Every bias correction method is based on the same assumption: the systematic error of the climate model in the future equals to the error in the past.

The largest errors usually occur in the precipitation datasets, which is problematic as crop models or biogeochemical models are highly sensitive to this parameter. Usually the climate models simulate too many rainfall events of too low intensity relative to individual stations within a grid cell. The difficulty of the precipitation correction is that wet days have to be created or removed so not just the precipitation rates have to be corrected.

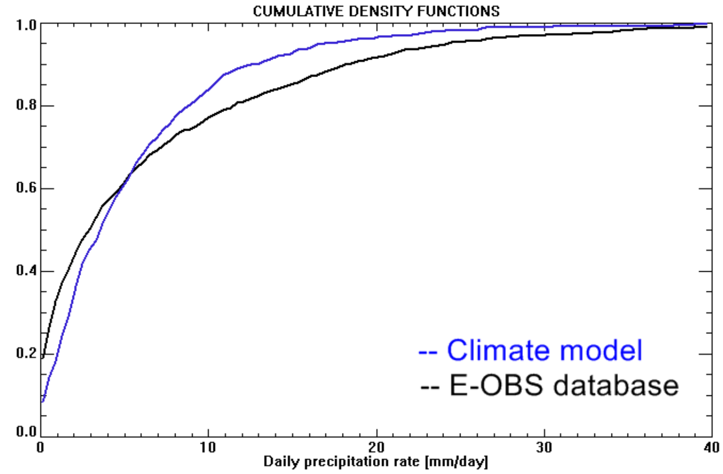


Figure 2.1-13 An example for cumulative density function differences between the reference (E-OBS) database and one of the climate model results (based on data from Januaries between 1951 and 2009)

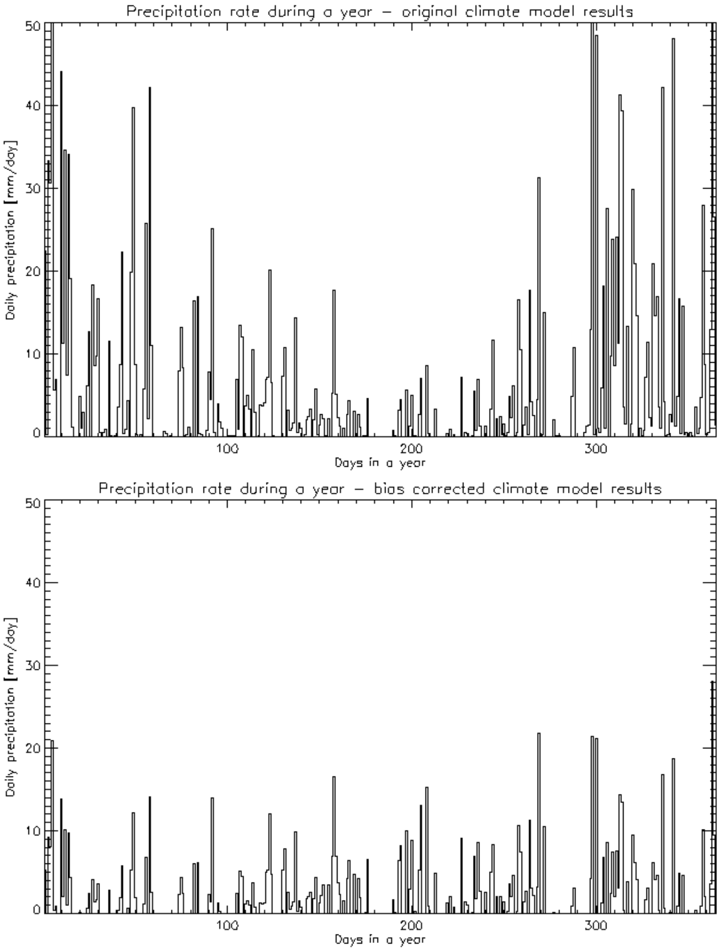


Figure 2.1-14 Annual distribution of daily precipitation for a selected pixel for year 2092 based on the original climate model output (no correction; upper plot) and the bias corrected climate model (lower plot).

Ines and Hansen (2006) present a procedure that calibrates both the frequency and the intensity distribution of daily simulated rainfall relative to a target station. If the modeled rainfall frequency is greater than the observed frequency for a given month (averaged across years), the modeled rainfall frequency is corrected by discarding rainfall events below a calibrated threshold. To correct the intensity distribution, each GCM rainfall amount above the calibrated threshold is mapped from the GCM intensity distribution onto the observed distribution (Fig. 2.1-14).

The Hungarian BioVeL group started to apply the bias correction to the daily datasets of the ENSEMBLES RCMs in order to feed them into Biome-BGC to predict the future carbon cycle in the Carpathian Basin. The newly created dataset is called as the FORESEE database.

2.1.6 Identification and description of typical and most challenging workflows

The scientific workflow concept is a new and emerging paradigm for the support of research (Gil et al. 2007; Goble and De Roure 2009; Ludäscher et al. 2009). A workflow can manage large, distributed data sources and can perform demanding computations within a simple framework. The scientific workflow concept is historically used in many different science domains (i.e. particle physics, bioinformatics, cosmology or mathematics), and it has the great potential to support biogeochemistry, biodiversity and ecology in general.

Biome-BGC based workflows

The application of Biome-BGC by the end-user requires the selection of appropriate data sources and the creation of different input files for the simulation. This procedure can be performed in a linear fashion (step-by-step) which means that the application of the model perfectly fits the scientific workflow concept. Considering the increasing interest in carbon cycle and biogeochemistry and the simplicity of the workflow concept, construction of Biome-BGC related workflows (and associated web services) might be beneficial for the scientific community. Hence, in the BioVel project we are undertaking this.

A typical workflow scheme could perform a single run of the Biome-BGC model at a given location of a selected ecosystem stand as showed in the Fig. 2.1–15. It goes through several simple steps in a sequential way, however the final workflow implementation could be more complex. In the preparatory phase the user feeds the model with monthly dataset, which has to be disaggregated into daily meteorological dataset and preprocessed and reformatted according to the Biome-BGC input requirements. The preparatory web service has to incorporate submodel for disaggregation (C2W model for example; Bürger 1997) and MT-Clim mountain climate simulator (Running et al. 1987, Kimball et al. 1997, Thornton & Running 1999) for data preprocessing. The core of the workflow is the execution of the Biome-BGC model, which performs a so called ’spinup’ simulation first, than the ’normal’ run. The spinup phase integrates the model through several thousend of years while the specific ecosystem pools of the model (carbon and nitrogen content of litter, live and dead stem pools for example) reach a steady-state equilibrium and creates the initial conditions to start the normal simulation.

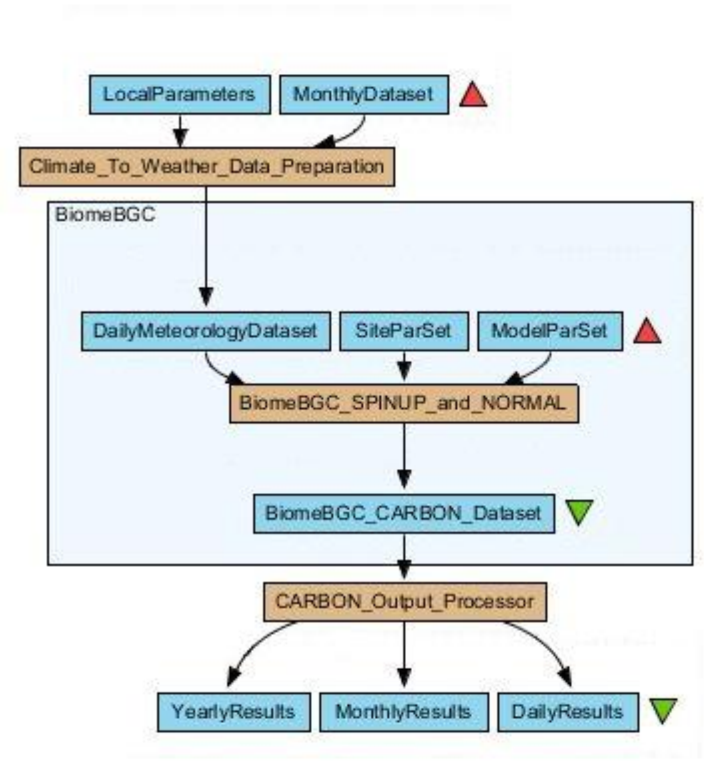


Figure 2.1–15 A typical workflow scheme to perform a single Biome-BGC model execution. Brown coloured boxes are representing ’functions’ or model components, blue coloured boxes are input (red triangle) or output (green triangle) data sets. The functions or components can be chained or embedded to each other.

A typical and challenging scientific workflow is the spatial extension of the model at a fine geographic resolution (called also as ’landscape simulation’, i.e. Kimball et al. 2000). One could consider it as a general parameter study similar to the data-model-harmonization (see in chapter 2.2.6), but it raises an important additional question: how can we get (i.e. give more details) the finer spatial resolution of grid cells for model inputs: spatial datasets of land cover types and parameters for soil, vegetation and meteorological characteristics? There are several solutions from global (i.e. Bonan et al. 2002) to regional scale (Barcza et al. 2009, Chiesi et al. 2011), but we can state the very clear trend to dramatically improve the thematic and spatial resolution and spatial extent of these projects. There are two preprocessing subcompartments of the Biome-BGC core simulation showed in the Fig. 2.1-16. The MTCLIM model spatially recalculate the daily meteorology dataset of the base met station considering the terrain and surroundings of the corresponding raster point (Bristow et al. 1984, Glassy & Running 1994, Kimball et al. 1997, Running et al. 1987, Thornton & Running 1999, Thornton et al. 2000). The ’parameterizer’ component of the workflow prepare the necessary parameter and initialization files of Biome-BGC. The Biome-BGC simulation (spinup and normal phase) performs for each raster points of the area of interest, which could runs up to millions. The execution of numerous simulation runs can be organized parallel if we apply a parallel computation environment just like SZTAKI desktop grid (Balaton et al. 2007).

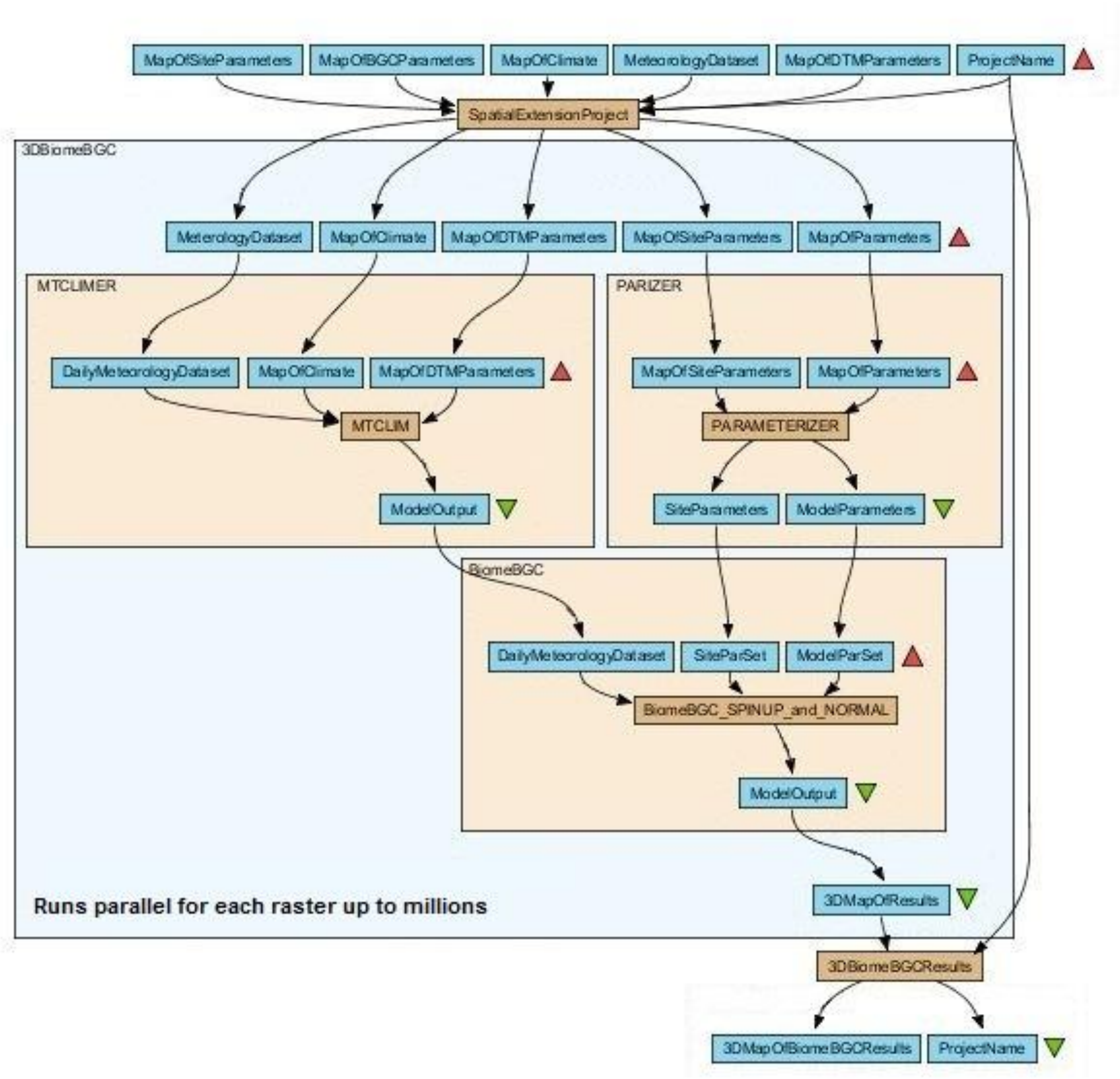


Figure 2.1–16 A challenging workflow scheme to perform a spatial extension of Biome-BGC model simulation. Brown coloured boxes are representing 'functions' or model components, blue coloured boxes are input (red triangle) or output (green triangle) data sets. The functions or components can be chained, parallelized or embedded to each other.

Metagenomics based workflow

The standardized, repeatable, and comparable utilization of metagenomics is hampered by the fact that samples and analytical procedures are rather complex. These complexities gave rise to a growing set of tools, services and platforms tackling the existing issues all individually at different levels of quality (MEGAN, MG-RAST, IMG/M, CAMERA, or MEGX.net). Currently the analytical results of none of the resources are comparable, while none of these platforms are able to compute all ecologically interesting features of microbial communities.

The metagenomics workflows and web services being developed in the BioVel project compute the community traits outlined in Barberan et al. 2011 "Exploration of community traits as ecological markers in microbial metagenomes" (Fig. 2.1-17). The traits calculated with these workflows range from GC (guanine-cytosine) content to functional diversity, and deliver a valuable set of ecological markers in order discriminate between habitats or geographic locations. Furthermore, inter-trait relationships can be used as habitat descriptors or indicators of artefacts during sample processing. Overall, these metagenomics community traits approach, when combined in the form of workflows can help to interpret metagenomics data to gain a full understanding of microbial community patterns in a rigorous ecological framework.

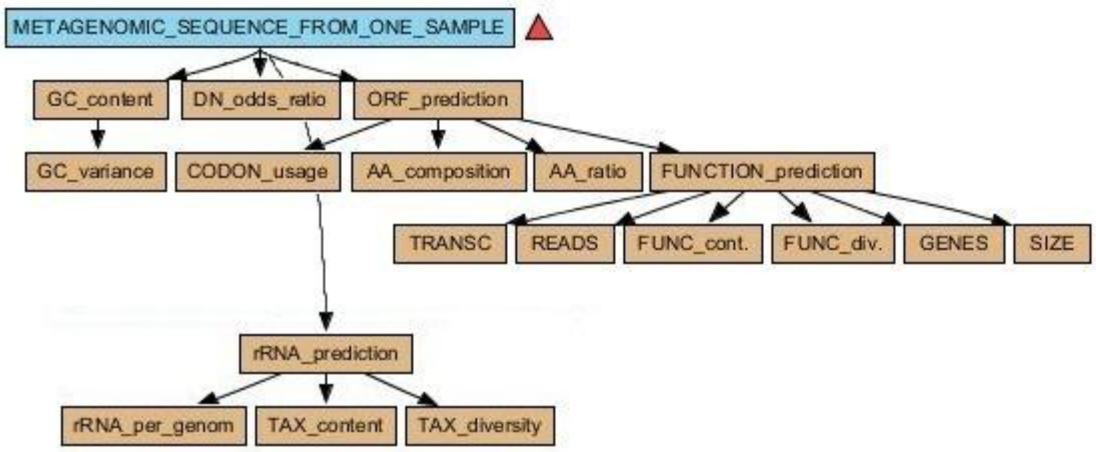


Figure 2.1–17 A simplified outline of a metagenomic trait workflow. Abbreviations: GC – guanine-cytosine content, DN – dinucleotide, ORF – Open Reading Frame, AA – amino-acid, TRANSC – transcription factors, READS – classified reads, GENES – genes per genom, SIZE – estimated genome size, TAX - taxonomic

2.1.7 Evaluation of web service requirements

Actually there are no existing open-source re-usable web services of terrestrial ecosystem model type on the web, so it is an open and opportunistic ‘niche’ to develop some. The existing functions of a simple or a complex model can be wrapped into a single web service according to the MaaS – ‘model-as-a-service’ concept of Roman et al. (2009), but a much more complex processing chain or a hierarchically embedded set of functions can be considered and developed as a separate web service as well. So there are multiple options to plan and build simple or more tricky services (Maué & Stasch 2010).

We have planned to develop a Biome-BGC web service to execute a single simulation (including the spinup and normal phase of model run) as a minimum (see Fig. 2.1-15), which functionality can be extended by a 'climate-to-weather' data preparatory service before and different post-processing sets to specifically profiling resulted outputs, like as a 'carbon-focused' or an 'ecosystem-service-indication' profile.

As it is shown in Fig. 2.1-16, one of the most challenging workflow could be the spatial extension of the model, when Biome-BGC simulation runs in each raster of the area of interest. That kind of task can raise an enormous computation and storage demand against the model hosting computer, but parallel distribution of the execution can reduce the processing time considerably. A BOINC-based desktop grid system (Anderson 2004) could provide a good solution, like as SZTAKI Desktop Grid, which is enhanced additionally by the so called 'GenWrapper' to support the execution of legacy applications (Balaton et al. 2007, Marosi et al. 2009). There are several options to define web service functionality and decide which processes are better to include in parallel computation to get an optimal performance.

There are a lot of other options too, because the high variety of open climate and weather datasets served by different providers (see section 2.1.5) offers possibilities to wrap the file-download-based services of dataset archives (i.e. NOAA NESDIS NCDC, ERA Interim reanalysis, WorldClim, E-OBS dataset, etc.) into web service or OGC web processing service.

According to the metagenomic trait workflow (Fig. 2.1-17) there are a set of high priority web services to develop. These are the GC Variance Web Service; Di-nucleotide Odds Ratio Web Service; ORF Prediction Web Service; Small and Large Subunit rRNA Prediction Web Service; Web Service for amino acid composition calculation; Web Service to calculate functional diversity; Web Service to calculate taxonomic diversity; Create Service for the prediction of transcription factors in metagenomes; Web Service for codon usage calculation; and Web Service to calculate number of rRNAs per genome in metagenomes (see more details in the deliverable report D3.1 – Prioritised list of service sets).

2.2 BIOSPHERIC CARBON SEQUESTRATION

by
Zoltán Barcza, Ferenc Horváth, Györgyi Gelybó and *Laura Dobor*

2.2.1 Science-policy context

Climate change is undoubtedly one of the greatest challanges of the 21st century. A large amount of evidence indicates that the chemical composition of the atmosphere has been changed since the beginning of the industrial revolution due to human activity (IPCC, 2007a). Huge amounts of greenhouse gases have been emitted to the atmosphere via burning of fossil fuels, cement manufacturing, land use conversion and other processes. The increasing quantity of atmospheric greenhouse gases can unbalance the energy budget of the Earth-atmosphere system and can trigger global warming (IPCC, 2007a).

Measurement shows that the surface temperature of the Earth has already increased by ~0.76 Celsius during the 20th century (IPCC, 2007a). We have ample evidence that proves the role of the increasing amount of atmospheric greenhouse gases behind the observed warming.

Carbon dioxide (CO_2) is recognized as the most important anthropogenic greenhouse gas. The atmospheric concentration of CO_2 has increased by ~40% since preindustrial times (Fig. 2.2-1). Due to its dominant radiative forcing CO_2 is considered as the major cause of the observed warming.

Ongoing and future climate change affects our everyday life, the society, the economy, and our environment including the land biosphere and the oceans. Among many other processes, climate change affects biodiversity, species distribution, vitality of ecosystems, outbreak of pathogens, plant growth and mortality (IPCC, 2007b). Considering land biosphere, plants build their own body through the process of photosynthesis when carbon is taken up from the atmosphere in the form of CO_2. This CO_2 uptake means that plants can decrease the amount of the atmospheric CO_2 concentration while mitigating climate change. Within the plant carbon is transformed into living biomass like leaves, roots, stems and branches. Like humans, plants also respire CO_2 to produce energy for their life processes. Soil and litter also release CO_2 since the organic carbon that is stored in these carbon pools is continuously decomposed by microbes. The carbon balance of ecosystems is determined by the amount of carbon uptake and respiration (and other forms of carbon loss) where both processes are very sensitive to the environmental conditions.

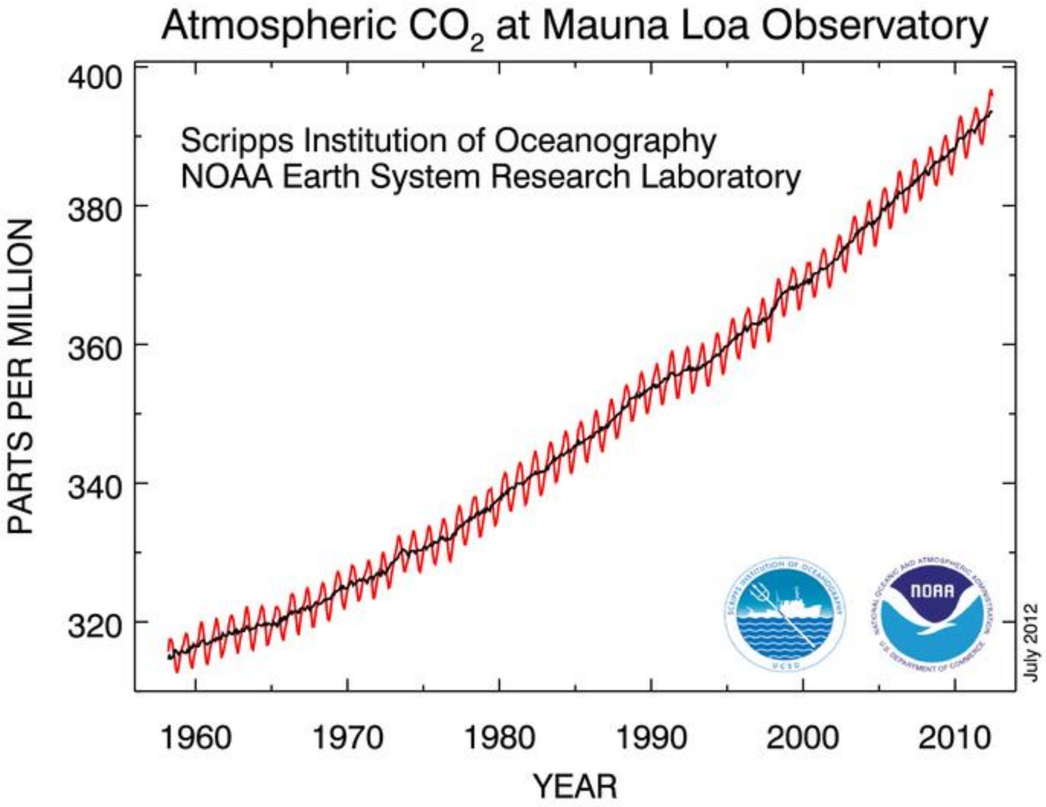


Figure 2.2-1 The so-called Keeling-curve showing the increasing amount of atmospheric carbon dioxide content since the beginning of the measurements at Mauna Loa (Source: www.esrl.noaa.gov/gmd/ccgg/trends/, accessed on July, 2012)

At present terrestrial biosphere (and also the oceans) mitigate climate change as biosphere and oceans together sequester about half of the CO_2 that is emitted to the atmosphere annually by human activity (IPCC 2007a; Le Quéré et al. 2009; Global Carbon Project website 2010). Climate change has already modulated the carbon balance of terrestrial biosphere (e.g. Ciais et al. 2008; Churkina et al. 2010), and it is reasonable to assume that it will further interfere with the carbon cycle (Friedlingstein & Prentice 2010). The interaction between the terrestrial biosphere and the climate means that the carbon balance of the ecosystems might change, which means that the carbon sequestration of the biosphere can increase or decrease (it means negative or positive feedback to climate change, respectively). However, it is not only the meteorological parameters (temperature, amount and timing of precipitation, radiation, etc.) that affect terrestrial carbon balance, but other environmental parameters are also important. For example, it is well established that increasing atmospheric CO_2 amount can stimulate photosynthesis through the so-called CO_2-fertilization effect (Leakey et al. 2009), and also nutrient availability (most importantly, nitrogen availability) plays an important role in plant growth (Churkina et al. 2003, 2010; Magnani et al. 2007; De Vries et al. 2009; Högberg 2012). At present there is no consensus about the direction of carbon cycle feedback mechanism that will be caused by the interaction between the changing environmental conditions and the carbon cycle (Friedlingstein & Prentice 2010). Lack of knowledge about the future evolution of the terrestrial (and oceanic) carbon sequestration is a major problem which causes uncertainty in the climate projections. Ironically, in spite of our increasing understanding of the carbon cycle and the climate system it seems that the uncertainty of the climate model predictions is increasing instead of decreasing (Maslin & Austin 2012).

In order to reduce uncertainty in the climate projections efforts are clearly needed in the field of carbon cycle research. This involves the establishment of new and long term field experiments (including ecosystem manipulation to study the long term effect of changing environemnt), development of existing biogeochemical models, and creation of information technology solutions in order to foster *in silico* experiments that are computationally intensive (e.g. model-data synthesis, spatial ecosystem modelling, etc.).

Besides scientific efforts, national legislation and international negotiations are urgently and seriously needed to reduce greenhouse gas emission and thus mitigate the hazardous effects of climate change. It is the responsibility of politicians to recognize the importance of climate change mitigation and to initiate legislation to control greenhouse gas emission. The Kyoto protocol and its predecessors are good starting points for such efforts, though it has been recognized that up to today the realized emission reduction is too small to have a significant influence on the CO_2 concentration of the atmosphere.

The following sections will focus on the terrestrial component of the global carbon cycle. Although the share of oceanic components from the global carbon cycle is quite big, these processes are rather driven by physical courses and very dependent on ocean water transport and dynamics, than biological processes (Doney et al. 2004). The oceanic sink of CO2 is mainly a physico-chemical response of the ocean to increasing atmospheric CO2, which dissolves in surface waters and is transported from the surface to the deep ocean by ocean currents (Le Quéré 2010). We review the most important open questions in relation with the terrestrial carbon budget, and we describe the methods that can be used to estimate the past, present and future carbon balance using state-of-the-art methods and computer technology. We also describe the possibility to use the scientific workflow concept and the applicability of the grid technology on carbon balance related research.

2.2.2 Review on the main scientific questions

In the last 10,000 years (i.e. during the Holocene) the terrestrial carbon budget has been approximately balanced (Friedlingstein & Prentice 2010). Due to changes in the chemical composition of the atmosphere and in the climate system the land biosphere has turned into a net CO_2 sink in the past few decades (Le Quéré et al. 2009). Further increases in temperature and changes in precipitation patterns, coupled with changing nutrient availability and air pollution, will most likely interfere with the carbon sequestration capacity of terrestrial ecosystems, resulting in a biosphere that might even strengthen the greenhouse effect in the future (Friedlingstein and Prentice 2010). In order to estimate the amount of CO_2

concentration in the atmosphere (and therefore climate change) it is necessary to quantify the present and future carbon balance of the biosphere at different spatial scales (from patch to global scale).

Data from direct field measurements and computer model based simulation results are jointly used to improve our understanding of the biogeochemical processes of the biosphere. Computer models are able to quantify the different carbon balance components even under environmental conditions that differ from the present day (Churkina et al. 2009; Friedlingstein & Prentice 2010; Zaehle et al. 2010). However, we can only rely on models that are capable to reproduce the present day carbon balance of the ecosystems with acceptable accuracy. Model-data fusion techniques (model calibration and validation, data assimilation) are used to improve our understanding of the fundamental processes (Wang et al. 2009).

In the early phase of carbon cycle related research models were developed to simulate biogeochemical cycles of undisturbed ecosystems (Vetter et al., 2008). Most recently, the research has focused on managed ecosystems because in certain parts of the world human alteration has a dominant role in the formation of the land surface (Vitousek et al. 1997). It is not only the environmental factors (e.g. temperature, radiation, precipitation, nitrogen availability, etc.) but also human activity (e.g. deforestation, afforestation, reforestation, fire suppression, agricultural management, harvest, biofuel production, use of fertilizers, abandonment of agriculture, etc.) has a measurable and significant impact on the carbon sequestration capacity of ecosystems (Chapin et al. 2006; Ciais et al. 2011). For example, in Europe, the majority of the land surface (forests, pastures, croplands, wetlands) is managed. Human activity includes the horizontal displacement of carbon (Ciais et al. 2007) in the form of e.g. harvest, forest thinning, residue management, grazing, mowing, and other forms of disturbance, which results in changes on the carbon sequestration of ecosystems.

As natural processes and human decisions jointly control the carbon balance of the terrestrial biosphere, management practices can be potentially changed to maximize the carbon sequestration capacity of ecosystems (Canadell & Raupach 2008). Historically, mitigation efforts focus on forest ecosystems due to the possibility of long term carbon sequestration in tree biomass (e.g. Somogyi 2010). However, not only forestry, but also agriculture can mitigate the potential climate change (Smith et al. 2001). Long term measurement projects and advanced modelling experiments are needed to improve our understanding of the carbon balance of managed ecosystems, and to attempt to predict the future evolution of the land carbon sink in a world that is continuously transformed by human activity. This represents a major challenge to the scientific community.

Considering present and future carbon sequestration of terrestrial ecosystems, the main scientific questions can be summarized as follows:

- What is the amount of carbon dioxide that is taken up by the vegetation in each year?
- How large is the interannual variability of carbon uptake?
- What is the amount of carbon that is removed from the ecosystems via human intervention? What is the amount of carbon that is sequestered in the plant/soil system?

- What is the spatial pattern and complete carbon balance of different locations (regions, countries, continents)?
- Can we manage carbon sequestration at the ecosystem level? How can we detect changes accurately in the soil and in the standing biomass?
- How will terrestrial carbon uptake and carbon sequestration evolve in the future? Will it mitigate or strengthen climate change?
- What is the role of nitrogen availability in the past and future evolution of carbon balance?
- Can we reliably simulate the effect of elevated CO2 concentration in the ecosystem processes? Can we improve our models based on field experience?
- What is the accuracy of the state-of-the-art carbon cycle models of different ecosystems under different climate and management conditions?
- Considering the ever increasing complexity of biogeochemical models, can we accurately use and optimize the models? Can we handle the enormous computational demand of the models?
- What is the spatial and temporal variability of model parameters? Can we construct generalized model parameters for regional, country, continental or global scale studies?
- Is it possible to adequately describe nitrogen related processes in a wide range of terrestrial ecosystems? Can we detect nitrogen limitation and the possible interaction of nitrogen availability with other nutrients?

2.2.3 Most relevant research groups, networks or projects

Due to the strong interaction between the global biogeochemical cycles and the climate system, carbon cycle related research has high priority in environmental sciences. Not only scientists, but stakeholders and policymakers also recognized the importance of carbon balance related research. Due to the available funding, several national and international research projects have been initiated to address the most relevant questions of the carbon cycle. Below we introduce a number of past and ongoing carbon cycle related research projects and initiatives without attempting to be comprehensive. First we focus on global scale issues, and then we move to the terrestrial component, mostly dealing with the European efforts. Note that the contents taken directly from the websites were collected in the end of 2011 and beginning of 2012, so the website content might have changed since then.

The Global Carbon Project

The Global Carbon Project (GCP) is an international initiative which was established in 2001. The main aim of the GCP is to describe and quantify the global carbon cycle. It also addresses questions related to the future evolution of the carbon cycle and the magnitude of the possible carbon-climate feedback. GCP is a fundamental data source for components of the global carbon cycle (including oceans, terrestrial biosphere, anthropogenic emission, land use change related emission). GCP periodically reports updates on the global carbon cycle which includes the realization of emission versus those predicted in the IPCC SRES scenarios (Nakicenovic & Swart 2000). As GCP is led by a collection of experts on the field of carbon cycle, the results are continuously published in international, peer reviewed journals (e.g. Le Quéré et al. 2009; Canadell et al. 2010). GCP hosts a good collection of related Internet resources as well.

Fluxnet

Field measurements are essentially needed to collect basic information about the carbon cycle of terrestrial vegetation. In response to this challenge long term measurement projects were initiated in many regions worldwide to determine the carbon balance of the ecosystems. Fluxnet is a global network for these measurement sites where components of the carbon cycle are monitored. The measurements are basically performed by the so-called eddy covariance technique (Baldocchi 2003), which is a micrometeorological method. Fluxnet integrates different regional networks.

Vertical fluxes of momentum, water vapor and carbon dioxide are measured at the Fluxnet sites using half hourly or hourly basis, usually covering many years of semi-continuous measurements. Fluxnet collects information about the geographical location of the flux towers, and provides infrastructure to archive and disseminate measurement results. Fluxnet also fosters the cooperation between researchers and supports synthesis studies that can improve our understanding of the terrestrial carbon balance.

The growth of Fluxnet is shown is Fig. 2.2-2 with the contributing sites on different continents.

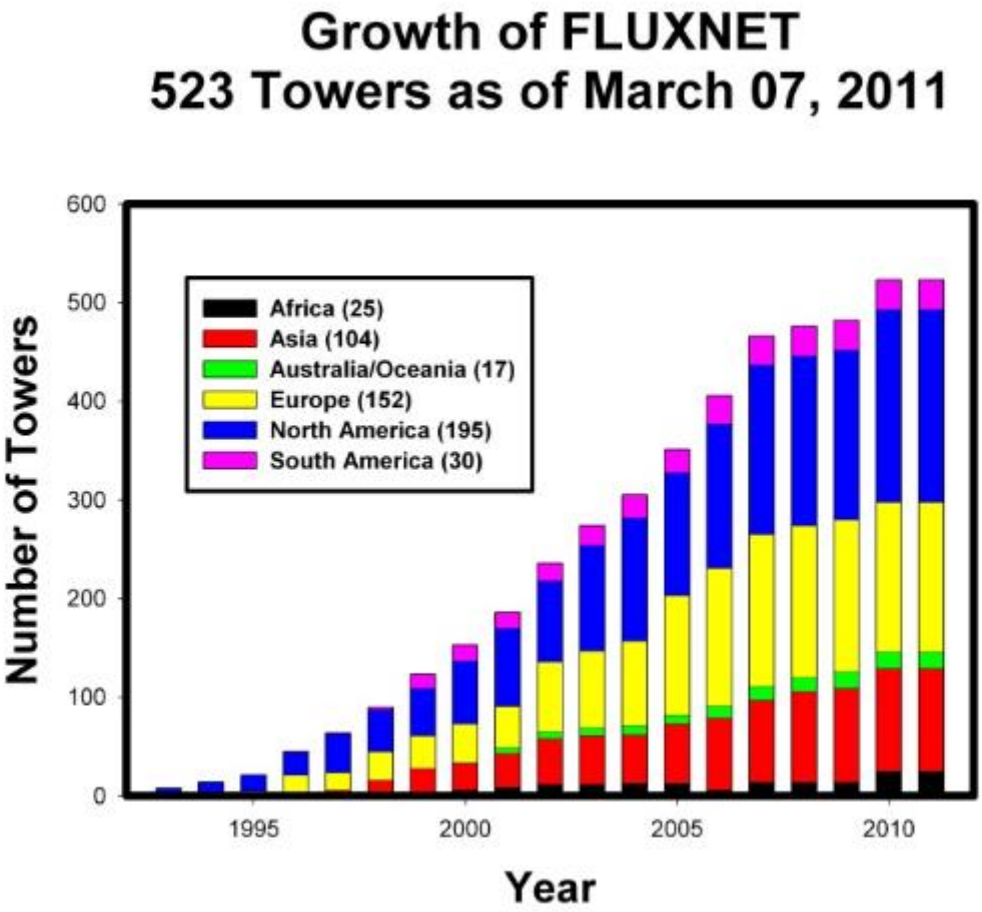


Figure 2.2–2 The growth of Fluxnet.
Source: www.fluxnet.ornl.gov/fluxnet/graphics.cfm

GHG Europe and its predecessors (CARBOEUROPE cluster)

In Europe the carbon cycle related research is historically performed in a coordinated way. Since the beginning of the 2000s the carbon cycle related projects were integrated into the CARBOEUROPE cluster (www.bgc-jena.mpg.de/public/carboeur/). This cluster consisted of different projects with emphasis on specific questions (e.g. dealing with airborne measurements, deployment of tall tower based greenhouse gas measurements, age related dynamics of carbon balance, carbon balance of grasslands, etc.). The projects were funded by the European Commission (DG Research). The cluster included projects AEROCARB and CHIOTTO, where some of the BioVeL partners were also included.

The CARBOEUROPE coordinated effort was continued in the framework of the CARBOEUROPE-IP project (www.carboeurope.org; also funded by the European Commission, within the 6th framework programme). The aim of the 5-years-long project was to quantify the European carbon balance using different approaches at local, regional and continental scale. Atmospheric (tower-based and airborne) concentration measurements, biospheric eddy covariance measurements and remote sensing was combined to provide an integrated picture about the European carbon cycle, and its associated uncertainties. The main findings of the project are summarized in Schulze et al. (2009).

The follow-up roject of CARBOEUROPE-IP is the GHG-Europe project (Greenhouse gas management in European land use systems, funded by the 7th framework programme of the European Commission). The main aim of the project is to gain better understanding on the European carbon and greenhouse gas balance with special emphasis on management of the carbon sequestration and minimization of the greenhouse gas emission. Following the logic of CARBOEUROPE-IP the project also deals with measurements and modelling of nitrous oxide and methane emission on the European scale. Advanced modelling experiments are performed within the framework of GHG-Europe using different, state-of-the-art biogeochemical models including Biome-BGC.

ICOS

Based on experiences of the European, carbon cycle related research projects (GHG-Europe and its predecessors; see above) it became clear that the operation of the long term measurement sites are highly depend on the availability of fundings. It means that some measurement sites that already provided invaluable information about specific ecosystems has to be shut down due to closure of funding. ICOS (Integrated Carbon Observing System) is a new research infrastructure that provides the long term observations that are essential to carbon cycle research. In the framework of ICOS the standardized, high precision, well developed monitoring sites can be secured. ICOS will build a coherent, precise database that can be used in the estimation of the continental scale greenhouse gas balance. ICOS also contributes to the of the Integrated Global Carbon Observation System (IGCO) and supports the monitoring obligations of Europe under the United Nations Framework Convention on Climate Change (UNFCCC). Ultimately, ICOS will suppurt the estimation of the present state and forecast of the future behaviour of the carbon cycle.

Similarly to the CARBOEUROPE approach, advanced modelling experiments will be performed within the framework of ICOS to support the estimation of the carbon cycle and the estimation of the magnitude of the climate-carbon feedback.

University of Montana, Numerical Terradynamic Simulation Group

This cutting-edge research group is referred in the ecosystem functioning and valuation part of the report (see chapter 2.1.3).

2.2.4 Evaluation of existing models and methods

Carbon cycle is a deeply interdisciplinary research area. Ecologists, biologists, soil scientists, hydrologists, mathematicians, foresters, agronomists, meteorologists, and scientists from other scientific fields are working together to address the complex questions related to the global carbon cycle. The main aim of the researchers is to understand the present state, and to estimate the future evolution of the carbon balance components and its interaction with the climate system.

Based on the quickly increasing amount of experimental data (including in situ measurements and remotely sensed readings; e.g. Baldocchi et al. 2001) it is possible to construct and develop mathematical models that attempt to quantify the elements of the carbon cycle. There are different types of models: the complexity ranges from simple, regression based models to complex, process oriented models. The models are designed to give answers to specific questions. For example, a model can be designed to estimate the amount of carbon sequestered by newly planted forests. Other models address the competition of species under specific environmental conditions. The most sophisticated models can be used to predict the future of the carbon cycle and its interaction with the changing climate.

A typical process based biogeochemical model handles many different “pools”, and a number of “fluxes” between the pools to simulate the plant-soil system. These pools usually include foliage, aboveground biomass, belowground biomass (roots), litter, soil carbon pool, and in some cases nitrogen content of different compartments. The pools can be differentiated as e.g. soil organic matter (SOM) with different turnover times (e.g. quickly decomposing SOM, more stable SOM, and stable SOM like humus). As water cycle is closely coupled with the carbon cycle of plants the models usually predict the water balance within the plant-soil system including canopy water interception, runoff, soil moisture content and evapotranspiration.

The models are usually driven by meteorological data (air temperature, precipitation amount, solar radiation, relative humidity or vapor pressure deficit, etc.) and soil parameters are also essential for the simulation (Vetter et al. 2008). Some models can handle nitrogen cycle (or even phosphorous cycle) which means that nitrogen (or phosphorous) availability has to be provided by the user. Some models use a number of ecophysiological parameters which control the main processes (e.g. photosynthesis, autotrophic respiration, heterotrophic respiration), the allocation of carbon (and sometimes nitrogen) into the different plant pools, plant phenology, plant mortality, management, disturbance, etc.

In case of process based models the simulation has two phases. The first is the spin-up (self-initialization) simulation, which runs until a steady state is reached with the climate in order to estimate the initial values of the state variables. The second phase is the normal simulation that provides results that can be analyzed by the user.

Traditionally, carbon cycle models were developed to simulate biogeochemical cycles of undisturbed ecosystems. However, as large areas of the land surface are managed, the undisturbed assumption is not applicable and turned out to cause significant bias in the model simulations. Therefore, some of the existing biogeochemical models have already been extended to simulate the carbon and water cycles of managed ecosystems (forests, croplands) with higher accuracy.

Model structural developments and model calibration techniques (model-data fusion) can jointly be used to improve the biogeochemical models (Wang et al. 2009; Hidy et al. 2012). Improved modelling techniques might provide invaluable information about the future of our climate system, and can inform policy-makers about the possible dangers of the climate-carbon cycle feedback mechanism. Carbon cycle related modelling efforts can also support food security and sustainable development in our changing world.

There are a number of biogeochemical models that have been developed for the quantification of the carbon balance components (ORCHIDEE-STICS, LPJmL, SiBcrop, JULES-SUCROS, BIOME-BGC, MOD17, CCASA, NETWORK_ANN, PIXGRO, CERES-EGC, PASIM, PnET, CENTURY, DNDC, GOTILWA+, ROTH C, CO2FIX, CASMOFOR, JSBACH, plus many more; see Vetter et al. 2008 for the detailed description of some typical models). As Biome-BGC was chosen to be used within the frame of BioVeL, and additionally as Biome-BGC is a typical biogeochemical model, in the following sections we mainly deal with Biome-BGC. Note that Biome-BGC is also rather typical considering the practical application of biogeochemical models in general (e.g. meteorological data requirement, parameterization, etc.).

We also describe a typical, data-oriented model called MOD17 which also demonstrates the applicability of remote sensing in carbon cycle research. Note that Biome-BGC and MOD17 were developed by the same institute described above (University of Montana, Numerical Terradynamic Simulation Group).

Biome-BGC

Biome-BGC is a process-based, mechanistic biogeochemical model that can be used to simulate carbon, nitrogen and water fluxes of different terrestrial ecosystems, including evergreen and deciduous forests, grasslands and shrubs (Running & Hunt 1993; White et al. 2000; Churkina et al. 2003; Vetter et al. 2008; Trusilova et al. 2009) as we described it in general in chapter 2.1.4.

MOD17

The MODerate resolution Imaging Spectroradiometer (MODIS) sensors onboard NASA EOS Aqua and Terra satellites provide remotely sensed information in global coverage in every 1 to 2 days. The MOD17 product (which is one of the several products derived from the measured radiance signal and ancillary information) provides Gross Primary Production (GPP) estimates with 8 days, and Net Primary Production (NPP) estimates with annual temporal resolution and 1 km spatial resolution.

The GPP model of the MOD17 product (i.e. the MOD17 model) is a light use efficiency based model (Monteith 1972, 1977). In this simple model, the theoretical maximum of light use efficiency is decreased by abiotic stress factors according to environmental conditions. GPP is determined by the actual value of light use efficiency and the amount of available photosynthetically active radiation (APAR). APAR can be calculated as a product of incident PAR and fraction of PAR absorbed by the vegetation (FPAR), which shows the amount of radiation absorbed in percentages.

The model can distinguish between 11 plant categories (Plant Functional Types, PFTs). PFT specific model parameters are stored in the biome properties look-up table (BPLUT) for each PFT. These parameters do not vary with geographical location, as they characterize biomes globally.

Net photosynthesis (GPP minus maintenance respiration of fine roots and leaves) calculations in the MOD17 model are based on exponential function of daily average temperature and the amount of biomass. Further parts of autotrophic respiration that are necessary to determine net primary production (NPP), such as growth respiration and annual maintenance respiration, cannot be calculated on daily basis with the algorithm logic used in the model (for details, see Running et al. 1999); therefore, NPP is given in annual data files.

The algorithm of the MOD17 model requires input databases from other MODIS products in case of FPAR (MOD15 LAI & FPAR product; Knyazikhin et al. 1999) and land cover information from the MOD12 product (Strahler et al. 1999). Data requirements for GPP calculations include daily global radiation, vapor pressure deficit and minimum temperature.

2.2.5 Evaluation of data source requirements of Biome-BGC

The three kind of datasets (site characteristics, vegetation eco-physiological parameters and past-present-future meteorological datasets) are discussed already in very detail in the chapter 2.1.5.

2.2.6 Identification and description of typical and most challenging workflows

A basic and typical workflow scheme to run Biome-BGC model is given in the chapter 2.1.6, so we identified here a more specific one with a great potential to gain a lot from scientific workflow and web service approach.

The Biome-BGC model has a long history, especially in carbon cycling simulations (Running & Coughlan 1988, Running & Gower 1991, Running & Hunt 1993, White et al. 2000, Thornton & Rosenbloom 2005, Hidy et al. 2012) and has further perspectives, because the model algorithm itself is under continuous and various improvement by several research teams. The newer versions of the model needs exhausting testing, validation and calibration by field-measured datasets. On the other hand, local or regional modeling and calibration of model parameters is one of the best approach to improve the results of field-based research projects. The model has a non-linear behaviour, so the model calibration requires a hugh demand of computational resources due to the high number of independent parameters. Accordingly, one of the most challenging scientific workflow is the ’data-model-harmonization’ (or in other words data-model fusion, data assimilation or calibration) by global optimization (Van Oijen et al. 2005, Wang et al. 2009, Trusilova et al. 2009, Wang et al. 2009, Hidy et al. 2012) as it is demonstrated in Fig. 2.2–3.

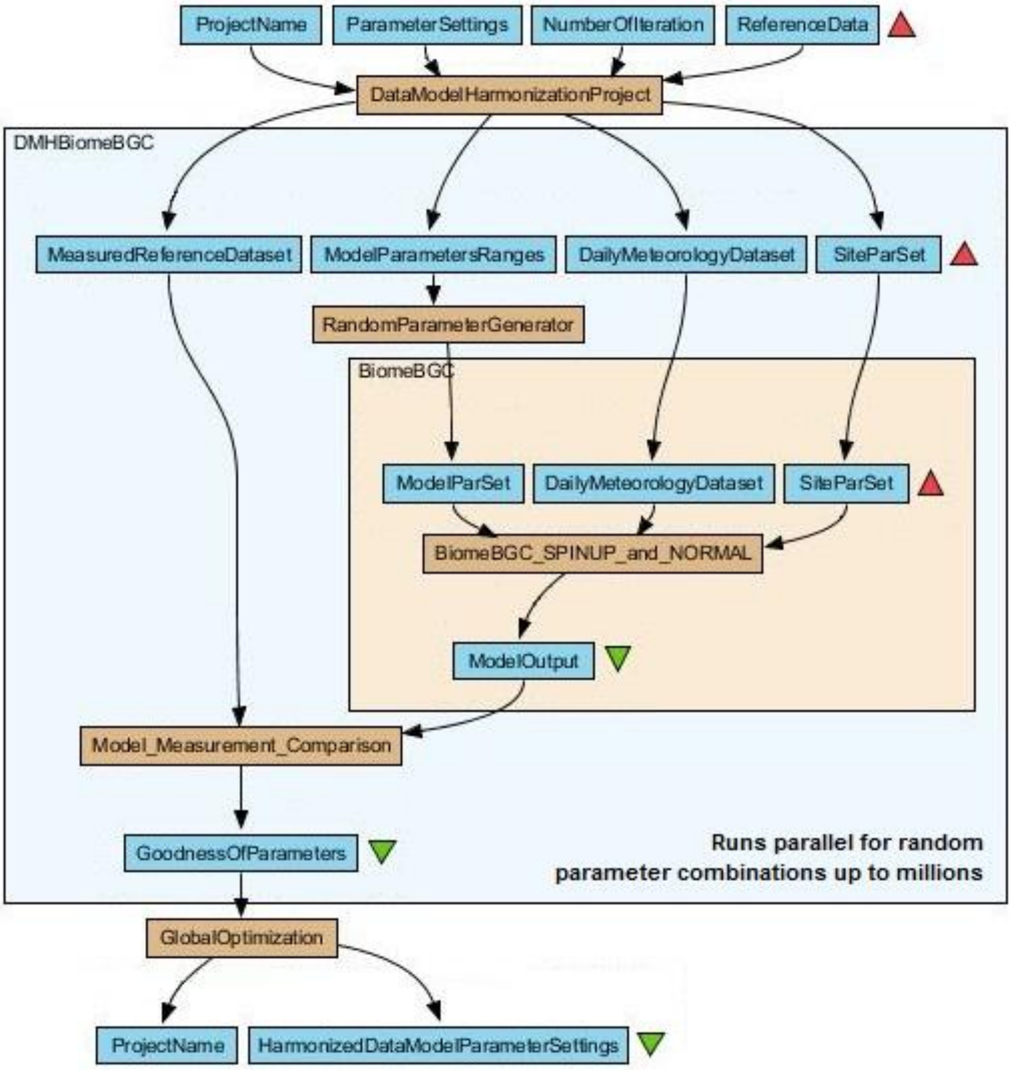


Figure 2.2–3 A possible workflow scheme to perform a complex 'data-model-harmonization' project run of the Biome-BGC model. The parallel parameter study can counts millions of executions

In this workflow the Biome-BGC model is embedded in a 'parameter sweep study' loop, which could achieve hundreds or thousands of runs, up to a millions in some cases. The huge number of simulations costs enormous computation time (i.e. weeks) on a standalone computer, but parallel service on desktop grids can provide an affordable solution (i.e. Anderson 2004, Kacsuk et al. 2009). The presented workflow scheme points out the main methodological steps (randomization of parameters, running the model, comparison of model output to reference measurements, global optimization of the model parameters), but does not deal with technological components of the workflow necessary to manage workunit packages for parallel computation.

2.2.7 Evaluation of web service requirements

Based on literature review we have found only two projects that already started to work on web service technology related to carbon sequestration modeling. The ARIES Consortium recently published a Bayesian statistical modeling approach based on conditional probability calculations developed in several case studies (Bagstad et al. 2011). They are working on an on-line GIS tool linked with Bayesian models to calculate basic ecosystem service indicators to support decision making. Existing carbon inventories and results of deterministic modeling (i.e. Biome-BGC) were noticed to apply as possible future improvements.

Another on-going project is the Digital Observatory for Protected Areas (DOPA) that has to be mentioned here. It was created by the Joint Research Centre of the European Commission (JRC) in collaboration with other international organizations. DOPA is conceived as a set of distributed databases combined with open, interoperable web services to provide end-users with information to assess, monitor and forecast the state and pressure of protected areas at the global scale. One of the planned modules will focus on ecosystem services (see: http://dopa.jrc.ec.europa.eu, and www.earthzine.org/2012/06/27/remote-sensing-emerges-as-an-important-tool-for-habitat-and-species-conservation/).

In the light of these trends and the Model Web concept (Geller & Turner 2007, Khalsa et al. 2009) we have to consider our efforts as a hot topical work. The proposed web services are very important elements of scientific workflows. These could easily embed access to large datasets, complex modeling processes and computation demanding tasks, which three are the main requirements for web service development.

2.3 INVASIVE SPECIES RESEARCH AND MANAGEMENT

by
Annamaria Fenesi, Päivi Lyytikainen-Saarenmaa, Hannu Saarenmaa, Sarah J. Bourlat, Norman Morrison, Matthias Obst, Gerard Oostermeier and *Vera Hernandez Ernst*

2.3.1 Science-policy context

2.3.1.1 Ecological impacts and invasive dynamics

The introduction of non-native organisms beyond their natural range was highly facilitated by the increases in the extent and volume of trade and transport over the last decades (Hulme 2009). The number of deliberately or accidentally introduced species (adventive or alien taxa) show surprisingly high numbers on each continent (e.g., > 11,000 alien species in Europe, Hulme et al. 2009a), and habitats completely free from non-native species no longer exist. Invasive alien species (IAS) are capable of rapid population expansion threatening ecosystems, habitats and species, and causing ecological, economic and human-health impacts (Convention on Biological Diversity 2008). Therefore, interest in the science and management of biological invasions has expanded rapidly over the last decades.

Biological invasions affect biodiversity worldwide at various scales (Manchester & Bullock 2000; Davis 2003). At local and regional level they were shown to affect native species, reduce biodiversity, threaten endangered species and alter communities (Vilá et al. 2011). At the global level, invasive alien species have been pointed out as the second cause of species extinction (after habitat deterioration or loss, Wilcove et al. 2008). They are also widely heralded as the cause of homogenization of floras, because due to many introduction events, the originally different phytogeographical units become similar (Hejda et al. 2009).

The vast majority of introduced alien species (also called non-indigenous, alien, non-native, or exotic species) is not invasive. So, the establishment of an introduced species does not necessarily constitute a problem, but the ability of some species to rapidly attain sufficiently high abundance can alter both abiotic and biotic processes of the invaded community (Siemens & Blossey 2007). The impact of IAS is most pronounced on the performance and population dynamics of individual resident species within the same trophic levels (Vilá et al. 2011). For example, invasive plant species can reduce local plant diversity in several ways: competitive replacement through shading, resource competition and/or allelopathy (Werner et al. 2010; Callaway & Ridenour 2004), reduction in colonization rate of native species (Yurkonis & Meiners 2004), altered abundance and structure of soil pathogens and mutualists (Klironomos 2002), competition for pollination services (Brown et al. 2002), modified fire regime (Epanchin-Niell et al. 2009), hybridization with native species (Huxel 1999), and so on.

At the same time, biological invasions can also alter community structure at higher trophic levels (Levine et al. 2003). Several studies report different impacts of plant invasions on the composition, diversity and behaviour of consumers, pollinators and decomposers. For instance, plant invasions have a high potential to affect soil fauna, thus modifying the resource cycling of the conquered habitats, altering this way the processes of the whole ecosystem (Levine et al. 2003). The most often cited ecosystem level changes after the establishment of IAS are the impacts on nutrient cycling and soil properties, on hydrology, on fire regime and on physical structure of habitats (Simberloff 2011; Strayer 2012). For example, the invasive annual yellow star thistle (Centaurea solstitialis) increased summer water use by 105-120 mm yr^{-1} in the invaded dry sagebush ecosystems in California (Gerlach 2000).

Climate change, with associated temperature increases, sea level rises and changes in ocean chemistry is expected to increase the impact of invasive species on ecosystems (Mainka & Howard 2010). For example, the common carp (Cyprinus carpio), a native of Asia, is already invasive in many parts of the world, and has the effect of decreasing water quality by increasing turbidity and thereby destroying nesting habitats for other native species of fish. It is expected that increases in water temperature due to climate change will provide more suitable habitats for this species to invade (Kolar & Lodge 2000).

Native invasive species. In addition to invasive alien species, also many native species have been observed to change their status as damaging agents as a consequence of climate change. This includes population dynamics, outbreak cycles, and the intensity and the spatial scale of epidemics. Climate change and more extreme weather patterns (drought, storms, high temperatures) can magnify the intensity of disturbances by biotic agents in different ecosystems, altering e.g. the geographical species range and plant productivity, particularly at higher latitudes (IPCC 2007). During global warming, increases in stress factors and insect outbreaks have been predicted (Volney and Fleming 2000, Walther et al. 2002). Due to rapid responses to changing temperatures pest insects can flexibly change their survival, development, reproduction, dispersal and geographic distribution (Bale et al. 2002; Musolin 2007; Régniére 2009). This can involve both a simple demographic adaptation and a genetic adaptation. Increasing numbers of pest insects have already begun to expand from their normal geographic ranges within native areas, either poleward latitudinally or upward altitudinally (Battisti et al. 2006; Musolin 2007; Vanhanen et al. 2007), or changed their pest status within their native ranges (De Somviele et al. 2007). Increased outbreak frequencies and spatial scales of e.g. forest pests evidently have already taken place during the most resent decade in Finland, particularly with pine sawflies (Virtanen et al. 1996; De Somviele et al. 2007) and bark beetles (Pouttu and Annila 2010).

Prediction of the changes in the distribution of species at different scales – both global and local - has become a topical issue in ecological research (Lyytikäinen-Saarenmaa et al. 2006; De Somviele et al. 2004, 2007). In addition to long-term trends, short-term projections are also highly needed, due to e.g. enlarged occurrences of native defoliators (Lyytikäinen-Saarenmaa 2008) and wood-boring insects (Lindelöv & Schroeder 2008), as well as plant diseases (Hantula 2010; Hantula et al. 2010; Nevalainen et al. 2010). Development of modern methods to improve projection of distributions of climate-driven disturbance agents is urgently needed.

In general, the knowledge on second and third grade ecological implications of invasions is scarce, while many potentially important mechanisms have been described. For example, a surprisingly large number of non-indigenous species benefit indirectly from interactions with other introduced or native species (Simberloff & von Holle 1999; Richardson et al. 2000; Ricciardi 2001). Simberloff & von Holle (1999) coined the term ‘‘invasional meltdown’’ to describe the positive interactions between non-indigenous species that facilitate eachother’s survival and accelerate the rate of successful invasion. This can take many forms. For example, introduced animals such as insects, birds, rats, and mammalian herbivores act as pollinators or dispersal agents for exotic plants (Loope & Snowcroft 1985, Barthell et al. 2001). Non-indogenous species can also have habitat-modifying effects by altering the physical or biological environment in their invaded range, making it more suitable for some species (facilitation), and less so for others (inhibition) (Stachowicz 2001; Bruno et al. 2003). For example, filtering by zebra mussels (*Dreissena polymorpha*) has improved water clarity in light-limited lakes, thereby accelerating the spread of a number of introduced macrophytes (MacIsaac et al. 1992, MacIsaac 1996).

Populations that can rid themselves of parasites and pathogens face altered selection pressures and may exhibit changed population dynamics (Colautti et al. 2004). Introduced populations often start from a very small founder population, and this is likely, by chance, to capture only a subset of the parasites and pathogens that exist in the parental population. Thus, introduced populations usually exhibit lower parasite and pathogen diversity than their parental population (Mitchell & Power 2003; Torchin et al. 2003). This release from the full effect of parasites and pathogens (‘enemy release’) is a likely cause for the spectacular success of many introduced species (Williamson 1996; Keane & Crawley 2002).

2.3.1.2 Economic impacts on ecosystem services and human well-being

Biological invasions of nonindigenous species today are among the most significant threats to global biodiversity. The direct economic impact caused by invasive species through lost ecosystem services, expensive prevention and eradication efforts, and increased human health problems are calculated to exceed $120 billion annually just in the United States (Pimentel et al. 2005). At the same time, the number of reports of new alien species is growing rapidly on a global scale (Ricciardi & MacIsaac, 2008; Richardson & Pyšek, 2008).

All the shifts in the structure and function of communities and ecosystems caused by the spread of IAS and the impact of climate change to native species are translated to global consequences of well-being (Millennium Ecosystem Assessment 2005), including the wholesale loss or alteration of ecosystem goods and services. However, the environmental and societal costs are often ignored in impact analyses of even the best-documented IAS (Pejchar & Mooney 2009). The repercussions of invasive species on ecosystem services are highly variable. Among the provisioning services (e.g. food, timber, fiber and water), some invasive species can fundamentally change the flow of water for drinking and irrigation, others can jeopardize the agriculture and food security. For instance, yellow star thistle (*Centaurea solstialis*), the above mentioned unpalatable invasive annual plant species costs California US$7.65 million annually in lost livestock forage and at least the same amount as control expenditure (Eagle et al. 2007). Among the regulating ecosystem services IAS may have severe impacts on pollination, water purification, pest control and natural hazards. These services are fundamentals of agriculture, forestry and fisheries, and therefore are an indispensable basis of human well-being (Pejchar & Mooney 2009). Another example, the chinese mitten crab (*Eriocheir sinensis*), a native of the yellow sea in China, and introduced to Europe through shipping and ballast water releases, is a migrating species, which breeds in sea water and migrates to inland waters as a juvenile. During these mass migrations, it can cause clogging of water intake filters of industrial cooling waters and drinking water plants (Gollasch 2011). Invasive species can also influence climate regulation by altering the carbon storage capacity of the invaded plant communities (Pejchar & Mooney 2009). For example, the replacement of native sagebush ecosystem in California by invasive annual grasses leads to a -0.5 µmol $m^{-2}s^{-1}$ loss of carbon sequestration over a large land area (Prater et al. 2006).

Because the management of invasive species is becoming central to many areas of environmental policy decision-making, economic valuation of IAS' damages is urgently needed. Several attempts have been made to quantify the economic impacts at national (e.g. US$14.45 billion in China, Xu et al. 2006, US$ 128 billion annually in the USA, Pimentel et al. 2005) or continental levels (US$13 billion in Europe, Hulme et al. 2009a). However, usually these figures are underestimates, as the potential economic and environmental impacts are known for just a small fraction of IAS (Hulme et al. 2009a). Besides, the mentioned damages on ecosystem services are difficult to convert into monetary terms therefore are regularly overlooked.

Invasive insects can cause yield losses in different agro-ecosystems. In forest ecosystems, for example, the estimated economic value of losses due to decreased radial growth and mortality of trees after consumption by insects could annually be € 50 – € 300 per hectare, depending on the intensity of damage and the feeding habits of the damage agent (Lyytikäinen-Saarenmaa & Tomppo 2002). During outbreak peaks, economic losses could annually be as high as € 500 - € 1000 per hectare. The ongoing, climate-impacted outbreak of the mountain pine beetle (*Dendroctonus ponderosae*) in British Columbia has spread over 18 million hectares and killed 435 million m^3 of timber. 80% of pine forests are expected to be killed by 2013. This will release almost a billion tonnes of carbon dioxide equivalent greenhouse gases into the atmosphere by 2020 (Kurz et al. 2008).

While there is certainly a need to increase existing knowledge of mechanisms, impacts and costs of biological invasions, it is also imperative that this information is translated into appropriate management responses. Early detection, implementation of optimal management options and of proper regulatory instruments are needed to control invasive species and to alleviate their salient ecological and economic impacts. Comprehensive national and international policy is crucial for ensuring coherent and effective planning and implementation of measures to master alien species invasion (McGeoch et al. 2010).

2.3.1.3 Countermeasures

Biological invasions are of a complex nature and to-date there are only a few general rules that govern the processes of invasive species management (Bright 1998). While many concepts of mechanisms behind invasions are only beginning to emerge (especially with regard to secondary or third grade implications), appropriate strategies for prevention and management of exotic species are under development. For example, many countries have ratified the IMO "International Convention for the control and management of ships´ ballast water and sediments" from 2004. Article 4 states that each country (party) shall ” develop national policies, strategies or programmes for Ballast Water Management in its ports and waters under its jurisdiction that accord with, and promote the attainment of the objectives of this Convention”. The aim of this convention is to prevent the potentially devastating effects of the spread of harmful aquatic organisms carried by ships' ballast water from one region to another.

Most policies agree on a few essential counter measures. These are

- Rapid discovery of invasive species greatly increases the chance that they can be eliminated (Myers et al. 2000). Eradication and control efforts for alien species are usually most efficient, and sometimes only possible, if the incursion is detected while populations are still relatively small and restricted in space (Parker et al. 1999; Myers et al. 2000; Bax et al. 2001). For this purpose, monitoring programs and sustained observations are essential as they facilitate early detection and eradication. Just as important, they may serve as a trigger for quarantine or control measures to limit their spread and impact on valuable resources.
- Identifying potential future invaders and taking effective steps to prevent their dispersal and establishment is much less costly than post-entry control (Ruesink et al. 1995; Reichard & Hamilton 1997; Kolar & Lodge 2002; Marchetti et al. 2004). At the same time, control of biotic invasions is most effective when it employs a long-term, ecosystem-wide strategy rather than a tactical approach focused on battling individual invaders.
- Analytical methods that evaluate the risk of an exotic species to an ecosystem need to be developed as well as new methods at the science-policy interface to increase the effectiveness of prevention of invasions.

Biotic invasions, especially human-mediated invasions typically consist of several successive stages: (A) engagement of propagules with a transport vector in a source location, (B) transport from source to recipient location, C) establishment of a propagule at the new location, then (D) development of a self-sustaining population, (E) spread through the new habitat, and (F) spread to other vacant habitat patches (cf. Mack et al. 2000, Sakai et al. 2001). In most cases the discovery of potential invasives takes place at the point of establishment, for example at Bodega Harbor, Bodega Bay, California, USA, nonnative species currently represent 71% of the total cover of the dock fouling community based on annual surveys conducted from 2006 through 2009 (Sorte et al 2010).

2.3.2 Main scientific questions

As in the case of greenhouse gas emissions, to handle the problems of invasive species, both scientific efforts and also national and international legislation are urgently and seriously needed. The theory of invasion ecology comprises many hypotheses designed to explain invasion success at a variety of temporal and spatial scales. However, this theoretical information can be highly different from what managers and policy-makers need to know to control the problem. Therefore we highlight several scientific issues which can help the science of invasion ecology to become more applied.

- Further research is needed to put invasion in an ecosystem context, instead of focusing narrowly on how a single invader affects a chosen ecosystem function.
- Consider how multiple drivers of ecosystems (other anthropogenic changes, habitat destruction, land-use change, climate change) may broaden our horizon to handle the IAS problem.
- Decide which changes to ecosystem function can be managed or mitigated, and which are unmanageable (Strayer et al. 2012), focusing research better.
- Use cutting-edge technologies for remote sensing (e.g. multi- and hyper-spectral imagery) to map invasions.
- Use cutting-edge molecular techniques for the early detection and accurate identification of invasive species, for example marine larval stages from ballast water tanks.
- Once an IAS has arrived, or a native species is becoming invasive, determine how the risk of spread, and damage can be predicted. Use new tools for modeling species distributions, abundance and spread from survey data, such as hierarchical spatial modeling, e.g. “spatial predictive process” model (Banerjee et al. 2008, Latimer et al. 2009), ecological niche modeling (Soberon & Peterson 2005), and ecological (meta)population modelling (Brook et al. 2009; Guisan & Thuiller 2005; Keith et al. 2008).
- What is the mechanism of introduction of a newly arrived alien species? Determine at which stage(s) in the life cycle the invasive species is most vulnerable, and whether those stages can be used as targets for more effective control or eradication? This requires demographic monitoring of populations followed by analyzing the population dynamics with transition matrix models (e.g. Ellis & Elphick 2007; Hansen 2007; Jongejans et al. 2006; Kanary et al. 2011; Morris et al. 2011).
- Are species rich native communities more or less susceptible to invasion by exotic species? Although fine-scale patterns have been taken as evidence that native richness protects ecosystems against invasions (Case 1990; Knops et al. 1999; Levine 2000; Kennedy et al. 2002), broad-scale patterns have led researchers to suggest the opposite (Stohlgren et al. 1999, 2003; Davis et al. 2000; Huston 2004).
- Are invaders drivers of rapid ecosystem change? A positive correlation between exotic dominance and decline in native diversity has been documented, but there is still little evidence of a cause–effect relationship (Gurevitch and Padilla 2004, Didham et al. 2005). Alternative explanation for such patterns are, that invaders often are successful in becoming established within communities that have been altered by human perturbations (Hobbs and Huenneke 1992).
- How strong are the ecological impacts of invasions from indirect mechanisms, like disease/parasite introduction by alien species (so called ‘spillover’), positive interactions among invaders (so called ‘invasional meltdown’),

population explosion due to host liberation from the parasite in the new area (so called ‘parasite release’).

- Are species rich communities more or less susceptible to invasion by exotic species?

2.3.3 Most relevant research groups, networks or projects

Delivering Alien Invasive Species Inventories for Europe (DAISIE).

The DAISIE project (www.europe-aliens.org) was funded by the European Commission (2005–2008) to create an inventory of European alien species in order to understand the environmental, economic, social, and other factors involved in alien invasions (Hulme et al. 2009b). The contributors are leading experts in the field of biological invasions, other European partners and stakeholders. The DAISIE database has collated information from terrestrial, marine and freshwater habitats, for fungi, plants, vertebrates, and invertebrates from up to 63 countries/regions (including islands) and 39 coastal and marine areas in both Europe and adjacent regions. Over 248 datasets, constituting more than 45 000 records on individual species alien to Europe were assembled and verified by experts (Vilà et al. 2010). This represents the largest database of alien species in the world, with more than 10 000 species alien to Europe. The database includes information on both the ecological and economic impacts of alien species in particular regions (Vilà et al. 2010).

Global Invasive Species Programme (GISP): 1997-2011

The mission of this independent not-for-profit association supported by the World Bank was to conserve biodiversity and sustain human livelihoods by minimizing the spread and impact of IAS. The programme follows two major objectives, (1) building of a well-coordinated and effective global network for control and management of IAS, through development and dissemination of information and best practice, and (2) to strengthen the capacity to address IAS at local, national and regional level through development of new assessment tools and delivery of training modules to assess and manage IAS. A part of the GISP is the Global Invasive Species Database (www.issg.org), which aimed to increase awareness about invasive alien species and to facilitate effective prevention and management activities. It was/is managed by the Invasive Species Specialist Group (ISSG) of the Species Survival Commission of the IUCN-World Conservation Union.

Global Invasive Species Information Network (GISIN)

GISIN (www.gisin.org) provides a platform for sharing invasive species information at a global level, via the Internet and other digital means. The GISIN encourages invasive alien species (IAS) data providers to share their data directly through GISIN, and then consider sharing with other networks. GISIN supports the sharing of types of invasive species data or data models (e.g. SpeciesStatus, Dispersal, Impacts, Management) that other networks such as the Global Biodiversity Information Facility

(GBIF) do not. GISIN works closely with representatives of many other data sharing networks, including GBIF and GEOSS, to better leverage our collective knowledge and technologies for data sharing and pursue effective solutions for avoiding duplication.

NOBANIS - European Network on Invasive Alien Species

NOBANIS (www.nobanis.org) is a gateway on to information on Invasive alien species in North and Central Europe. One of the main goals is to provide tools for implementing the precautionary approach against the unintentional dispersal of invasive alien species. It also establishes regional cooperation to aid countries in eradication, control and mitigation of these species. NOBANIS provides a a portal with access to information about the alien and invasive species of the region. This includes a central database with updated information from all the NOBANIS countries, factsheets of the most invasive species, access to an identification key to marine invasive species, newsletters, a species alert function for new invasive species to the region, an invasive species photo bank, and information about the national legislation on invasive alien species.

IUFRO division 7 on forest health

This division of the International Union of Forest Research Organisations (IUFRO) (www.iufro.org) includes among other things research on impacts of air pollution and climate change on forest ecosystems, physiological and genetic interactions between trees and harmful biotic impacts, environment/ pathogen interactions in forest decline, and the biology and control of forest tree insects and diseases. The division has over 30 working groups that are carrying out research on both invasive alien and native species, and applying methods of population modelling, niche modelling and climate change projections.

2.3.4 Evaluation of existing models and methods

2.3.4.1 Ecological niche modelling

The ecological niche is a widely used concept in analysis development. The ecological niche of a species can be defined as the conjunction of ecological conditions within which a species is able to maintain populations without immigration (Grinnell 1917). A species' fundamental niche is the set of conditions that allow long-term survival (Phillips et al. 2006), without being limited by biotic factors (Soberon & Peterson 2005). Realized niche is limited by external factors, as biotic interactions (e.g. competition, parasitism, predation) and historical factors (Fig. 2.3–1). Historical factors, such as geographic barriers and lack of sufficient dispersal opportunities may also influence species distribution (Patterson 1999). An ecological niche model can be an approximation of the fundamental niche, considering environmental dimensions and indicating its response to physical interactions. The main hypothesis for developing the ecological niche model will address the question of whether a species could survive and reproduce in certain kinds of conditions at any given place. A species is seldom able to occupy all of its potential geographical range, and the presence of other species as well as historical factors can reduce distributions to a subset of the potential range (Chase & Leibold 2003).

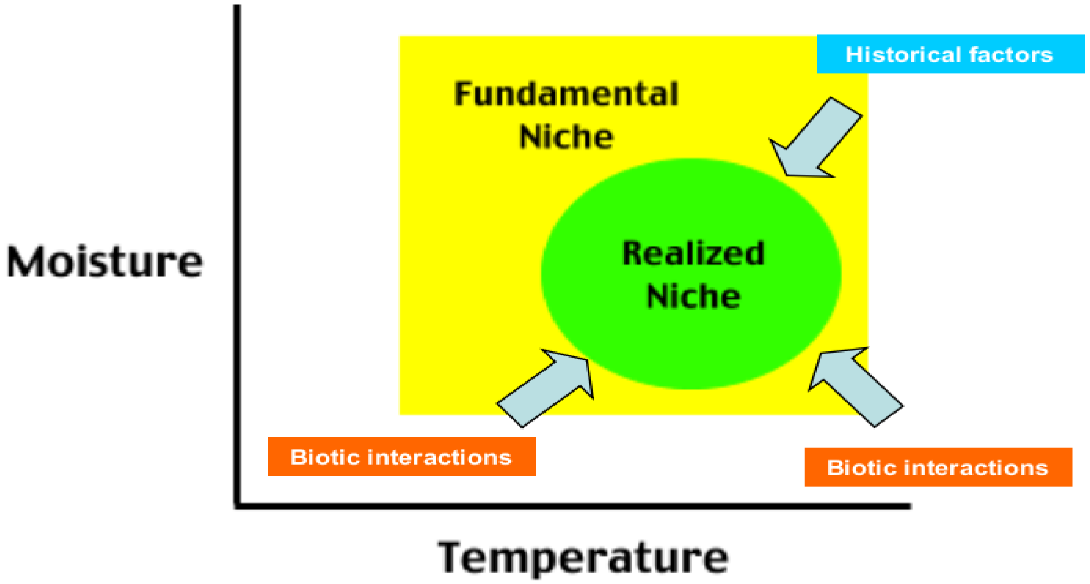


Figure 2.3–1 The yellow area represents a geographic area with appropriate set of abiotic factors for the species and may represent the geographic expression of a fundamental niche. The green area represents the right combination of abiotic factors, and an interaction of a species with biotic and historical factors, representing a geographic extent of a realized niche.
(Original image by Healy Hamilton).

A main challenge has been to ask which factors exert the highest impact while shaping the distribution of species. Much of the difficulty stems first from the lack of objective means for identifying areas of suitable habitat. Second, it is difficult to integrate how ecological and/or historical factors shape the species' actual distribution (Costa et al. 2008). Novel GIS (Geographic Information Systems) models may identify previously unsampled areas where species have a high probability of occurrence and have been applied successfully to predict the geographic distributions of several animal groups in a variety of ecosystems (Peterson 2001, Luoto et al. 2002, Guisan & Thuller 2005). However, these GIS niche-based models do not present species interactions or historical factors.

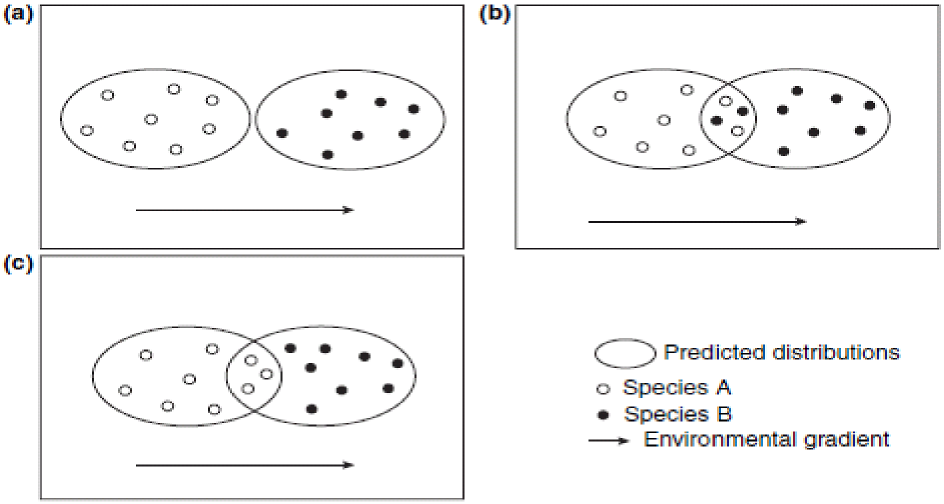


Figure 2.3–2 Predicted results of using niche modeling to investigate factors affecting distributions of closely related species along an environmental gradient. (a) Species do not overlap in their predicted distributions. (b) Both species occur in their predicted overlap zone. (c) Only one species occupies the predicted overlap zone. For more detailed explanation, see Costa et al. 2008.

Models focusing on the occurrence of closely related species in adjoining or overlapping areas along an environmental gradient will be useful when exploring competitive interactions and/or environmental characteristics in limiting and shaping species' distributions. According to Costa et al. (2008), this kind of analysis could provide three patterns (Fig. 2.3–2). First, if based on the niche-based model, two species do not overlap in their present predicted distributions. The explanation is that the distribution of both species is limited by unfavourable environmental factors, preventing expansion (Fig. 2.3–2a). Second, the model may predict an overlap zone in which both species can occur during prevailing favourable environmental conditions (Fig. 2.3–2b). Niche segregation (e.g. microhabitat, diet, activity time) allows the coexistence of both species. In the third possible pattern, only one species can occupy the predicted overlap zone. Favourable conditions may exist for both species, but one species competitively excludes the other. A historical factor may also exclude one of the species from the area in question (Fig. 2.3–2c). There is a need to analyze natural history data in order to unravel the possible impact of historical factors. Costa et al. (2008) found that niche models can predict overlapping niches for two pairs of amphibian species. In reality, the areas were occupied by only one species, indicating the role of competition and evolutionary history on a realized niche.

There are only a few studies exploring the idea of seasonal shifts of distribution of ecological niches as a part of species' migratory systems. Therefore the pattern of temporal niche changes is not so clear at the moment. Studies of migratory birds revealed patterns suggestive of some species being niche followers (i.e. using the same climatic niche year-round) and others acting as 'niche switchers' (i.e. changing niches between seasons) (Joseph 2003). According to Nakazawa et al. (2004), many nearctic-neotropical migrant bird species (ca. 28.6 %) effectively switch niches from one season to the other. A consistency with a hypothesis on niche conservatism in winter, but a derived state in breeding season was found with Passerina buntings (Martinez-Meyer et al. 2004).

A similar seasonal shift of ecological niche was found with an eastern migratory population of monarch butterflies (*Danaus plexippus*) (Oberhauser & Peterson 2003). Monarch butterflies overwinter in restricted areas in montane oyamel fir forests with specific microclimates in Central Mexico, preferring dry and cool conditions. According to projections of the monarch overwintering areas, no overlap was found between future potential overwintering areas and any present winter distribution. Ecological niche models identified the key limiting environmental parameters in species' response to climate change on switched niches (Oberhauser & Peterson 2003).

To summarize, environmental predictors can exert direct or indirect effects on species, arranged along a gradient from proximal to distal predictors, and are optimally chosen to reflect the three main types of influences on the species (see Huston 2002):

- limiting factors (or regulators), defined as factors controlling species eco-physiology (e.g. temperature, water, soil),
- disturbances, defined as all types of perturbations affecting environmental systems (natural or human-induced), and
- resources, defined as all compounds that can be assimilated by organisms (e.g. energy, water). These relationships can cause different spatial patterns to be observed at different scales (Fig. 2.3–3), often in a hierarchical manner (Pearson et al. 2004, Guisan & Thuiller 2005).

Increasing numbers of studies suggest that global warming effects are dramatically increasing at the present. Populations of different organisms, as well as communities and ecosystems are affected by changing environmental conditions (Parmesan and Yohe 2003, Root et al. 2003). These effects could be direct, through the influence the weather can have on the insect's physiology or behaviour (Parmesan 2007, Merrill et al. 2008), or may be mediated by host plants, competitors or natural enemies (Bale et al. 2002). Biological response is particularly prevalent in the northern sub-boreal, boreal and subarctic ecosystems, where the warming signal is strongest (IPCC 2007). Mass extinction of species and losses in biodiversity at the global level are accelerating due to climatic change (Harte et al. 2004). The need to understand the impact of climatic change and make past, present and future scenarios of species distribution is important, in order to present recommendations and solutions to policy-makers. This situation calls for approaches that have greater anticipatory potential, whereby extrapolation and prediction based on quantitatively validated models become key steps.

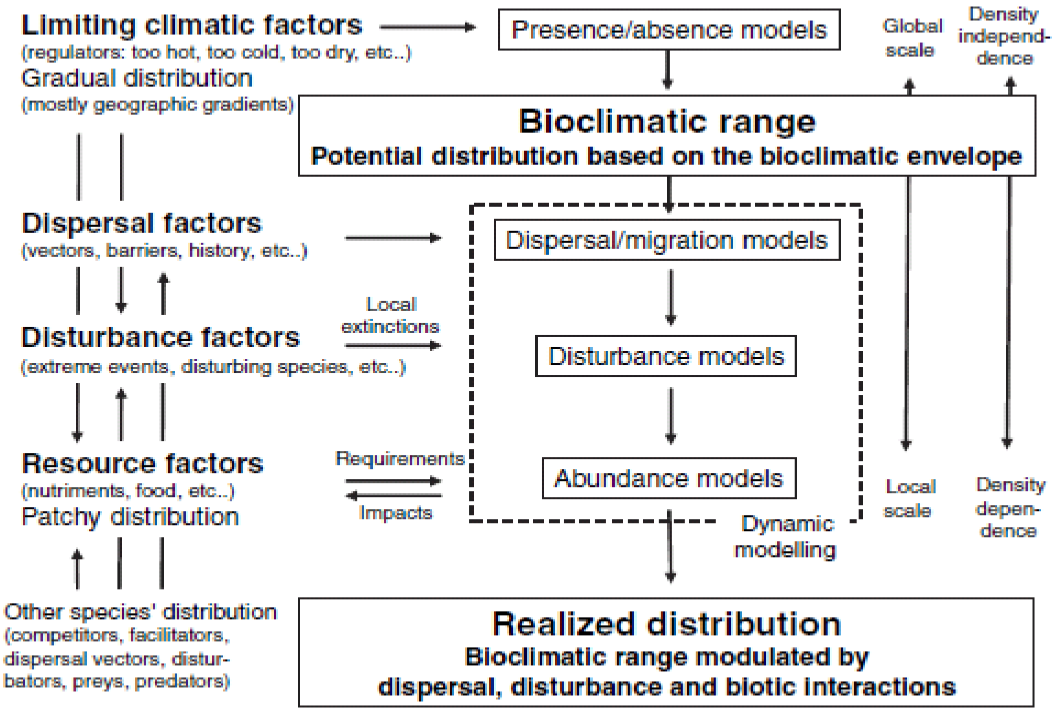


Figure 2.3–3 General hierarchical modelling framework illustrating the way to integrate disturbance, dispersal and population dynamics within currently static species distribution models. For more details, see Guisan & Thuiller (2005)

In recent years, predictive modelling of species distributions has become an increasingly important tool to address various issues in ecology, biogeography, evolution and conservation biology, connected with climate change research (Guisan and Thuiller 2005). Researchers have used GCM-derived (General circulation models) climate projections to predict a variety of climate change impacts. For example, there are projections to predict the future extinction rates of butterfly species (Oberhauser & Peterson 2003) or plants (Araujo et al. 2004), to evaluate conservation policies (Harrison et al. 2006) and to assess the risk of invasive species (Peterson et al. 2007, Mika et al. 2008). Another option is to use IPCC climate change scenarios. The global average surface temperature is projected to increase by 1.4 to 5.8^{o}C by the year 2100. Calculations are based to SRES emission scenarios A1, A2, B1, and B2 (IPCC 2001). Vanhanen et al. (2007, 2008) projected distributions of two moth and three bark beetle species, which were based on IPCC scenarios. Hsu et al. (2012) simulated climate change impacts on forests and associated vascular epiphytes in the mountains of Taiwan. For wider areas than continents, the US Geological Survey's Hydro-1K data set (US Geological Survey 2000) as well as the WORLDCLIM dataset (Hijmans et al. 2005) have been applied. Native climate data has also been adopted for distribution models, as data produced by the Finnish Meteorological Institute. The climate data included mean values for the period 1991-2003 at 10 x 10 grid system and were successfully used for predictions of 17 butterfly species (Luoto et al. 2005).

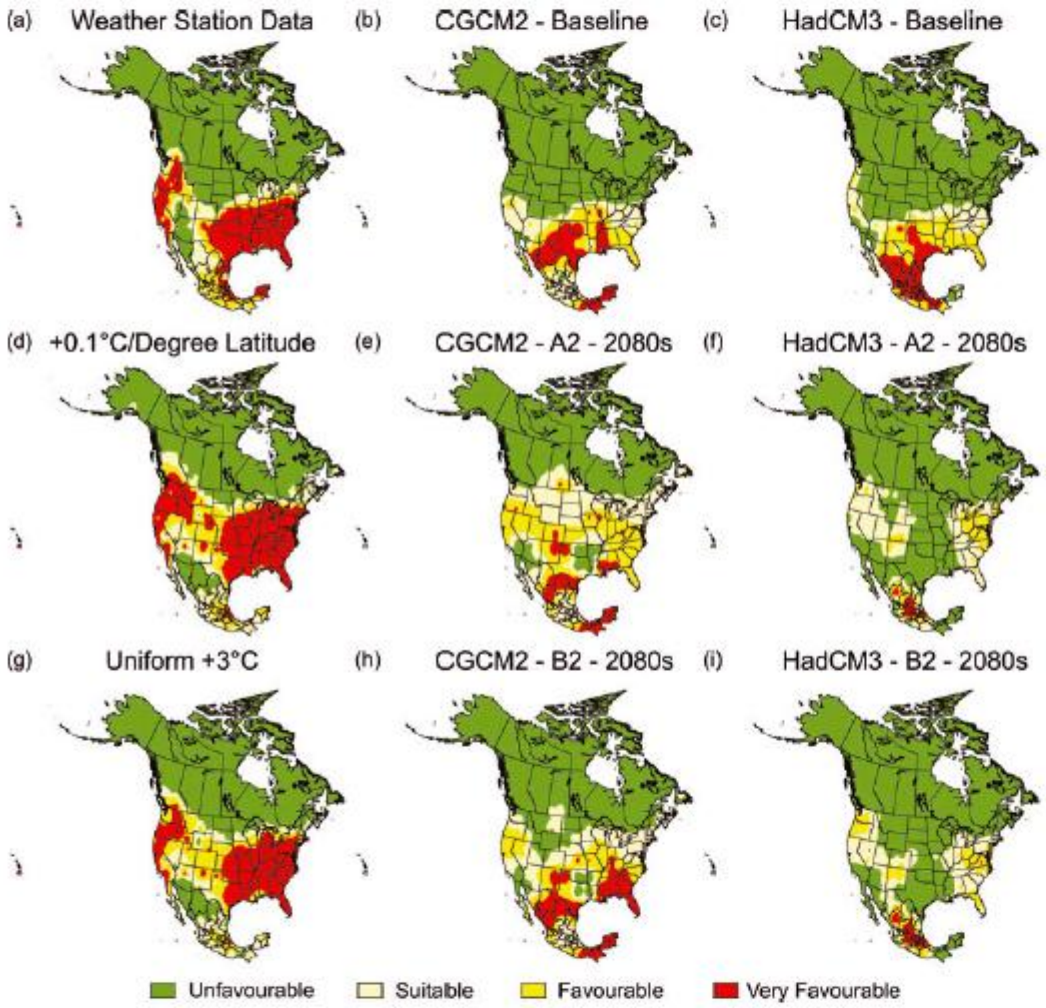


Figure 2.3–4 Ecoclimatic Index (EI) values for *Liriomyza huidobrensis* in North America using the (a) weather station data and (b) Canadian Centre for Climate Modelling and Anasysis GCM (CGCM2) and (c) Hadley Centre climate model (HadCM3) baseline period (1961-1990). The results from the bioclimatic envelope model (BEM) when using (d) an increase of 0.1 ^{o}C per degree latitude or (g) a uniform increase of 3 ^{o}C everywhere are shown. The BEM results when using GCM climate change projections in combination with the A2 scenario for (e) CGCM2, and (f) HadCM3 are shown for the 2080s. The B2 scenario projections for (h) CGCM2 and (i) HadCM3 are also shown for the 2080s. Unfavourable climate represents EI<10, suitable is 10<EI<20, favourable is 20<EI<30, and very favourable climate is EI>30. For more details, see Mika & Newman (2010).

There are two options to consider with respect to climate projections: (1) which models to use and (2) which climate scenario to use. The choice of climate scenario may impact the conclusion of the study. E.g. Mika & Newman (2010) assumed that the projected areas will depend on a choice of climate change scenario (Fig. 2.3–4). Kriticos et al. (2006) found that the variability between different GCM climate projections was as large as the difference between different emission scenarios. Several scientists have suggested that modelers should always use climate change projections from more than one GCM when studying the impacts of climate change on a biological system (e.g. Newman 2006). Therefore, model projections have often used GMC results from the Hadley (Pope at al. 2002) and Canadian (Flato et al. 1999) climate change modelling centers as the basis for future climate projections. Furthermore, from the Hadley Centre (HadCM3 model) and the Canadian Climate Change Modeling Centre (CGCM1 model) two scenarios have been assessed: one conservative and one less conservative of how climates could change over the next 50 years using the B2 and A2 emission scenarios (e.g. Peterson et al. 2004).

The major unanswered issue in species distribution modeling is environmental data selection. Which environmental factors we choose depends largely on data availability and to a lesser extent on our understanding of the causal mechanisms behind species distributions (Dormann 2007). Selection of environmental data may reflect the typical practices. In general, the environmental data used for each region are determined according to the relevance to the species in question. Most of the studies do not address the problem of environmental data selection, which is typically met with a limited number of data sets available. There are no statistics provided for the power of the environmental datasets. E.g. monthly climate variables may be much more effective than annual climate averages, suggesting the variables typically used are not the best possible variables (Stockwell 2006). In addition, many researchers employ only climatic variables, neglecting all the biotic interactions.

An overview of the questions associated with the species distribution models will be the following. For a review on the role of environmental drivers, see Dormann (2007).

- How to solve the serious problem with several national institutes not willing to share their data?
- How to choose environmental variables?
- Are all the algorithms freely available in order to compare the projections?
- Would the poor performance of some algorithms be connected with a wrong decision of climate variables? See e.g. performance of BIOCLIM according to Elith et al. (2006).
- How do limiting factors act throughout a species' range? Would their impact change with environmental change?
- How does environmental change affect biotic interactions / genetic structure / phenotypic plasticity / evolutionary changes of species?
- Are trends valid beyond the range of present data?
- Environmental change scenarios may be spatially uncertain?
- Do environmental drivers have non-linear effects on species distribution patterns?
- Do drivers have interactions and do they correlate with each other?
- Are data points in space independent?
- Are there georeferencing errors / misidentification with species occurrence?
- Presence – absence data have low information content. Can we add some additional information into data points?

- Do we have too low sample size, which may lead to an inadequately simple model? What is the minimum number of occurrence points required to produce an accurate model?
- Can we increase awareness of climate change impacts on biodiversity to garner support for expanding conservation?

According to Dormann (2007), the following steps are vital to a development of species distribution model-based forecast. Firstly, there is a need to identify where the largest contribution to projection uncertainty comes from, i.e. what introduces most variability (e.g. quality of raw data, choice and collinearity of variables, type of modelling approach etc.). A second step is a critical comparison and parallel construction of static statistical and dynamic individual-based species distribution models. A third step is a validation of model projections, which must play a more prominent role, e.g. with data sets from different time periods, or using field experiments in various parts of a species range to assess drivers.

Algorthims used for ENM

There are several methods for niche or species distribution modelling. Some of them are targeted for this purpose, such as BIOCLIM (Mika & Newman 2010) and GARP (Genetic Algorithm for Rule-Set Production) (Stockwell & Noble 1992). Other methods include e.g. statistical approaches, such as regression analysis, discriminant analysis, and machine learning techniques. There is a need either to develop one’s own software application or to use general packages for statistical and numerical computations (R, GNU, MATLAB etc.), in order to use the algorithms. Statistical packages are quite often flexible, but with modelling process the user needs to learn a programming language or to use complex statistical software (Munoz et al. 2011).

There has been activity in modeling species’ potential distribution and creating new algorithms and tools for niche modelling. Elith et al. (2006) compared 16 modelling methods using 226 well-surveyed species (birds, plants, mammals, reptiles in six regions of the world and created most the most comprehensive set of model comparisons to date. Regions represented with the evaluation were Australian Wet Tropics (AWT), Ontario, Canada (CAN), New South Wales, Australia (NSW), New Zealand (NZ), South America (SA), Switzerland (SWI). The individual data sets had up to 54 species wit ha range of geographic extents and rarities. Foe each region, two sets of data were available: 1) presence only data, from unplanned surveys or incidental records, including those from museums and herbaria, and 2) independent presence-absence data from planned surveys, with accurate location records.

The environmental data used for each region were selected for their relevance to the species modelled. Eleven to thirteen predictors were supplied per region, with grid cell sized ranging from ca 100 by 100 m (all regions, excluding CAN) to 1000 by 1000 m (CAN). Predictor variables were climate (several variables), topography, distance, vegetation, soil, site moisture, disturbance, substrate (Elith et al. 2006).

Eleven distinct modelling methods were used by Elith et al. (2006). A number of these were implemented in more than one way, resulting in the 16 approaches. The methods formed two broad groups based on the type of data use: those that only use presence records (BIOCLIM, DOMAIN, LIVES), and those that characterized the background with a sample (all other methods). The first group included one envelope-style method (BIOCLIM) and two distance-based methods (DOMAIN and LIVES).

The second group of methods included several regression approaches. Generalised linear models (GLMs) and geenralized additive models (GAMs) are used extensively in species' distribution modelling because of their strong statistical foundation and ability to realistically model ecological relationships (Austin 2002). BRUTO provides a rapid method to identify both the variables to include and the degree of smoothing to be applied in a GAM model. Multivariate adaptive regression splines (MARS) provide and alternative regression-based method for fitting non-linear responses, using piecewise linear fits rather than smooth functions. They are faster than GAMs and simpler to use in GIS applications. Elith et al. (2006) implemented two versions of GARP, the widely-used desktop version (DK-GARP) and an openModeller implementation (OM-GARP) that has updated algorithms for developing rule sets. Two methods were evaluated within the machine learning community: maximum entropy models (MAXENT and MAXENT-T) and boosted regression trees (BRT, also called stochastic gradient boosting). MAXENT estimates species' distributions by finding the distribution of maximum entropy (i.e. closest to uniform), subject to the constraint that the expected value of each environmental variable under this estimated distribution matches its empirical average (Phillips et al 2006). The final algorithms within the evaluation were generalized dissimilarity models (GDM), which model spatial turnover in community composition between pairs of sites as a function of environmental differences between these sites. The approach combines elements of matrix regression and generalized linear modelling (see e.g. Ferrier 2002).

All the analyses were performed by modellers, blind to the evaluation data. Elith et al. (2006) provided modellers with the presence-only locations for each species and random background locations. The evaluation focussed on predictive performance at sites. Three statistics were used: the area under the Receiver Operating Characteristic curve (AUC), correlation (COR) and Kappa, to assess theagreement between the presence-absence records and the predictions.

Presence-only data were effective for modelling species' distributions for many species and regions. Predictive success varied markedly across regions (Fig. 2.3–5). AUC scores vere high for SWI and SA, intermediate for NSW, NZ and AWT and poor for CAN. Some patterns and exceptions to model performance by region were apparent. Performance of methods in NSW, NZ, SA and SWI was similar with BRT, MAXENT and MAXENT-T. MARS-Comm and GDM-SS useally performing well. In NZ, presence-only methods (BIOCLIM, DOMAIN and LIVES) performed poorly. In most regions DOMAIN and LIVES had lower COR values in relation to AUC than average method (Fig. 2.3–5). The novel methods consistently outperformed more established methods. Elith et al. (2006) concluded that the results were promising for the use of data from museums and herbaria, especially as methods suited to the noise inherent in such data improve.

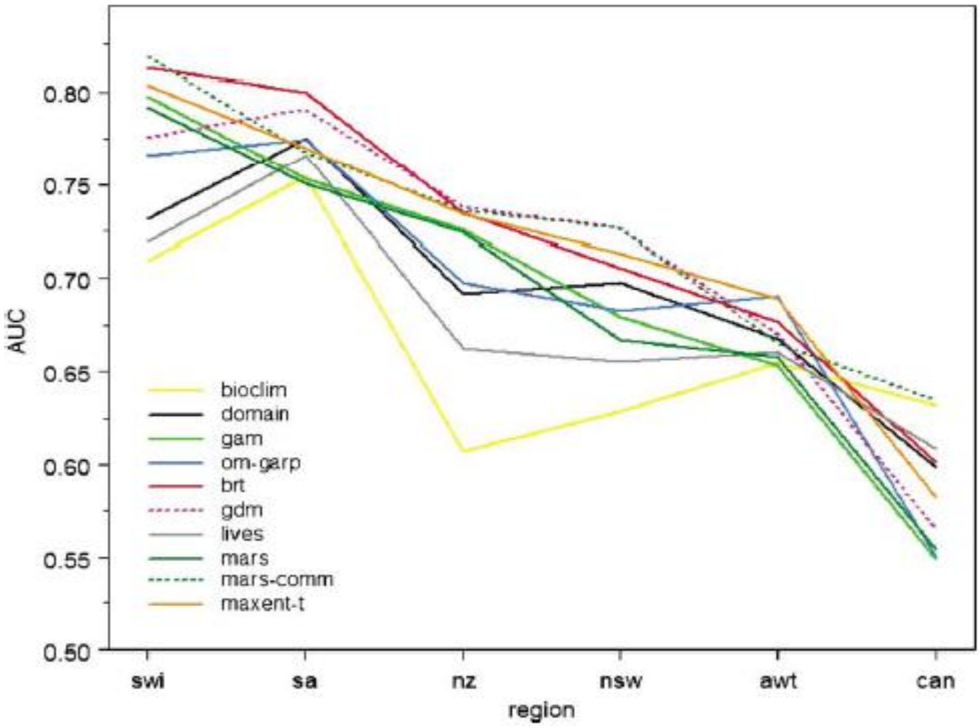


Figure 2.3–5 Predictive success across regions for ten methods. Regions are sorted by the mean AUC across all 16 methods and all species in region. Regions: Australian Wet Tropics (AWT), Ontario, Canada (CAN), New South Wales, Australia (NSW), New Zealand (NZ), South America (SA), Switzerland (SWI).
AUC = area under the Receiver Operating Charasterictic curve.
For further information, see Elith et al. (2006)

Finally, we must note that there has been an obvious gap between devising a new algorithm and implementing it as a usable software package. This gap is due to the different kind of expertise needed for the various areas involved. In addition, the level of difficulty of model generation has increased, due to demanding knowledge in computer techniques that a biodiversity or ecology researcher may not usually have (Santana et al. 2008). Therefore, a software package for niche modeling should be able to accommodate changes and inclusions with a minimum of programming skills. This requires a user-friendly software architecture with specific characteristics (Santana et al. 2008). Until the present time, most software development has been carried out in isolation, developing software packages for single algorithms, as e.g. DesktopGARP (Scachetti-Pereira 2002) and Maxent (Phillips et al. 2006). There are some potential distribution modelling frameworks available that can run different algorithms (e.g. Thuiller 2003), but none of them are open source and easy to use, i.e. lacking openness and accessibility.

2.3.4.2 Population modelling

After the ecological niche of a species has been modelled, the next step is to determine the variation in population performance in different parts of its range, in different habitat types and under variable degrees of habitat suitability. Suitable habitat of a species can be defined as the concurrence of ecological conditions (abiotic and biotic) that result in stable or growing (i.e. viable) populations over a specified time interval (e.g. Bass et al. 2006). Establishing whether or not populations are viable requires data on temporal and spatial variation in population growth rates, preferably in relation to variation in important ecological variables (Oostermeijer et al. 2003; Marrero-Gomez et al. 2007). This data can be derived from long-term studies or monitoring programs that in its simplest form consist of annual counts of the number of individuals in a certain area (count-based data, e.g. Sierdsema et al. 2006; Thomson & Schwartz 2006; Johnson et al. 2010). More detailed demographic studies involve following the fate of individual plants in permanent quadrats (Morris & Doak 2002) or animals by means of capture-mark-release-recapture techniques (Hagler & Jackson 2001; Celik 2012) or genetic monitoring (Koelewijn et al. 2010; Swenson et al. 2011). This leads to complex data on recruitment, survival, growth and reproduction that can be integrated into different types of population models that allow detailed statistical analyses. The most widely used type (e.g Crone et al. 2011) is the matrix projection (or transition matrix) model (Caswell 2001). In this type of model, individuals in a population are classified in either age, size or stage-based classes. Transition probabilities from year to year (or any other time step) between any two classes are calculated from field monitoring data and entered into a projection matrix. The dominant eigenvalue of the projection matrix represents the finite rate of increase of the population (λ), and the left and right eigenvectors the stable stage distribution and the reproductive value for each stage (Caswell 2001). The contribution of each matrix element to lambda can be estimated by determining the change in lambda after small changes in each of the elements (sensitivity analysis, resulting in a sensitivity matrix). Scaling the sensitivities so that they sum to one facilitates direct comparison of the relative contributions of each life cycle transition to population growth rate. This matrix of elasticities is called the elasticity matrix (de Kroon et al. 2000). The elasticities can be used to identify the stages in the life cycle that – under the given environmental conditions – have the strongest effect on population growth. This knowledge can be used to guide population management aiming either at conservation (increasing growth rate) of endangered species, or eradication (decreasing growth rate) of invasive ones (Jongejans et al. 2008; Crone et al. 2011). Matrix models can also be used to analyze effects of past variation in specific transitions or vital rates on lambda's (a type of analysis of variance that is also called Life Table Response Experiment, or LTRE, Caswell 2001).

Integral Projection Models (IPM's), based on regressions between size of individuals and their survival, growth and reproduction (Easterling et al. 2000), are a good alternative for matrix projection models. They can for example be used when data is scarce (Ramula et al. 2009) and for species for which individuals are difficult to place in discrete size- or stage-classes (Childs et al. 2004; Rees & Ellner 2009).

Although single projection matrices comprise a lot of data, multiple annual matrices are required to obtain a good insight into population dynamics and viability. As a result of stochastic or deterministic changes in the environment, nearly all populations will show considerable variation in lambda (Kaye & Pyke 2003). Detailed knowledge of this variation and its causes forms the key to understanding and managing populations (Crone et al. 2011). Many applied researchers incorporate the set of transition matrices into stochastic simulation models that can be used to estimate extinction risks under different environmental scenarios (climate change, harvesting, habitat management, herbivory, invading non-native species, etc., e.g. Ellis & Elphick 2007; Lennartsson & Oostermeijer 2001; Pfab & Scholes 2004; Keith et al. 2008; Smith et al. 2005). It is important to realize that even though the models are able to accurately describe the population trajectories during the parameterization period, these estimates are not realistic, and should preferably be used in a comparative way (Crone et al. 2011).

So far we have discussed the use of matrix models for analysis of the dynamics of single populations, but when relationships between matrix elements and lambda and environmental (habitat) parameters are sufficiently known, matrices can also be used for metapopulation models (Akçakaya et al. 2004). In these, we first use niche models to create Habitat Suitability (HS) maps for the species, which we then translate into a metapopulation map with occupied and vacant habitat patches. Habitat area and average habitat suitability can be calculated for each patch. With knowledge of population densities and relationships between HS and l, patch-specific carrying capacities and mean and maximum population growth rates can be specified. When we add data on dispersal rates, e.g. from population genetic studies and assignment tests, we can simulate metapopulation dynamics and quantitatively compare effects of (scenarios of) landscape changes, management-induced habitat dynamics, human disturbance (habitat loss or gain), etc. (Bossuyt & Honnay 2006; Hansen 2007; Jongejans et al. 2008; Wang et al. 2011).

2.3.4.3 Molecular phylogenetics

The field of molecular phylogenetics is concerned with the reconstruction of the historical relationships among organisms and their features. Within this field, especially the application of phylogeographic methods are appropriate for the study of invasive patterns. Phylogeographic analyses study the historical relationships of geographically separated populations in a species, and can be used to understand the origin and dispersal ability of an introduced species. As an example, an analysis of the genetic divergence in populations of the Ponto-Caspian amphipod *Echinogammarus ischnus* originating from the Black Sea and the Caspian Sea show that a single mitochondrial genotype of Black Sea origin has colonized sites from the Rhine River to North America (Cristescu et al. 2004). In contrast, a phylogeographic analysis of the comb jelly shows multiple introductions (Reusch et al. 2010). In addition to single species phylogeography, novel comparative approaches are emerging to alayse the historical biogeography of serveral species, which helps disclosing typical disperal routes for alien organisms (Ilves et al. 2010). In this context, A combination of phylogeographic methods with niche modeling and population modeling methods would be very powerful to analyse and predict invasive patterns.

In addition to historical biogeography, phylogenetic methods can also be used to identify DNA sequences with tree based taxonomy assignments. Such methods provide an alternative to the otherwise direct genetic matching of unknown marker sequences with reference libraries auch as BOLD. Since, inavsives are usually not a part of local genetic reference libraries, direct matching may not identify the origin of the alien DNA. In tree based identifications, unknown sequences are mapped onto a phylogenetic guide tree (Fig. 2.3–6). Existing tools for this purpose include the open source software pplacer (Matsen, Kodner et al. 2010), which is already available as a web-service. Robust guide trees with corresponding alignments can be obtained from treebase (www.treebase.org).

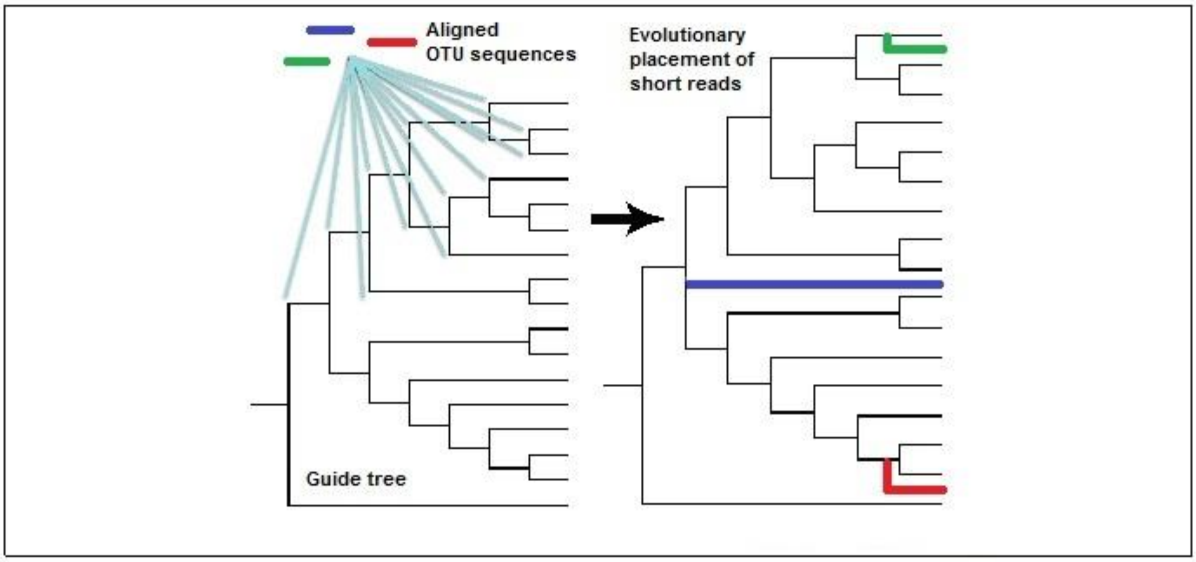


Figure 2.3–6 Operational taxonomic unit (OTU) reference sequences can be placed into an evolutionary context using tools such as ”pplacer” or the evolutionary placement algorithm, which place short reads into a guide tree framework constructed from full-length reference sequences. For each pre-aligned OTU or sequencing read, likelihood scores are calculated for all possible positions in the tree, and the sequence is subsequently inserted at the node exhibiting the best score.

2.3.4.4 Taxonomy

Taxonomy, as a scientific discipline is used to organising information about biodiversity, including species observations, character descriptions, identification methods, classification system(s), and links to associated information in literature and other resources. Taxonomic resources are essential when gathering information on invasive species. Important taxonomic methods for the large scale analysis of invasive patterns are essential support functions for all other the methods relevant for studying invasive biology, i.e. niche modeling, population modeling, molecular phylogenetics. The ability to combine these methods when and large data from many species depend on the ability to aggregate, formate, harmonize, and refine taxonomic data such. The ability to collect occurence records, synonyms, and taxonomic classifications for invasive species are among the most important features neccessary for studying invasive biology over large spatio-temporal scales.

In addition to the basic taxonomic functions, also genetic identification methods bear great potential for invasive species research**.** Correct species identification is essential when managing the risks posed by potential invasive species, and methods for correct species identification need to be much more cost-effective in the future, as well as technically accessible, accurate, and applicable across a wide range of taxa and life stages. Often, beause of lack of local taxonomic expertise, non-native organisms are identified only to family, or higher ranks, which makes it impossible to efficiently track many alien species over large distances. The accuracy of morphological identification is obviously even more attenuated when it comes to invasive species monitoring and early warning mechanisms since the difficulty of identifying early life history stages (eggs and larvae) by morphological criteria is well known (Besansky et al. 2003).

DNA-based tools for monitoring and identifying invasive species have great potential. At present the most appropriate technology for the identification of unknown specimens is called DNA barcoding, an approach involving direct matching of unknown sequence with the gentic information in a reference library (Hebert et al 2003). In invasive species research DNA based identification methods can be used for (i) early detection of invasives (e.g. larvae, eggs, adults) by screening a genetically known habitat for ‘new sequences’, and (ii) for studying the ecological impact of invasives through identification of the stomach contents of invaders (Fig. 2.3–7).

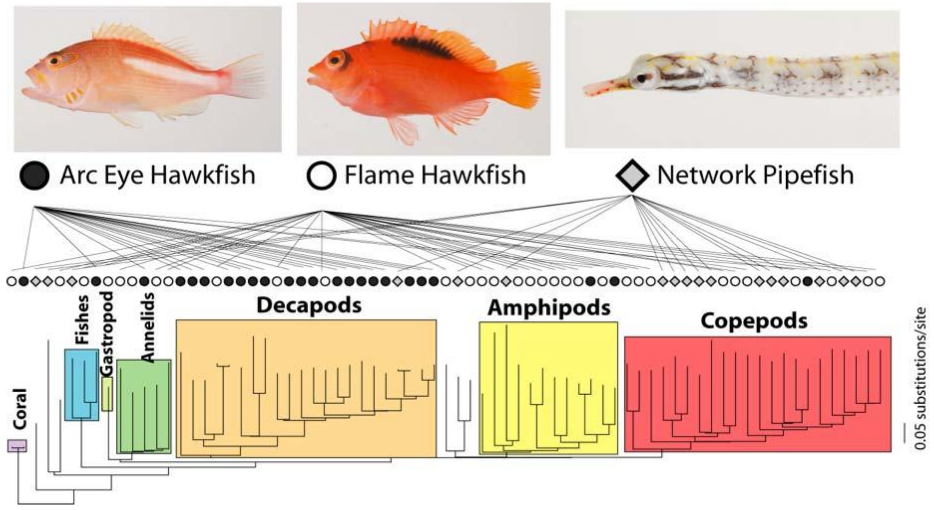


Figure 2.3–7 Food web ecology revealed by fish stomach identifications (Leray at al., 2012). The ecological footprint of invasive species can be studied using DNA based methods that identify stomach contents to the species level, given that a reference library is avaialble (Courtesy of Christopher Meyer, Smithsonian Inst.)

2.3.5 Identification and description of typical and most challenging workflows

2.3.5.1 Taxonomic workflows

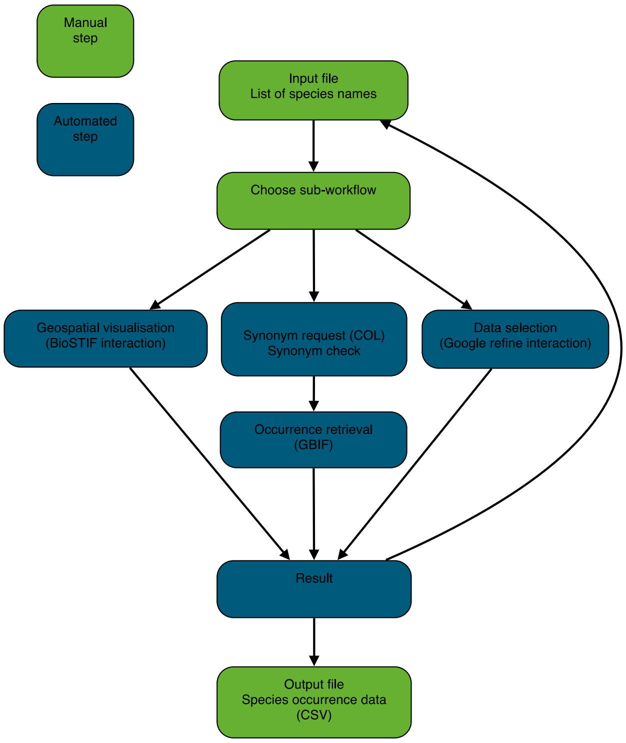


Figure 2.3–8 Taxonomic data refinement input generator workflow

Taxonomic workflows are used to access, harmonize, format, clean, and refine taxonomic data. In this example illustrated in Fig. 2.3–8, the input file is a list of scientific names (genus, species). The workflow is divided into three sub-workflows that can be selected by the user: 1) synonym request and occurrence retrieval, 2) geospatial visualisation and data selection, or 3) data selection and refinement in Google Refine.

The first sub-workflow is used to automatically retrieve synonyms for the species in question from the Catalogue of Life (www.catalogueoflife.org) and the GBIF checklist database. Synonyms can then be checked and accepted by the user through a graphical user interface. Occurrence data are thereafter automatically retrieved from GBIF (www.gbif.org) for all species names and their associated synonyms.

Through the data selection sub-workflow, occurrence records can be browsed using Google refine (http://code.google.com/p/google-refine), a tool for cleaning up data, which allows filtering, editing and clustering data. The Google refine step was used in this study to remove records without a latitude or longitude, to check the consistency of spelling of species names and to reconcile synonyms. In addition, the provenance of the data can be used as criteria to exclude dubious or low quality records.

In the geospatial visualisation sub-workflow, all occurrence records are visualized and can be refined using the Biodiversity Spatial Temporal Interactive Interface (BioSTIF), which allows selection of the occurrence points on a map and in tabular format with graphical tools and export of the selected data points in csv format.

2.3.5.2 Ecological niche modelling

Literally hundreds of papers using ENM to tackle particular problems have been published in recent years. However, only a handful of papers are specific about the data processing methods and workflows that have been employed. This is understandable, as most papers are aimed for an ecological and not data processing audience.

There are two main methods for modelling the potential distribution of species. Firstly, most of the data-driven methods are based on a correlative approach. This approach builds a representation of the fundamental ecological requirements of a species, based on the environmental characteristics of the site. Three types of data are needed for the model: occurrence data, environmental data and algorithm-specific parameters. Projected maps will show areas with similarities to those areas already occupied by the species in question (Soberon & Peterson 2005). In addition to individual species' modelling, models for communities follow a similar approach. Secondly, mechanistic modelling is based on the physiological responses and constraints of species to the environment (Kearney & Porter 2009). However, its use is limited due to a need to understand species' physiology.

Species occurrence data, i.e. collected or observed individuals or populations, is comprised of identifier, taxonomic identification, location, abundance, and a corresponding date. Biological collections and records are maintained by institutions such as natural history museums, herbaria and culture collections. Observation data are gathered during surveys by researchers and volunteers. Data on estimated records (appr. 2.5 billion records) is quickly becoming available over the Internet (Guralnick et al. 2007). GBIF (Global Biodiversity Information Facility) is one of the most prominent data sources of species occurrence, and is growing at a rapid rate. However, plenty of data is kept by individual scientists and institutes, beyond the common share of the data.

Environmental data is typically available in the form of georeferenced raster layers, representing abiotic conditions (e.g. temperature, precipitation, radiation, topography, vegetation etc.) that will be used to determine species distributions. Raster data associates a geospatial reference system and a matrix of cells containing data for the region. Environmental raster data is based on satellite data, weather station data or some other means to measure environmental conditions. These physical variables influence macro-distribution of species (Anderson et al. 2002). According to Munoz et al. (2011), these data are produced and made available by many different organizations, e.g. NASA, USGS, IPPC, UK Met Office, WorldClim and others. WorldClim, which has been described already in chapter 1 of this review, is the most widely used dataset in ENM. However, all these datasets are global, and there is often a need to crop them into a smaller area of interest, such as Europe or country / region. Furthermore, subselection needs vary between marine, coastal and terrestrial or freshwater ecosystems. Any modelling environment needs to support these subselection functions.

Munoz et al. (2011) describe the openModeller framework for executing ENM tasks. OpenModeller is a workbench that includes the steps of data retrieval and selection, and choosing and running the models. openModeller is a platform that packages several algorithms and does not require additional learning effort from the user when different algorithms are used. In addition, data preparation and comparison between algorithms becomes simplified when using just a generic computing environment. OpenModeller also exposes its functions as web services that can be used by external tools such as those of BioVeL.

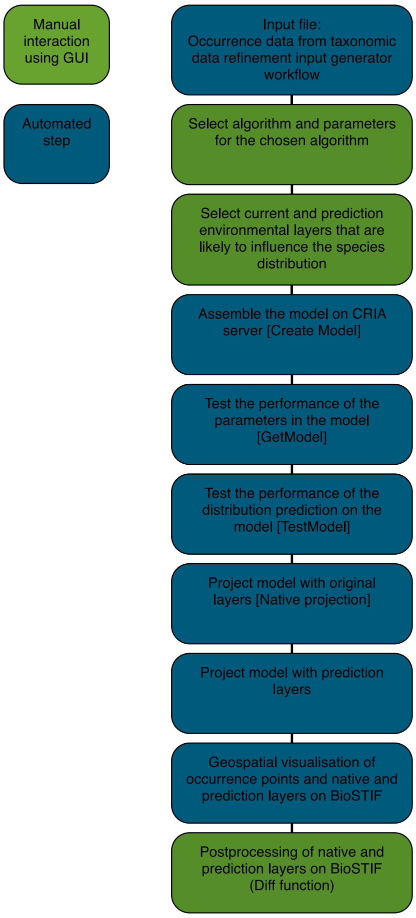


Figure 2.3–9 The niche modelling workflow takes as input occurrence data from the taxonomic workflow (Fig. 2.3–8), a set of environmental layers and a choice of a modeling algorithm. The workflow interacts with a niche modeling Web Service to generate models remotely using OpenModeller (Munoz, de Giovanni et al. 2011). A manual interaction step allows algorithm selection and parameter selection for the chosen algorithm, and another manual step allows the user to select environmental layers that are likely to influence the species distribution.

Santana et al. (2008) describe ENM as a business process. They note that „the process to generate an ecological niche model is complex. It requires dealing with a large amount of data, use of different software packages for data conversion, for model generation and for different types of processing and analyses, among other functionalities". They describe a service-oriented architecture to build such systems, and describe a reference business process for ENM for build a system on SOA concepts.

Nativi et al (2009) describe a workflow for ENM, and the required discovery of data and processing services through external infrastructure (community catalogs) of the GEOSS.

The ENM workflows being constructed in BioVeL include elements from these 3 papers. They include steps of 1) selecting the species, 2) retrieving data from GBIF and adding one's own data set, 3) cleaning the data for outliers and taxonomy, 4) selecting the environmental data layers, 5) selecting the algorithm and its parameter values, 6) running the model and testing it, and 7) projecting the model. These steps are illustrated in Fig. 2.3–9.

2.3.6 Evaluation of web service requirements

Below is a description of services that have been identified to support the study of invasive species in each of the relevant research fields.

2.3.6.1Taxonomy services

Taxonomy services can facilitate bio-identification tools, geographic distributions, classification systems, and links to ecological information systems for invasive and alien species. Examples are (1) the **Catalogue of Life checklist web service.** This service is used to expand given names into associated names, i.e. accepted name, synonyms, etc **(**www.catalogueoflife.org/webservice**)**; (2) **GBIF web services for occurrence data retrieval,** a service to retrieve occurrence records for any given scientific names (http://data.gbif.org/ws/rest/occurrence); (3) **GBIF checklist web service** (http://ecat-dev.gbif.org), which is used to expand given names into associated names (i.e. accepted name, synonyms, etc).

2.3.6.2 Phylogenetics services

Phylogenetics services relate to data mining, alignment, core phylogenetic inference, trait evolution on phylogenies, phylogeographic inference, and tree information storage. Examples are (4) **Alignment web service**, available trough European Bioinformatics Institute, which performs and cleans a DNA alignment; (5) **User interface to describe model of substitution.** The service guides the user trough possible choice of the subsitution model and produces a model description useful for the program of phylogenetic inference; (6) **Infer Phylogeny service.** This service is built around the program MrBayes 3.2 and requires nexus format input of the aligned sequences, as well as the model block and the MCMC integration parameters; (7) **Assess overall goodness of fit of phylogenetic inference with Posterior predictive test.** This service controls the fit of the model on the data based on simulation and checking overlap between simulated data and observed ones.

2.3.6.3 Ecological niche modelling services

Ecological Niche Modeling services are based on the OpenModeller services at CRIA, point data services at GBIF and speciesLink, GISIN for invasive species information, WorldClim for climate layers, and IPCC for climate change scenarios. Examples are (8) **Ecological Niche Modelling (ENM) Service**, which allows ecological niche models to be created, tested and projected into different environmental scenarios. A new instance of the service was configured for BioVeL with its own set of environmental layers, including WorldClim bioclimatic terrestrial data in different spatial resolutions and AquaMaps marine layers - both available for current and future conditions.

2.3.6.4 Ecological population modelling services

The workflows which have been (and are being) created in BioVeL up until now use (annual) monitoring data on individual organisms classified by life stage, age or size **(a)** to produce and **(b)** analyze annual transition matrices, **(c)** perform an LTRE, **(d)** estimate and analyze the same parameters for stochastic lambda and **(e)** perform stochastic simulations. Because many researchers nowadays use R to calculate this, the already existing R-scripts have been used as a basis for the BioVeL population modelling service set. For this, the **RServe service** (9) has been developed, which executes R-scripts on a remote host. In addition, **Interaction services** (10) for configuration of a workflow were created to support the input data. In collaboration with the Max Planck Institute for Demographic Research in Rostock (Dr. R. Salguero-Gomez) and the Radboud University Nijmegen (Dr. E. Jongejans), recently developed R-scripts for Integral Projection Modeling will also be incorporated into BioVeL.

For links between single population models, metapopulation models and habitat suitability maps produced with Species Distribution (Niche) Models, the most frequently used software package is RAMAS-GIS (www.ramas.com, see Yates & Ladd 2010; Pellet et al. 2006; Schtickzelle & Baguette 2004). Important components of RAMAS are being converted into R-scripts, which will enable their inclusion in BioVeL as well. This will eventually result in a service set that can convert data from individual organisms into models at the individual population and the metapopulation/landscape scale.

2.3.6.5 Geospatial visialisation services

Geospatial Visualisation services have a strong focus on providing mechanisms for exploration, computation, and presentation of data with spatio-temporal attributes. Those data can be divided into raster data (or coverages), which holds multidimensional values distributed into a homogeneous grid, and vector data, which may have one or more attributes representing a geometry. The usage of existing standard interfaces from the Open Geospatial Consortium (OGC) and ISO/TC211 contributes to support interoperability within BioVeL, allowing standard software to access and use the data and services. The (11) **BioVeL GeoServer** (https://biovel.iais.fraunhofer.de/geoserver/web) is based on the open source application GeoServer (http://geoserver.org), which supports the following protocols: the Web Map Services (WMS) for mapping of raster and vector data, the Web

Coverage Services (WCS) for querying raster data, the Web Feature Service (WFS) for querying vector data, and the Web Processing Services (WPS) for making computations on both data types. The GeoServer application is the OGC reference implementation for WMS, WFS, and WCS. With so-called SHIM Services (connectors or adapters to workflow services, e.g. providing transformation) biodiversity data and computation results can be transformed and uploaded to the WMS/WFS/WCS services.

For discovering of spatio-temporal data the (12) **BioVeL GeoCatalogue** (https://biovel.iais.fraunhofer.de/geonetwork/) was deployed based on the open source application GeoNetwork (www.geonetwork-opensource.org), which is the reference implementation for OGC Catalog Services for the Web (CSW). The GeoCatalogue allows harvesting metadata using standards like the OGC-CSW 2.0.2 ISO Profiles, the OAI-PMH, and the Z39.50 protocol. The GeoCatalogue provides an interactive web application, where the user can search for data applying textual, temporal, and geographical constraints. This application will be extended to be used as an interaction service within tavern workflows.

(13) **OGC-SHIM Services** will support the integration of the OGC services into workflows. Since the OGC services are technically based on XML-RPC protocols, the OGC-SHIM services will provide REST interfaces facilitating the construction and interpretation of the transferred XML-documents and requests.

The user of the workflows need, on the other interactive tools to explore and select spatio-temporal data, as well as to perform computations and visualize their results. A main contribution to the Geospatial Visualisation Service Set is the web application (14) **BioSTIF-Spatio-Temporal Interactiv** interface (Jänicke et al. 2011), which can be integrated into Taverna Workflows as interaction service. BioSTIF is also available as standalone web tool (https://biovel.iais.fraunhofer.de/biostif) BioSTIF shows spatio-temporal point data e.g. species occurrences on a map. Different background maps can be chosen. The user can make selections on the data using spatial objects like polygons, circles or other geographical features loaded from web map services. Occurrences can be deleted. The user can browse through the data in a map, a tabular view, and a timeline plot. The supported formats for occurrence data are kml (OGC standard), Darwin Core (TDWG standard), JSON (open standard) and comma separated files (csv). The results of data manipulation will be sent back to the workflows as URL link to documents using the same format.

3 Conclusions

We can confirm that the needs of biodiversity and ecology sciences for new leading-edge integrative IT tools are growing rapidly, while existing, reliable and open web services and workflow management services to fulfill these needs are still scarce. The planned and on-going developments of the project, targeting new and improved IT facilities and demonstrating the success of the virtual laboratory approach for i) DNA sequence-based phylogeny and metagenomics research, ii) usage of taxonomy and species occurence data services, iii) ecological niche and population modelling, iv) modelling and simulating ecosystem functionality and valuation will reach big steps toward the main goals of the project. They will open new perspectives for biodiversity analysis. However several gaps will remain unbridged and we have to count some constraints also.

The main gaps and constraints

Shortage in relevant dataset services – One of the gaps is due to the lack of relevant ecological and biodiversity datasets or dataset services. Although the availability of various open environmental and biodiversity datasets is growing continuously, the demand for open, high quality, globally-regionally-locally relevant datasets for various ecological analyses is also growing. Furthermore, species have certain (narrow or broad) environmental, habitat based, biotic and temporal requirements and limitations, which researchers have to consider in addition, and which are used to then find the most relevant and accessible datasets for their analyses. Most of these datasets today have no or poor web service interface, incomplete metadata, incomplete geographical and temporal coverage, or limited spatio-temporal resolution.

Difficulty finding data and services – Even in cases where services and data are online, their discovery often requires knowledge of the people, projects and organisations behind them, and the terms and conditions of the data use. Still too few biodiversity data and services are discoverable through open registries such as BioCatalogue, GBIF, LTER, and GEOSS.

Bridging the inter-disciplinary gap – Although technology provides huge potential for chaining web services and build complex scientific workflows (see the ecological niche modelling workflow described in chapter 2.3 as a best practice example), several gaps remain. Bridging these gaps will soon open up new possibilities for research. For example, there are several missing links along the *’phylogeny – taxonomy – species distribution – community ecology* (as missing link, see Bekker et al. 2007, Dengler et al. 2011a, 2011b, Lopez-Gonzalez et al. 2011, Janßen et al. 2011) – *functional ecology* (as missing link, see Bonan et al. 2002, de Bello et al. 2010, Kattge et al. 2011, Scholes et al. 2012) – *ecosystem modelling’* chain for complex analysis. We can foresee, that other inter- and transdisciplinary workflow chaining, even across different levels of organisation will be possible in the near future, like *’species distribution – community ecology – population modelling – ecological nich modelling*’ or *’taxonomy – metagenomics – functional ecology – ecosystem modelling*’. As disciplinary and interdisciplinary services extend, so will the number of possible scientific interactions be able to grow exponentially. However, we have to keep in mind that the biodiversity and ecological knowledge represented in our databases, expert systems and scientific tools remains limited in contrast to the complex patterns, processes and interactions of the Earth's bioshpere.

Data consistency gap - When combining data from different sources and domains it becomes clear that interoperability is not the only obstacle to analysing complex patterns of biodiversity. Existing biodiversity information repositories generally provide high quality data with respect to the reliability of the information reported. However, data quality is rather low with respect to consistency. In other words, the data aggregated today have been collected for different purposes and on different spatio-temporal scales, leaving significant gaps in data sets assembled from different sources. Such gaps seriously inhibit the analysis of complex patterns. It is therefore of uttermost importance that dataset and analytical services are integrated components of the developing biodiversity observatory networks (BONs). Analytical tools will always be limited in their potential to discover and understand complex patterns of biodiversity until they become the drivers for the collection, aggregation, and discovery of data coming from BONs.

Model construction constraints – According to the well-known bon mot of George E. P. Box „Essentially, all models are wrong, but some are useful". This quote illustrates well that all models have strong limitations and a scope of validity. As a consequence, not all models can be sensibly pipelined into a workflow, even if creating a link seems to be technically possible. It will become necessary to develop and use a variety of models and find the appropriate parameters to partially overcome these constraints, as well as to provide and use model validation tools. When chained in a workflow it is important that the workflow presents (i.e. does not hide) the assumptions and limits of uncertainty that the models work under.

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