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Global Research Alliance Modelling Platform (GRAMP): An open web platform for modelling greenhouse gas emissions from agro-ecosystems.

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Abstract:

Carbon (C) and nitrogen (N) process-based models are important tools for estimating and reporting greenhouse gas emissions and changes in soil C stocks. There is a need for continuous evaluation, development and adaptation of these models to improve scientific understanding, national inventories and assessment of mitigation options across the world. To date, much of the information needed to describe different processes like transpiration, photosynthesis, plant growth and maintenance, above and below ground carbon dynamics, decomposition and nitrogen mineralization etc., in ecosystem models remains inaccessible to the wider community, being stored within model computer source code, or held internally by modelling teams. Here we describe the Global Research Alliance Modelling Platform (GRAMP), a web-based modelling platform to link researchers with appropriate datasets, models and training material. It will provide access to model source code and an interactive platform for researchers to form a consensus on existing methods, and to synthesize new ideas, which will help to advance progress in this area. The platform will eventually support a variety of models, but to trial the platform and test the architecture and functionality, it was piloted with variants of the DNDC model. The intention is to form a worldwide collaborative network (a virtual laboratory) *via* an interactive website with access to models and best practice guidelines; appropriate datasets for testing, calibrating and evaluating models; on-line tutorials and links to modelling and data provider research groups, and their associated publications. A graphical user interface has been designed to view the model development tree and access all of the above functions.

Keywords: Biogeochemical modelling, Integrated modelling platform, Unified modelling approach, Climate change, ecosystems, greenhouse gas emissions.

1 Introduction

Agriculture plays a vital role in food security, poverty reduction, rural employment and sustainable development (Foresight, 2009). There is a need to produce more food with fewer resources, while safeguarding the environment and reinvigorating rural economies to feed a growing population (Smith, 2013). The agriculture sector is particularly vulnerable to the impacts of climate change and faces significant challenges in meeting a dramatic increase in global food demand, while reducing its contribution to greenhouse gas emissions (GHG) (Smith and Gregory, 2013). The agricultural sector contributes ~14% of world's annual direct anthropogenic GHG emissions (Smith et al., 2008), and these emissions are expected to rise by 30-40% above 2005 levels, in line with the projected increase in food production by 2050 if current trends continue (Godfray et al., 2011). Farmers need new strategies to produce goods with anticipated changes in climate and agro-ecological conditions. Modelling can be used to support decision making that introduces new management practices to reduce GHG emissions and maintain productivity.

Recently, many models (Del Grosso et al., 2009; Giltrap et al., 2010.; Smith et al., 2010) have been developed and are in use to address the challenges of sustainable agricultural development (Shepherd et al., 2011). The active use of simulation modelling techniques is one of the few means to enable us to verify hypotheses about the operating principles in agro-ecosystems and their subsystems. Carbon (C) and nitrogen (N) process-based models are an important tool in the quantification, prediction and reporting of GHG emissions from different ecosystems. We need to evaluate, develop and adapt models that can be used to improve national inventories of GHG emissions by meeting Tier 2 and Tier 3 reporting requirements, as countries upgrade from Tier 1. If models are accessible enough, they can act as a medium for wider participation in environmental management. However, using, testing, calibrating and evaluating these models are far from straightforward. There are already several models that can address the questions related to C and N cycling and GHG emissions from soils (Del Grosso et al., 2009; Li, 2007) and there are about 4000 more general mathematical models in the field of ecology and environmental sciences (Jørgensen, 1999; Rivington and Koo, 2010) . These models represent a large collection of scientific knowledge and experience about structure, function and behaviour of ecosystems.

There have been many contributions to a more profound understanding of ecosystems in the past two decades (Smith et al., 2012) unifying approaches and identifying and removing artefacts contributes to the development of more comprehensive ecosystem theory. There are major benefits that can be delivered by the consolidation of existing models and theories in order to address the challenges of representing different spatial and temporal scales, avoiding the redundancy in model development (Rotmans, 2009). There has been debate about the different approaches used (e.g. empirical *vs.* process-based, simple *vs.* complex, importance of different processes) in ecosystem modelling. Most of the scientific knowledge associated with these models is heterogeneous and dispersed and, therefore, not directly available to the scientific and user community. Furthermore, there is limited information available on the mechanistic hypotheses used in most of the existing models. Lack of adequate model documentation has been described in previous studies (Russell and Layton, 1992). Because of this, there is often a gap in understanding model structure, or expectations and certainty of measured and modelled results between model developers and model users. There is a need for a resource that unifies thoughts, ideas and observations to achieve the state-of-the-art in ecosystem modelling. As of now, much of the critical information needed to describe different processes in ecosystem models can only be found with individual model developers and the “comment statements” found in their computer codes, hence it is often largely inaccessible by the broader community. In addition, experimental conditions influence the choice of model parameterization which can lead to differences in simulations. Hence, in addition to detailed documentation of the models themselves, the experimental conditions and choices made by modellers on how to set different parameters must also be fully documented. This information is very important for scientific understanding of different ecosystem processes and of model performance.

Acknowledging these challenges, and in an attempt to improve the communication and understanding, an open web-platform, GRAMP, has been developed (www.gramp.org.uk). This paper describes how the GRAMP web platform was initially developed, and demonstrates several uses in scientific projects, and for policy formulation. We also present the initial case study using the DNDC model, to illustrate its functionality and utility. Section 3 discusses the future development of GRAMP and the ways in which it can help with unifying environmental modelling and assessment.

2 GRAMP

2.1 Aim and scope of GRAMP

1) To create an open web-platform with existing data and prior knowledge, in collaboration with end-users, with every stage open to critical review and revision, to improve the predictions of soil C & N cycling in agro-ecosystems in the context of climate change. This will involve classifying the various models according to their capabilities and specificities.

2) Establish a vibrant network of specialist researchers, model developers and users who can work together, to examine strategically what the various models currently available can deliver in accounting for the effect of ecosystem management on GHG emissions, to identify promising mitigation options, and to assess the effect of future climate on emissions.

3) Link a global network of experimental sites to provide suitable data for testing, tuning and validation of models and their derivatives across different crops, management strategies, soil types, and climates.

4) Develop protocols for model development, application, calibration and evaluation with the aim of providing an unprecedented level of detail in describing models and simulations.

5) Allow network members to exchange information, experience and data and provide a forum for model development for future needs.

Users: four types of users are identified, viz; 1) researchers working on model development, 2) researchers using models for various outputs, 3) students who want to be trained in ecosystem modelling, 4) researchers interested in policy making, based on modelling outcomes.

Content and database management system: GRAMP will allow users to link databases for use by the modelling community. The GRAMP platform contains a list of management system and a database system which are searchable by region, crop etc. GRAMP will host a set of links to global databases like NitroEurope(C1 and C3 database), CarboEurope, GRACEnet and REAP databases (Del Grosso et al., 2013) etc., with associated metadata. It also contains a web-GIS linked mapping system with a reference library, a database system and training materials (case studies, demos, videos).

Functionality and outputs: The web platform will host the existing ecosystem models with a version control system. This will allow users and model developers to create version specific documentation. All the models entering the platform need to develop a model tree with documentation (Figure 1). GRAMP describes the performance of different model versions, which allows users to identify changes, and the implications of those changes on output variables.

2.2 GRAMP platform design:

The website was built upon Python's Django open source web framework. Django is a free and open source web application framework, written in Python programming language. Use of Django eases the creation of complex, database-driven websites like GRAMP. The website has a custom-built user authentication system which implements the Django Guardian project for multiple tiers of permissions depending on a user's GRAMP affiliation and offers several tools to implement management of those permissions. After initial access, the users are allowed to enter any of four categories:

1. *Data records system*: The database system has been classified into four categories: (i) project resources (ii) web resources (iii) model version records and (iv) application records. The project resources will include links to a global wide database, and metadata associated with each experimental dataset. Users can also add new database links to other databases by following the standard protocol provided on the website. Field databases identified by the collaborators will be collected from various sources, harmonized (where possible) and placed in the database system. Project resources store the records, for example of measured emissions of GHG from different ecosystems, which would be suitable for the further development, calibration or evaluation of the models. It will also store the records of a centralized database that is harmonized with clear and full attribution of the sources of the data, authorship, measurement methods, referencing, etc. Web resources provide links to data without harmonization. There are several good experimental databases in existence (e.g. Croplands research database : Liebig et al., 2013; Australian N_2O Network: http://www.n$_2$o.net.au etc.,), so direct links will be provided in this category.

Model version records keep the summary of model versions in a specific format that are used in the modelling portal. Application records are the bibliographic references which are classified according to a set criterion and linked to almost every other entity in the database; the corresponding information will be made accessible to all users.

2. *Model repository*: A repository where models can be stored and accessed with a detailed description of the most relevant processes, authors, version history etc. The repository uses version-control tools. This will also provide version-specific documentation, which is easily accessible, complete, standardized, mutually comparable and transferable to different applications. The database is accessed *via* a web interface which allows modellers to search and download different versions of the models in the form of ready-to-compile software. Modellers can also add their own models to the existing repository. This also provides best-practice guidelines, on-line tutorials and links to modelling and data provider research groups, and their associated publications.

3. *Model application*: Model performance with different model versions is documented in this category. Different statistical performance indicators are used to compare the performance of different versions of model. Model performance is also assessed by considering biological meaning (processes), in addition to statistical significance. Model versions that constantly fail to predict known patterns, or those that generate implausible estimates will be viewed as untenable for given applications.

4. *Research & education*: This category provides the training manuals, videos, tutorials for new users, and provides FAQs. Users are allowed to interact in the forums and raise questions and get help from worldwide colleagues to solve questions. Tools are provided for blogging, which allow experienced users, developers and other researchers to communicate

with the audience. GRAMP also has the capabilities to organize Webinars, which allow scientists across the world to attend web-based seminars.

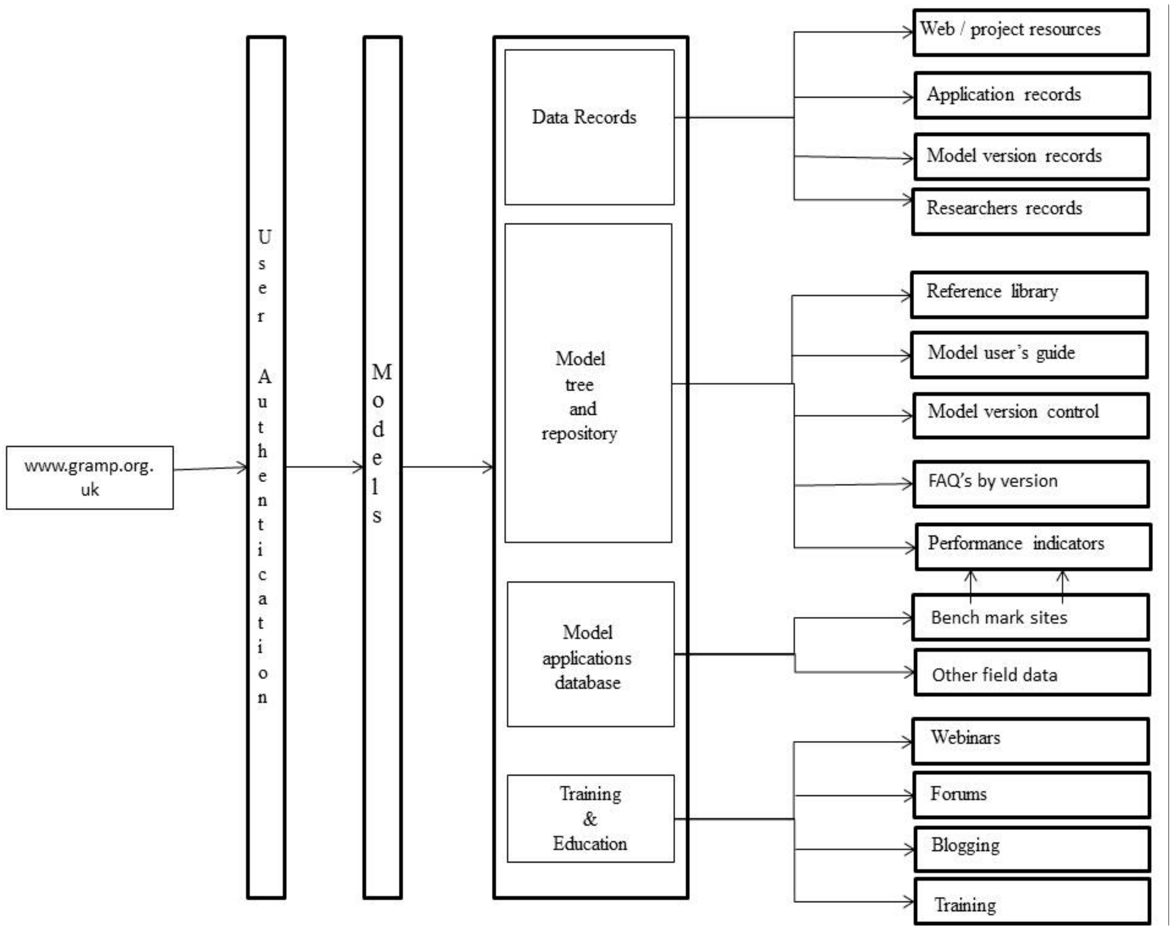

Figure 1. A schematic representation of the GRAMP network

2.3 Data record system under GRAMP

2.3.1 Project resources

We developed a simple template for researchers to document research projects that have measured emissions of GHGs from agricultural land, which could be suitable for the development, calibration or evaluation of models. The template is a Microsoft Word document that uses named fields for automatic extraction of the data. This will enable automatic generation of web-site pages from the records. The template will be available for download from the web-site, to allow researchers to submit formatted records of their projects for inclusion in the GRAMP database.

The template collates project information on (i) project location and duration (ii) contact details for the coordinator and organisation (iii) description of work done and method used (iv) published papers and reports (v) site measurements available for input to the ecosystem models such as site climate, soil properties, land use and grazing practices, fertiliser and manure inputs (vi) if site measurements are available, the type of site measurement parameters, (vii) expert opinion on best use of the dataset. To demonstrate use of the template, we have completed examples for 6 national and 2 European scale projects which are available on GRAMP (section 3).

2.3.2 Web resource records

A set of searchable 'card' records are created to summarize existing web resources relevant to measurement and modelling of GHG emissions that would be of interest to users of the different models. Each record is formatted according to a template, and can be stored in a relational database for easy search. Each web resource record provides a description of the purpose of the web site and the types of information available, along with contact information and any restrictions on data access. A total of 50 web resource records have been prepared to date, based on the standard template format. In the future, further records may be added by the user community using this template.

2.3.3 *Model version records*

GRAMP allows a set of searchable 'card' records to be created, summarising versions of the model that can be used in the modelling portal. Each model record will be a formatted record, stored in a relational database, and as such, each record follows a standard template format.

Each model record includes a description of model version, an explanation where possible of its link to the original model form; details of any modifications and version numbers; and a general description of any validation and specific data requirements. The biopic provides pointers to the home-page where the model executables and manuals can be downloaded, if available, and also provides citations of key papers describing each model version. As an example we produced eighteen model records for versions of the DNDC model by combining literature searches, web searches and DNDC community expertise.

2.3.4 *Application records*

This section contains a database of papers published in peer-reviewed journals that describe the development or application of the model. Each paper was classified according to a set criterion to enable the database to be searched for previous applications of the model to areas of interest defined by land use and region, and types of study outcome, such as a regional emissions inventory or an improved process description. For each publication, we have produced a study record. Each study record contains 12 classes (Figure 2). The Web Portal will display the list of papers, and the links to the source journals, as the paper abstracts are generally copyrighted and cannot be displayed. We have classified all of these papers into eight categories (Figure 2). The classification will allow users of the web portal to rapidly identify papers that are relevant to their needs. The classification system anticipates other GHG models, and other types of models. All the papers that belong to one model version are linked to the model tree (Figure 2).

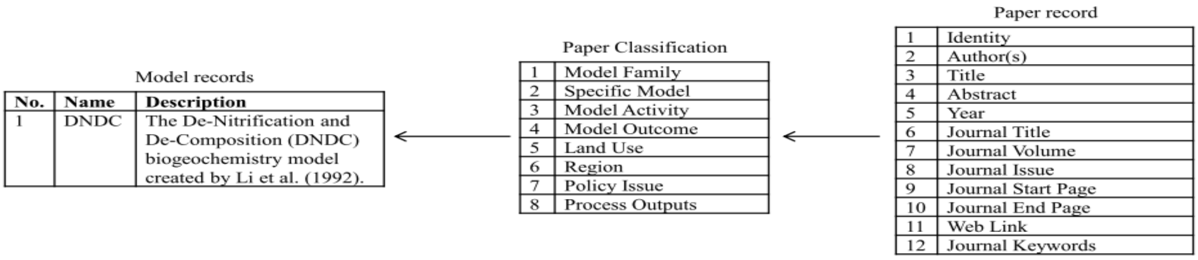

Figure 2: Description of the database structure describing the linkage between publications, their classification and the model to which they refer within GRAMP.

Here we present a bibliography associated with DNDC model as an example. Papers were identified by searching for the term '*DNDC*' in the 'Web of Knowledge' and 'Scopus' search engines. A total of 248 papers were identified. All these papers are categorized according to the classification system presented above. The papers collectively provide trends in DNDC model development and application. As shown in Figure 3a, the majority of research papers published have used the original DNDC model version. DNDC was initially developed in the USA, it has been used and tested extensively in Asia (Figure 3b), followed by Europe and North America. DNDC has been applied in many land uses, but the majority of applications have been in croplands, followed by agricultural grasslands and paddy fields (Figure 3c). DNDC has primarily been used for GHG quantification and soil C and N dynamics, as shown in Figure 3d. Sixty eight percent of literature focused on quantification of environment fluxes under present-day land management practices, such as fertiliser inputs, livestock grazing regime and crop rotations – at field, farm or landscape scale. Only 15% studies focused on quantification of the impact of changing climatic rainfall and temperatures on different ecosystems (Table 1).

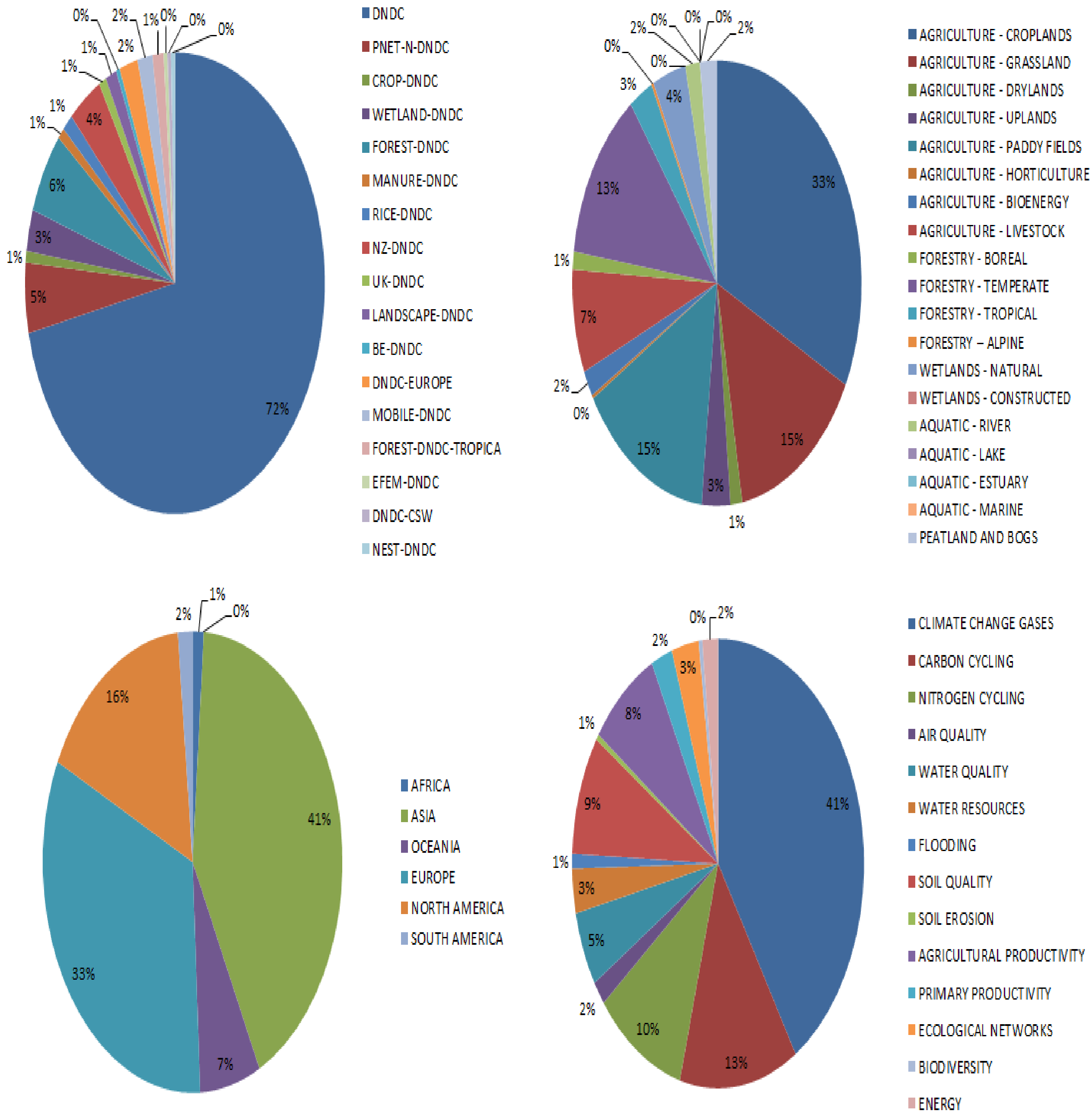

Figure 3. Percentage of publications that used (A) different version of DNDC (B) different regions (C) different land use and for (D) different research purposes.

No.	Name	Description	% of Papers
1	Development, integration and testing	Detailed description and testing of new algorithms for improved process representation.	25.0
2	Measurement and verification	Comparison of model outputs with measured fluxes at plot and field scale for verification and calibration of the model parameters.	57.0
3	Inter comparison	Comparison of the abilities of different models or model versions to reproduce measured fluxes	16.0
4	Sensitivity and uncertainty	Analysis of the sensitivity of model outputs to varying the scale and range of input data and internal model parameters.	27.0
5	Scenario evaluation	Application of the model to calculate the impact of, for example, a change in land management or climate change on simulated fluxes.	34.0

Table 1. Percentage of papers which cover different aspects of model use, development and testing.

2.4 Model tree and repository

Ecosystem model construction is an iterative process in which the modeller often develops a number of models or variants due to changes in the underlying assumptions made about the system. The number of assumptions and simplification of the system, increases or decreases depending on the contemporary understanding of the system and objective of the model. As a result, a number of model representations will emerge, with one of these ultimately being used for the desired purpose. During this refinement of models, the changes that are made to the model normally diverge from the original design or process of the model. There is a need for continued documentation which explains how each model version differs, and why each was created. Ultimately, the modelling community is interested to know how the existing model was changed to justify the creation of a new model, or model version. To improve current modelling practice, GRAMP describes a framework for developing a "Model Tree", in which other tools such as a model repository work together for greater productivity and transparency.

A Model Tree is a hierarchical collection of models which provide many different representations of the same system. These are collated in a manner which focuses on the similarities and differences between each model in the collection. The specific differences between individual models are recorded as model members. The use of Model Tree and model families makes it possible to store a large number of models of the same system, improving understanding of the system and allowing reuse of concepts or ideas. Each version in the Model Tree is associated with the model repository. The aim of the GRAMP model repository is to provide access to an up-to-date collection of ecosystem models or model versions. This model repository ensures that the model is curated, which is important to ensure that the model is able to accurately reproduce the published results. This tool brings together a rich set of features for the analysis, management and usage of large sets of process models. The repository holds models along with conceptual metadata, rather than as mathematical equations or programming language code. The conceptual representations of models in metadata enhance the use and improve the understanding of models by various stakeholders.

2.5 Model performance

Linking detailed model description with model performance might help in improving process understanding and detecting the origin of some model errors. Most of the time model calibration is carried out by trial and error or by using optimization techniques. Both of these methods are designed to search the parameter space for combination of parameters which provides the best fit. There is sufficient information provided in the literature on general aspects of model structure but little is presented about the values of model parameters. Without this information it is difficult to assess whether the lack of fit is due to the inadequacy of model structure or due to poor parameter choice. This information also helps in improving scientific interpretation and transparency in model analysis.

3 Pilot study of GRAMP using the DNDC model

We present here a case study with the DNDC (DeNitrification-DeComposition) model to demonstrate the functionality and utility of the major features of the GRAMP tree and model repository. Prototyping with the DNDC model presented in this paper demonstrates its feasibility, as well as an outlook to the further developments of GRAMP. We piloted this study with the DNDC model due to its wide-spread use throughout the world. To develop a DNDC Model Tree under GRAMP, we reviewed DNDC model versions and documented the important chronological changes made to the model. We reviewed papers published in peer-reviewed journals that describe the development or application of the DNDC model. Each paper was classified according to criteria to enable the database to be searched for previous applications of the DNDC model, to areas of interest defined by land use and region, and types of study outcome, such as a regional emissions inventory or an improved process description. A total of 248 papers were identified for this study. The aim was to build a Model Tree to identify the major processes in each version of the model. The ability within GRAMP to create an easily exchangeable model tree knowledgebase is relevant in this respect.

3.1 DNDC model families

Several standalone versions evolved from DNDC, sharing most of the sub-models of the original DNDC. Many standalone versions of DNDC were regionalized by incorporating regional-specific management or parameterization of the model (Figure 4). There were several versions of DNDC developed during the last few decades. Many of these modifications have been incorporated into the latest standalone versions of DNDC (Giltrap et al., 2010.). There are several standalone versions of DNDC, the most stable of which have been reviewed and tracked through GRAMP. Constructing models in this manner enables the modeller to retain various representations of DNDC in one location. This simple change in model typology dramatically improves the model repository by eliminating most of the repetition in modelling.

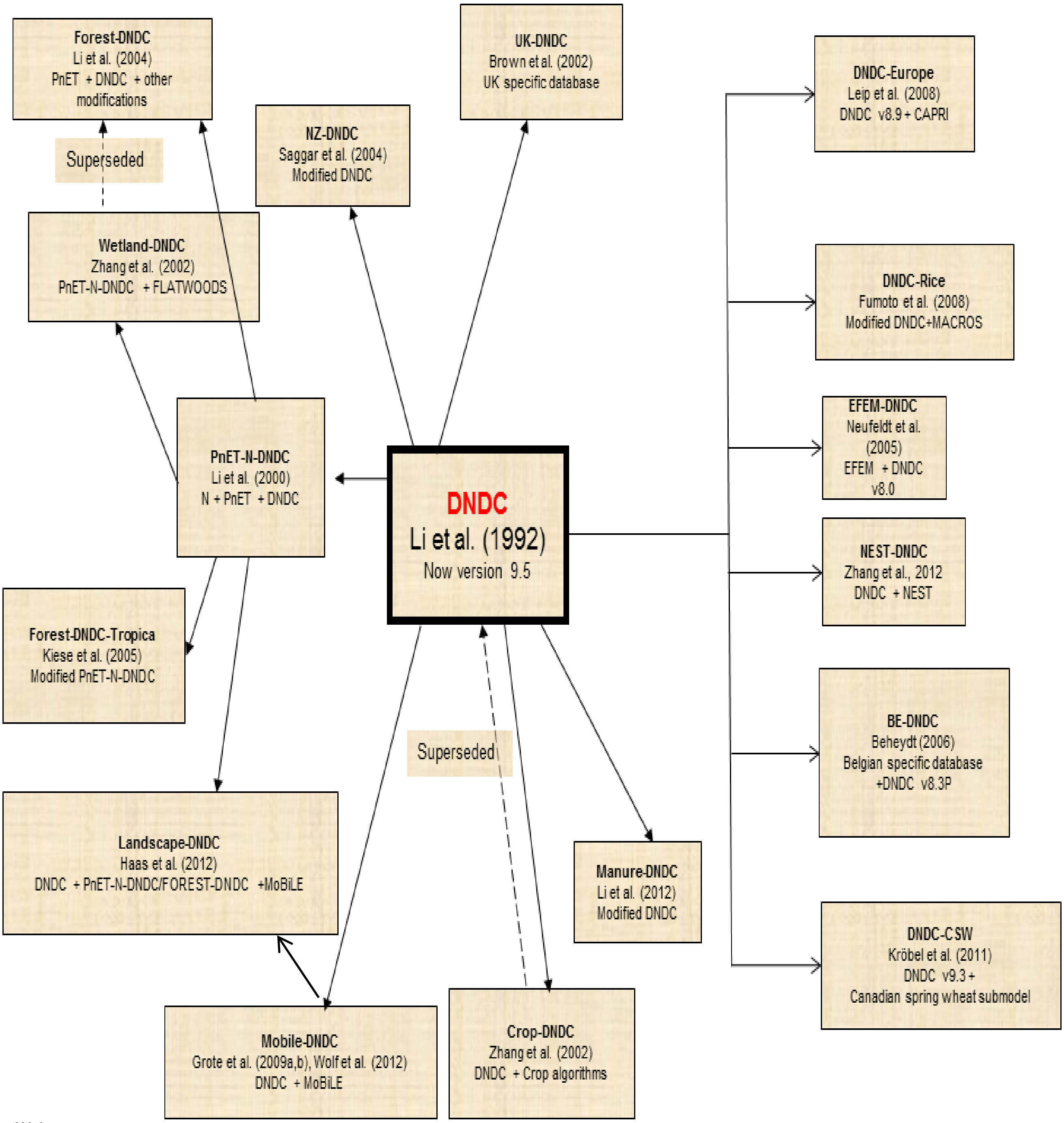

Figure 4: Schematic diagram of the DNDC extended family. By detailed literature review, we identified the following standalone versions of DNDC: 1) PnET-N-DNDC 2) Crop DNDC 3) Wetland DNDC 4) Rice DNDC 5) Forest DNDC 6) Landscape-DNDC 7) Forest DNDC-Tropica 8) Manure-DNDC 9) Mobile-DNDC 10) NZ-DNDC 11) DNDC - EUROPE 12) EFEM-DNDC 13) NEST-DNDC 14) BE-DNDC 15) DNDC-CSW 16) UK-DNDC.

3.2 Example of DNDC model performance

In an attempt to evaluate the current state of the DNDC crop model as an example we present a meta-analysis of 363 modelling studies published in the peer-reviewed literature between 1990 and 2013. GRAMP has the user interface to display the model with associated simulation results. The model performance tab shows the systematic goodness-of-fit assessment of the original models, i.e., plots in which simulated values were visually compared with observed data. The model performance window will have the capacity to show graphs comparing modelled and observed values in various formats. Under GRAMP a diagram has been devised that can provide a concise statistical summary of how well daily or annual field observations match the model simulations in terms of their correlation, their root-mean-square difference, and the ratio of their variances. Representing the results in this form is especially useful in evaluating complex biogeochemical models. It will also be capable of showing the location of these field sites on world maps. This process helps in identifying the parts of the model that needs to be improved. This is an important tool to evaluate the current state of ecosystem models and rigorously assesses what the model can or cannot predict. This tool can show statistically significant trends of the model performance.

Despite the heterogeneity of the modelling studies examined with respect to model complexity, type of ecosystem modelled, spatial and temporal scales, and model development objectives, this study revealed statistically significant trends of the DNDC model performance. Here we present the predictions of N_2O emissions by the DNDC crop model as expressed by the coefficient of determination (r^2). As shown in Figure 5 & 6, predictions of cumulative annual N_2O emissions improved over several versions. Our analysis is limited by the number of samples and heterogeneity in these modelling studies.

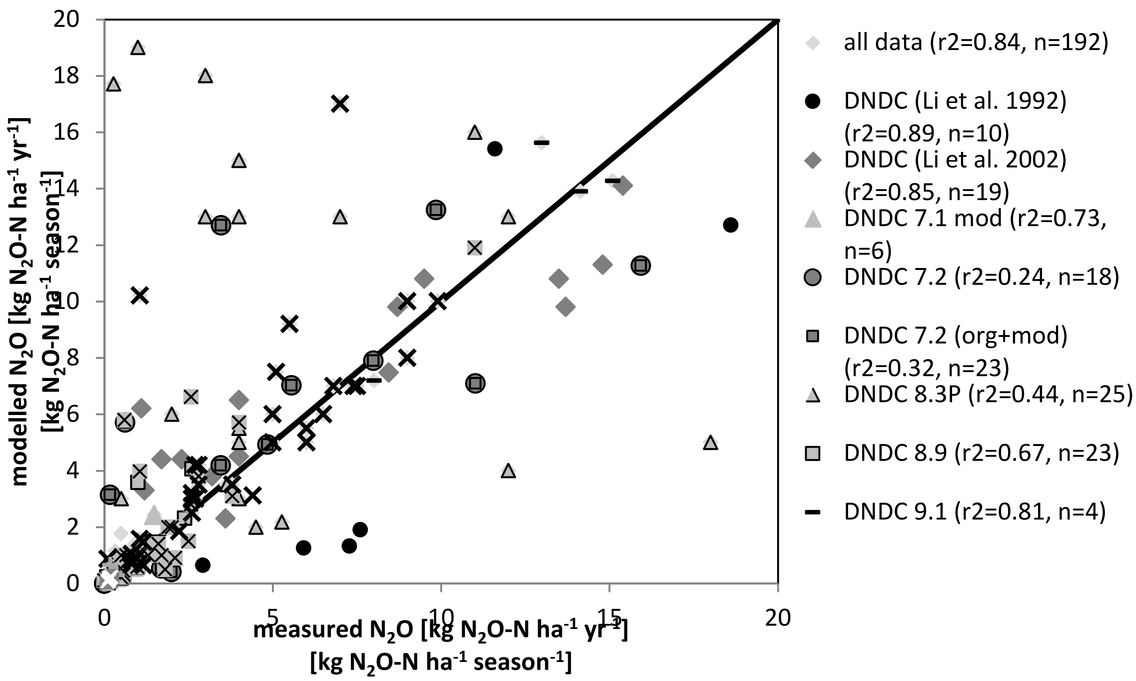

Figure 5 : Measured and modelled total or annual N_2O sorted by model version, extracted data from publications.

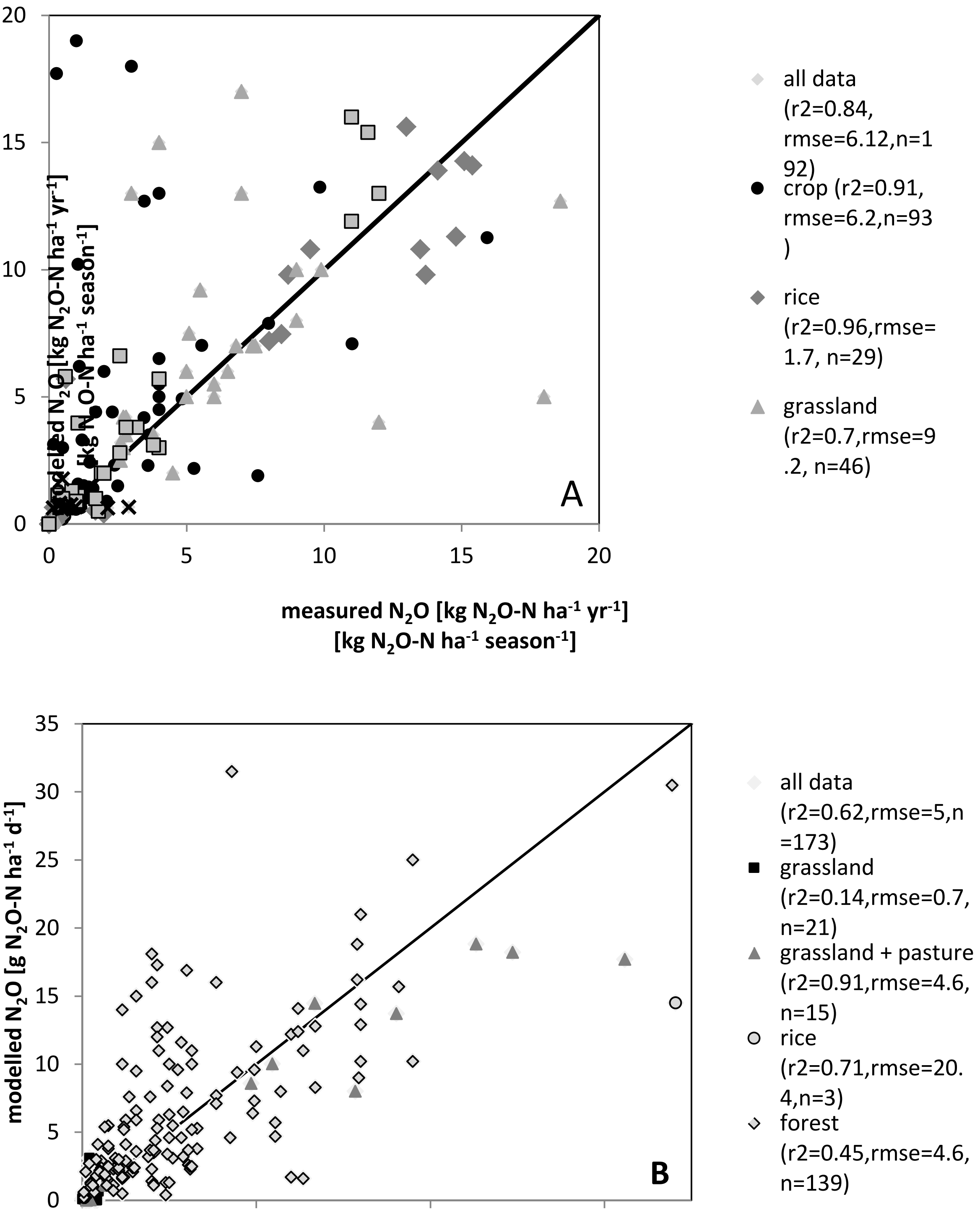

Figure 6: Measured and modelled N_2O emissions (A) Annual and (B) daily total N_2O sorted by model land use, extracted data from publications.

Registered users of GRAMP can upload the simulated results to an existing database. It is anticipated that database will grow over a period of time and give a snapshot of model performance. In this analysis, daily N_2O emissions were poorly modelled (r^2), indicating that the performance of DNDC model declines as we move from annual to daily time step (Figure 6A & 6B). This model performance tool can be used to summarize the relative merits of a collection of different models or to track changes in performance of a model as it is modified.

4 Discussion

The modeller's task is to identify or develop an appropriate model or methodology for a given modelling objective (Wagener et al., 2003). Experience shows that identifying or developing a best methodology is difficult due to several different conceptualizations of ecosystems, which may yield equally good results. This ambiguity has serious implications for models and limits the applicability of ecosystem models for the simulation of land use or climate-change scenarios, or for regionalization studies (Moore and Clarke, 1981). There is a rapidly growing literature on ecosystem models predicting soil C (Liu et al., 2009; Smith et al., 2010), N dynamics (Bell et al., 2012; Giltrap et al., 2010; Thorburn et al., 2010) , GHG emissions (Hutchings et al., 2007; Smith W. N et al., 2008), ecosystem services (Schröter et al., 2005) and climate change mitigation (Del Prado et al., 2013), from different ecosystems (De Gryze et al., 2010). As these models develop, the challenges of information accessibility, data comparability and unification of existing methods become more prevalent. New research approaches must be developed to support decision-making for the management of ecosystems and natural resources (Parker et al., 2002; Spielman et al., 2009; Walker, 2002).

GRAMP is an open-source platform, where scientists can collaborate freely and share data. GRAMP allows the creative and productive powers of numerous individuals and research groups to be harnessed with the common goal of quantifying GHG emissions and simulation of soil C & N dynamics across broad geographic regions and multiple spatial scales. It is an integrated, web-accessible knowledge base that allows temporally and spatially explicit data to be linked to dynamic simulation models. Anyone can participate by registering on the site as model users or as developers. It provides various services, such as: version control, code sharing, modelling tools sharing and support organizing online training sessions, tutorials and webinars. It allows greater interactions among different scientific communities across the world who are interested in the study of soil C and N dynamics and climate change.

In addition, the GRAMP meta-database resource provides information for researchers on the existence and availability of data applicable to a wide range of agricultural and environmental questions. The metadata base has proved useful for many applications and is freely available for many more *via* the GRAMP web portal. Working on a common platform using standardized models should enable the harmonisation of many existing methodologies.

5 Conclusions and future outlook

The aim of GRAMP is to develop a web resource that will serve as a central hub for information on agriculture GHG emission modelling. GRAMP is anticipated to increase the modelling research capacity and to accelerate improved reliance on models to predict GHG emissions and test mitigation practices. GRAMP will bring greater transparency in model development and application, which will help in the advancement of ecosystem modelling. GRAMP will collect and document a comprehensive and standardized set of metadata for ecosystem model simulations. Using this web-platform, the modelling community, along with end users, can build well-documented models and harmonise existing methodologies. The metadata archive and model repository will provide a much more comprehensive and up-to-date description of ecosystem models than is typically available in journal articles or reports. The open-source community managed GRAMP as a metadata repository is anticipated to spur the development of cutting edge modelling techniques. GRAMP will advance the fundamental understanding of C-N interactions at different scales, and improve the interaction between modellers, experimentalists and users, to synthesize solutions in the problem areas of model application and validation. GRAMP will act as a global communication tool between research teams and model users, specifically interested in the measurement and modelling of GHG mitigation.

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