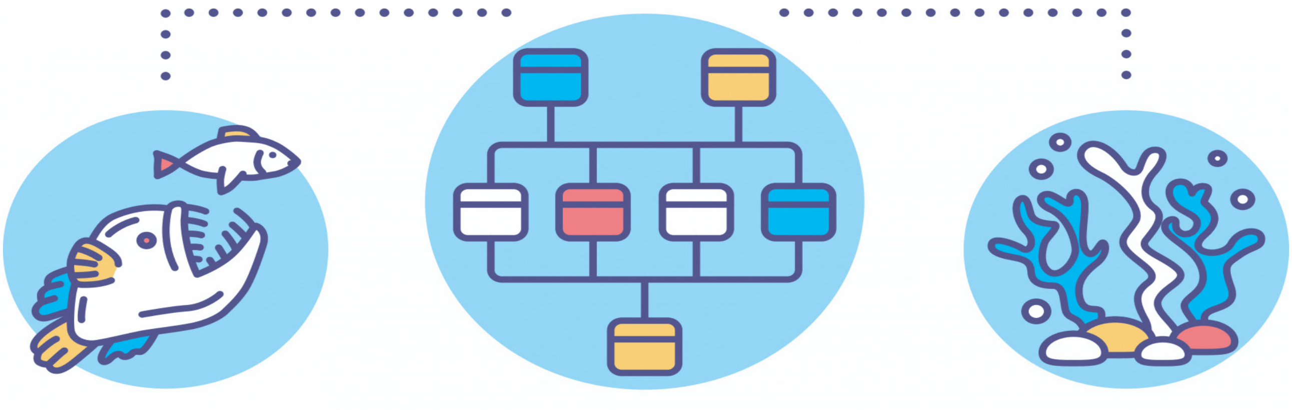
Best practices for ecological model evaluation I 2018

Workshop Report



The Nansen Legacy Report Series 6/2020

Best practices for ecological model evaluation I

Tromsø, November 6 – November 7, 2018

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Executive summary

The Nansen Legacy workshop on best practices for ecological model evaluation, chaired by Benjamin Planque (IMR) was held in Tromsø on the 6-7th November 2018. The meeting was attended by 13 participants from four institutions. The objective of the workshop was to develop recommendations for best practice in evaluation of the performance of food-web simulation models (deliverable 4-4.1.1 of the Nansen Legacy project).

The workshop first reviewed current practices in model evaluation for the five ecological models used in Task 4-4, namely: Gompertz, Norwecom, Atlantis, NDND and EwE. In addition, the NorCPM/ESM model was also presented. In a second phase, workshop participants engaged into open discussions around specific topics related to model evaluation methods. Finally, an attempt was made to develop a protocol for the standard reporting of model evaluation procedures.

Two important recommendations from the workshop are: 1) the definition of clear objectives for specific applications of a model are a pre-requisite for model evaluation. These clearly stated objectives are often lacking and will need to be specified; 2) a standard protocol for describing model evaluation will significantly contribute to standardisation, transparency, communication and quality of the evaluation of the ecological models used in the Nansen Legacy. The draft evaluation protocol outlined during the workshop will need to be further developed.

Content

1 Opening of the meeting

Benjamin Planque opened the meeting with a short presentation of the Nansen Legacy project and the role of the present workshop in the overall objectives of the Nansen Legacy.

The workshop is directly relevant to Task 4-4.1: *Performance evaluation of Barents Sea food web models*, and aims at deliverable 4-4.1.1: *Recommendations for best practice in evaluation of the performance of food-web simulation models*.

In the Nansen Legacy, ecological models can be used to understand, predict or give forecast on the ecological system. The aim of the workshop is to improve modellers practice in the evaluation of the performance of their models when performing these tasks.

The introduction presentation was followed by a round table self-presentation by all participants.

Bérengère Husson and Elliot Sivel were nominated as rapporteurs.

2 Individual ecological models, approaches and evaluations

Models were presented individually. This was important to get all participants familiar with the rational, structure, and evaluation of all the ecological models used in the Nansen Legacy. Individual presentations were prepared following the following structure: 1. Model purpose, 2. Model structure, 3. Model outputs, 4. Model evaluation.

2.1 NorCPM/ESM

Model purpose (why): NorESM is an Earth System Model, meaning that it can be used to investigate the role of different parts (ocean, atmosphere, land) of the Earth system in the Global climate, and how they interact.

When it comes to HAMOCC it is used to explore the role of ocean biogeochemical cycles in the Global climate, and to understand the influence the global climate system (i.e. ocean, atmosphere, sea-ice dynamics ..) have on ocean biogeochemical cycles (for example ocean productivity).

NorCPM: to produce reanalyses, to investigate the predictability of, and to predict, different aspects of the climate system. It is similar to NorESM, except that it employs data assimilation.

Model structure (how): NorESM and NorCPM consist of several coupled models (ocean dynamics, ocean biogeochemistry, atmosphere dynamics, atmospheric chemistry, and sea ice) that together build up the Earth System. The ocean biogeochemical model, HAMOCC, consists of several tracers representing i.e. phytoplankton, zooplankton, organic and inorganic nutrients and carbon, and oxygen. It is embedded in the dyamical ocean model, and is therefore affected by ocean currents, stratification and sea ice extent.

Model outputs (what): 4D (depth, latitude, longitude, time) fields of for example:

Ocean: currents, salinity, temperature, sea ice
Ocean biogeochemistry: nutrients (nitrate, phosphate, iron), phytoplankton concentration (carbon), carbon fixation, export production, air-sea co2/o2 exchange
Atmosphere: winds, clouds, precipitation

Model evaluation (skills): The model is evaluated by measuring how well it reproduces the (historical) state of the climate system. This can be done by comparing model output with time series from certain stations (for example primary production), 2D fields (for example sea ice extent), 3D fields (for example phosphate disribution in the ocean). The comparison can be done by correlations, RMSE, or looking at patterns (for example, does the model reproduce the spatial distribution of chlorophyll in the Barent's Sea?)

2.2 State-space multispecies models (Gompertz)

Model purpose (why): Model purpose is to quantify roles of processes that are potentially important for population and ecosystem dynamics and hence improve our understanding of the ecosystem.

Model structure (how): The ecosystem is simplified to a few, important players and processes. Dynamics are described by a process model, which is linked to data by an observation model. Parameters are estimated in a Bayesian framework by MCMC in JAGS or Hamiltonian MC in STAN.

Model outputs (what): Model outputs are parameter estimates, retrospective «what if» scenarios, and short-term predictions.

Model evaluation (skills): Model evaluation consists in assessing convergence, assessing validity of key model assumptions (e.g. for Gompertz function, independence, additivity), applying sensitivity analysis for uncertain assumptions (e.g. observation error), and investigating model output such as correlations between parameters and explanatory power (magnitude of different variance components).

2.3 The Norwegian ecological model system end-to-end (Norwecom.E2E)

Model purpose (why): To quantify state, growth and energy flow between key species with a special focus on climate impact (bottom-up) to improve our understanding of the marine ecosystems.

Model structure (how): The main characteristics of NORWECOM.E2E is high resolution in space and time and relatively few different species. The model is based on a detailed description of the physics from an ocean circulation model together with an NPZD model for nutrients, phytoplankton and zooplankton. On top of this a number of individual based models (IBMs) for key species is added and 2-way coupled. At present IBMs for *Calanus finmarchicus*, *Calanus hyperboreus*, mesopelagic fish, pelagic fish and fish boats are available. The model also has modules for ocean acidification and contaminants.

Model outputs (what): Model outputs are time series and fluxes of and between the different state variables. The model can be used to study the effects of climate, and for a number of "what-if "scenarios such as the effect of aquaculture, changes in fish stock size and fishing pressure, harvesting on lower trophic layers, cruise design and parameter estimates.

Model evaluation (skills): The model is evaluated against available observations of nutrients, chlorophyll and zooplankton biomass and stage distributions. Evaluation is clearly limited as available observations are few in numbers and their representativeness is unknown as plankton by nature is patchy in both space and time. For this reason, a proper quantitative evaluation is difficult.

2.4 Nordic and Barents Seas Atlantis (NoBa)

Model purpose (why): Built for exploring cumulative effects of changes in fisheries (management), climate and/or other stressors (e.g. pollution, invasive species)

Model structure (how): The NoBa model is a spatial, deterministic complex end-to-end ecosystem model, with 57 components representing the ecosystems of the Nordic and Barents Seas. The components are linked together through a predator-prey matrix, which describes the overlap between the predator and its prey. In addition, for any predation to happen, the components need to overlap in time/space, and prey needs to fit in predator's mouth.

Model outputs (what): NoBa provides information on biomass, numbers, weights (structural+reserve weights), mortality (natural+predation), diets, catches, production, consumption/grazing and distributions. All provided in time and space (polygons+layers).

Model evaluation (skills): Model evaluation is currently consisting of 'traditional' methods, such as root mean square, ME +++. However, these tools don't work as they should with models of the NoBa kind, as these are providing trends and not exact biomass/numbers. We are currently working on finding better methods for doing this.

2.5 Non Deterministic Network Dynamics (NDND) model

Model purpose (why): to explore the possible dynamics of the Barents Sea food web, from the likely to the extreme cases. To investigate how changes in climate and fishing may impact the range of possible futures.

Model structure (how): The NDND model is a simple food web simulation model. It consists of few species groups interacting via predator-prey interactions. It is grounded in the concepts of 'chance' and 'necessity'. The trophic interactions are stochastic (chance) but bounded by a number of simple constraints (necessity) such as maximum ingestion rate, positiveness of biomass and flows or maximum population growth rates.

Model outputs (what): Model outputs time-series of species biomass and trophic flows. From these time-series, multiple patterns are derived, which include: diet composition, density-dependence, top-down vs. bottom-up controls, food web stability and synchrony, etc...

Model evaluation (skills): The principle of NDND model evaluation is rooted in pattern-oriented modelling. The idea is that the multiple patterns produced by the model should match those observed in the natural system. The quantitative method for doing this is currently being developed.

2.6 EcoPath with EcoSim and EcoSpace (EwE-E)

Model purpose (why): To study structure, dynamics and spatial patterns in the Barents Sea ecosystem to gain knowledge about how climate, exploitation and other drivers affect the system.

Model structure (how): EwE is a simple data-grounded mass-balance ecosystem model concept that is flexible and the simulation and spatial module can be driven by observed (back in time) or hypothetical (future predictions and forecast) environment data.

Model outputs (what): Ecopath outputs biomass, mass flows, mortality rates and a range of ecosystem metrics. Ecosim outputs time-series for biomasses, mortality rates, mass flows and Ecospace outputs spatial fields of biomass over time.

Model evaluation (skills): Model output will be evaluated by comparison of model output with observed data, e.g., changing patterns over time in group biomass, diet and predator composition, consumption and spatial distribution.

3 Model evaluation protocols

The examination of the five ecological models used in RF4-4 reveals that the approaches used for model evaluation are diverse and do not follow common formats or protocols. They can focus on very different aspects of the model structure and outputs, for example: convergence of the optimisation (Gompertz), fit to historical data (Gompertz), quality of the input parametrisation (Ecopath), realism of the model structure (Norwecom), reproduction of ecological patterns (NDND, Atlantis). There is a general belief that if the structure of a model is 'good', then the performance of the model should also be 'good'. The diversity of evaluation criteria reflects to a large extent the diversity of objectives that can be targeted simultaneously with the same model: improving understanding of the generative mechanisms behind observed ecological patterns of variability, hindcasting of ecosystem trajectory, forecasting, or what-if scenario experiments.

The evaluation approaches can be broadly divided in two main categories: evaluation of the model construct and evaluation of the model outputs.

Evaluation of model construct is concerned with the overall quality of the model. The criteria considered can include: model realism and credibility, transparency, replicability, parsimony, communicability, parameters measurability. These criteria are often considered independently of a precise question being asked. They are important for the model to be accepted by the scientific community and by the community of users. A model that scores high on these criteria will be considered relevant to address a range of questions about ecosystem dynamics. As an analogy, a statistical catch-at-age model is considered performant for the assessment of a fish stock for which there is appropriate age-structured data and fisheries information. But this doesn't say how well the model will perform when applied on a specific stock, at a specific point in time, for a specific purpose.

Evaluation of model outputs is concerned with a quantitative evaluation of the model performance in addressing a well-specified objective. Usually evaluation of model outputs will involve some comparison between simulated and observational data. **Two critical aspects for the evaluation of model outputs are 1) the specification of the objective and 2) the identification of the observational data available and the uncertainty associated with this data.** As an analogy, the model output performance of a statistical catch-at-age model can be evaluated given a specific question, e.g. for conditional forecasting of the spawning stock biomass for given stock, and given specific fishery and survey data. The performance criteria can include convergence of the model, uncertainties in parameter estimates, distribution of residuals between numbers-at-age observations and model predictions, and retrospective patterns.

Multiple patterns: The five ecological models used in the Nansen Legacy can produce a wide range of outputs and these outputs can be interpreted in terms of ecological patterns (e.g. temporal or spatial variability, top-down vs. bottom-up controls, community structure, benthic-pelagic coupling,...). It is important that the key/dominant patterns that the models should (re)produce be defined in advance of the evaluation. Pattern Oriented Modelling (Grimm et al., 2005, Grimm and Railsback 2012) provides a useful framework for this.

Data quality and availability is a central issue for the evaluation of model outputs. There are substantial data on commercially exploited species, but this is not the rule for most benthic or planktonic species. When data exists, the quantity, precision, scale of observation, sampling design, etc. may not be appropriate to be used for model evaluation. In some cases, observational data may not cover a range that is wide enough to cover extreme events that models could be used for.

Use of data for model evaluation. This can be achieved in many ways. Allen and Sommerfield (2009) and Stow et al. (2009) advocate for approaches that are centred around the direct comparison of field observations against simulated observations in a univariate or multivariate framework. Wood (2010) and Hartig et al. (2011) provide a statistical framework for the analysis of emergent patterns in stochastic simulation models, based on summary statistics. The latter is consistent with Pattern Oriented Modelling. When observational data is used to fit models (i.e. estimate model parameters), it is common practice to perform cross-validation on a set of data that was not used for calibration. This can however be complicated when there is strong spatial or temporal structure in the data (Roberts et al., 2017). Data may also be used to parametrise input parameters during the model construction phase.

Recent advances in complex model optimisation. Numerical optimisation of models strongly depends on the specific objectives, the structure of the model and the type of simulation. So, defining the appropriate model optimisation protocol is a problem analogous to defining the appropriate model evaluation protocol. A network of French researchers called Mexico (Methods for numerical exploration of complex models, https://reseau-mexico.fr/) is currently working on a variety of tools to guide for the selection of optimisation methods to be used to answer a specific question and describe the model optimisation process. Those should be soon submitted to Ecological Modelling (Follow the guide! A handbook for conducting optimisation with complex ecological models based on feedback from practitioners, Stéphanie Mahévas, Victor Picheny, Patrick Lambert, Nicolas Dumoulin, Lauriane Rouan, Jean-Christophe Soulié, Dimo Brockhoff, Sigrid Lehuta, Rodolphe Le Riche, Robert Faivre, Hilaire Drouineau). Among those tools are decision trees and an adaptation of the ODD (Overview, Description and Details) protocol originally designed to describe ecological models (Grimm et al., 2010). The ODD-O (ODD-Optimisation) is being designed as a protocol for describing the optimisation procedure for a specific model. In a similar way, it could be useful to develop decision trees for the selection of appropriate model evaluation methods and protocols for the description of the evaluation approach used.

The ODD protocol, a useful template? The ODD protocol was developed to respond to a problematic situation faced by ecological modellers: the lack of standardise protocol for describing individual based models (IBMs). This situation made it problematic to communicate about models, to understand or to replicate them. The ODD protocol consists of three blocks (Overview, Design concepts, and Details), which are subdivided into seven elements: Purpose, State variables and scales, Process overview and scheduling, Design concepts, Initialization, Input, and Sub-models (Grimm et al., 2006). Four years after its initiation, the protocol was reviewed and updated (Grimm et al., 2010) and it is now commonly used by ecological modellers, beyond the original IBMs community, to describe their models in reports and publications (the original article has been cited 1,111 times according to ISI-Web of knowledge on the 16th November 2018). Based on the success of this approach and the ongoing development of the ODD-O protocol (section above), we suggest developing a similar protocol for the reporting of ecological model evaluation procedures: ODD-E (ODD-Evaluation).

The draft ODD-E. The workshop format did not allow much time for the construction of the ODD-E protocol but two hours were used to draft a first structure. The elements of the draft ODD protocol are as follows:

1. Specific objectives for the application of the model

   These can fall in several categories related to e.g. hindcasting, forecasting, what-if scenario simulations, improved understanding of ecological mechanisms. Vague objectives are not appropriate (e.g. "investigate the impact of climate and fishing on ecosystem functioning"). Precise objectives are required (e.g. "forecast the possible range of biomass for all demersal fish species combined one year in advance" or "hindcast the annual primary production from 2000 to 2017 with the highest possible precision, and no more than X% uncertainty").

2. Assumptions related to the objectives

   Assumptions that are general to the model, are usually included in the ODD protocol. The assumption listed here relate to the specific application of the model to the objective stated above. e.g. "it is assumed that in the coming year fishing regulations will remain as they are today" or "it is assumed that there has not been significant year-to-year changes in nutrient inflow during the period studied")

3. Specific deviation from the odd of the model

   To address a specific objective, a model can deviate from the general description provided in the model ODD. This should be specified in this section. e.g. "a sub-model has been added to simulate current fishing harvest control rules, the sub-model is [description] "

4. Data (and observations) used for evaluation, relative to the objective and how they are used,

This section describes the ensemble of observations and data (including already processed observations, e.g. total biomass of a species) that are used for parameter estimation and for model performance evaluation in relation to the objective (section 1). The section provides information on data potential bias, representativeness, uncertainties, quality and quantity.

5. Patterns in relation to the objective. Inferred from the data that should be reproduced by the model

   This section presents which part of the model outputs (in terms of output data or patterns) are considered in the evaluation process. These can include raw outputs in the form of point estimates (e.g. number of individuals of a given species at a precise location and timing), aggregated outputs (e.g. mean or total production over a period of time and area) or more complex emerging patterns (e.g. spatial structure described by a variogram, occurrence of regime shifts, degree of spatial overlap between species).

6. Method for evaluating model against data and evaluation criteria

   The methodology used to evaluate the model (described in the ODD and section 3) against data (section 4) to address the specific objective (section 1) is described in this section. Optimally the method includes evaluation metrics than can quantify the coherence between model and observations. For example, the residual patterns (difference between model output and observations) for the spatial distribution of a species should not be spatially autocorrelated and the standard error should be as low as possible and no exceed a predefined value.

7. Sensitivity

   General (of global) sensitivity analysis of the model can already be described using the ODD-O protocol (if this has been completed). This section describes sensitivity analysis in relation to the specific objective outlined in section 1. For example, analysing how residual patterns in spatial distribution vary depending on assumptions about individual daily vertical migration patterns.

Because of the variety of models employed in the Nansen Legacy, it appears very difficult to establish a common set of guidelines for best practices in conducting model evaluation. Instead, we have adopted a non-prescriptive approach in which we don't tell modellers how to best evaluate their models, but rather ask modellers to explain and document how they evaluate the performance of their model for a specific task. The ODD-E draft protocol is a concrete step in this direction.

4 Recommendations for future work

The two-day workshop revealed that several steps are needed to develop guidelines for good practices in ecological model evaluation:

> First, the definition of a precise question is a pre-requisite to model evaluation.
>
> Second, there is a need for a standardised way of reporting model evaluation procedures.

Third, the standardised reporting protocol must be experimented on the models used in the Nansen Legacy.

For this purpose, it is recommended that a second workshop takes place in 2019, to develop further the ODD-E protocol and test it on some of the models used in the Nansen Legacy.

It is also recommended that scientists and leaders in RF4 jointly work towards the definition of precise objectives/questions against which their model performance can be assessed.

5 References

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Annex 1: List of participants

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Annex 2: Agenda

6 November

11:00 Introduction to the workshop, motivations, expected outcomes. Nomination of rapporteur

Introduction to ecological models used in the Nansen Legacy

- Model purpose (why)
- Model structure (how)
- Model outputs (what)
- Model evaluation (skill)

11:15 NorCPM/ESM (Filippa Fransner)

11:35 Gompertz (Leif Christian Stige)

12:25 Norwecom (Morten Skogen)

13:15 Lunch

14:15 Atlantis-NoBa (Bérengère Husson)

15:05 Non Deterministic Network Dynamics (NDND) (Benjamin Planque)

15:55 Ecopath with Ecosim (EwE) (Torstein Pedersen)

16:45 end-of-day-1

19:00 joint dinner

7 November

09:00 Model evaluation: motivations and tools

10:00 Structured discussion

- What are the common evaluation approaches currently used in Nansen Legacy models?
- What are other candidate approaches?
- Model evaluation through pattern oriented vs. point-estimate?
- Evaluating parameters (sensitivity), past dynamics (fitting) and projections (predictive skills)
- Predictability horizon, what is it and how can it be measured?
- How could my model be improved? Improved with regard to what? Can I evaluate it?

11:30 Lunch

12:30 Discussion continues

14:00 Report structure and writing allocation

15:00 end-of-day-2

The Nansen Legacy in numbers

6 years

The Nansen Legacy is a six-year project, running from 2018 to 2023.

200 people

Currently, there are 204 persons involved in the project. By the end of the project period, the Nansen Legacy will have educated a total of 50 PhD students and postdoctoral fellows.

1 400 000 km² of sea

The Nansen Legacy investigates the physical and biological environment of the northern Barents Sea and adjacent Arctic Ocean.

10 institutions

The Nansen Legacy unites the complimentary scientific expertise of ten Norwegian institutions dedicated to Arctic research.

Norwegian Meteorological Institute

UNIS The University Centre in Svalbard

NERSC

NTNU

Akvaplan niva

>10 fields

The Nansen Legacy includes scientists from the fields of biology, chemistry, climate research, ecosystem modelling, ecotoxicology, geology, ice physics, meteorology, observational technology, and physical oceanography.

50/50 financing

The Nansen Legacy has a total budget of 740 million NOK. Half the budget comes from the consortiums' own funding, while the other half is provided by the Research Council of Norway and the Ministry of Education and Research.

Norwegian Ministry of Education and Research

With funding from The Research Council of Norway

>350 days at sea

The Nansen Legacy will conduct 15 scientific cruises and spend more than 350 days in the northern Barents Sea and adjacent Arctic Ocean between 2018 and 2022. Most of these cruises are conducted on the new Norwegian research icebreaker RV *Kronprins Haakon*.

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