Enhancing the ecosystem modeling cycle: Machine learning approaches for parameter sensitivity and model calibration

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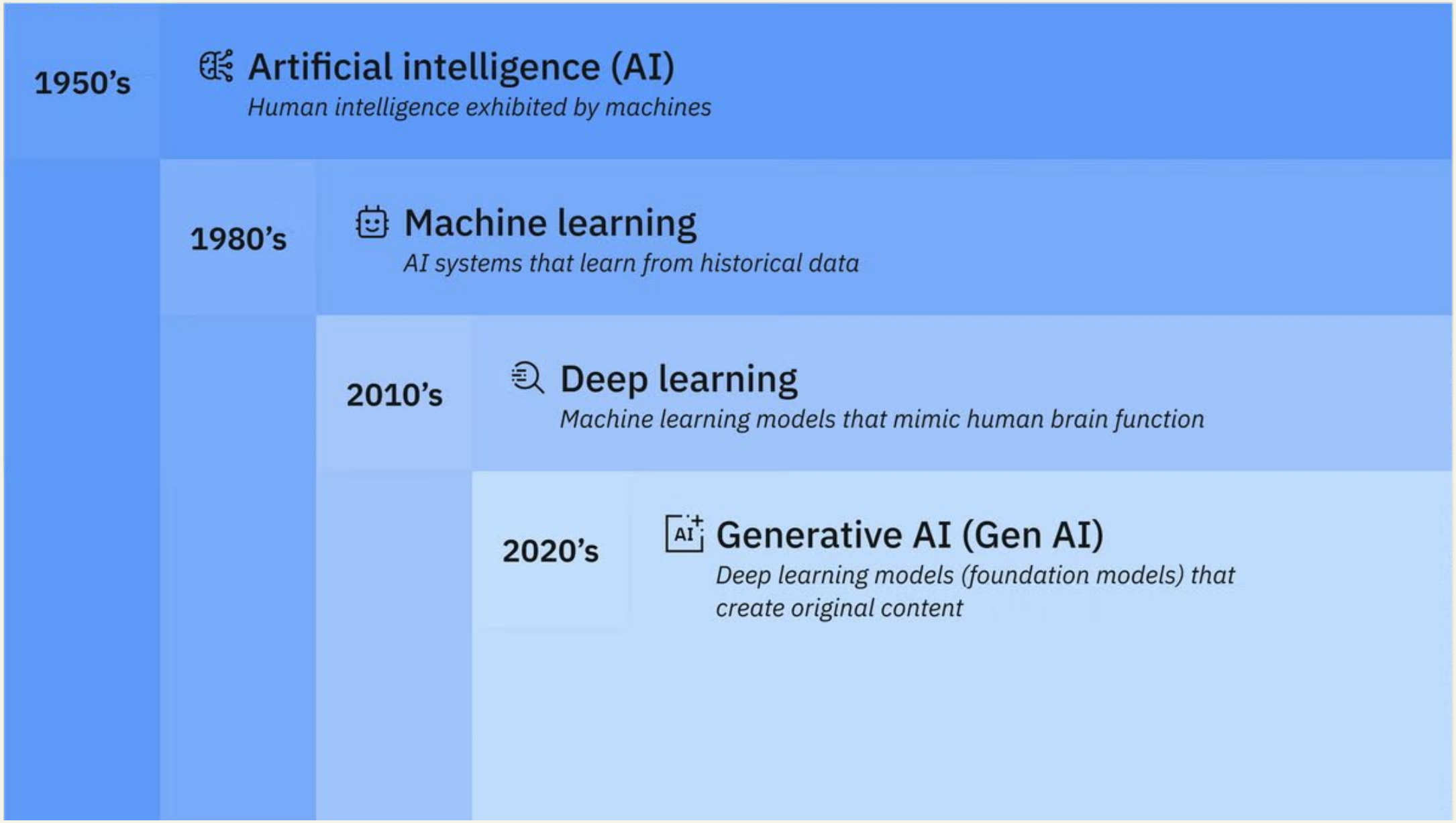
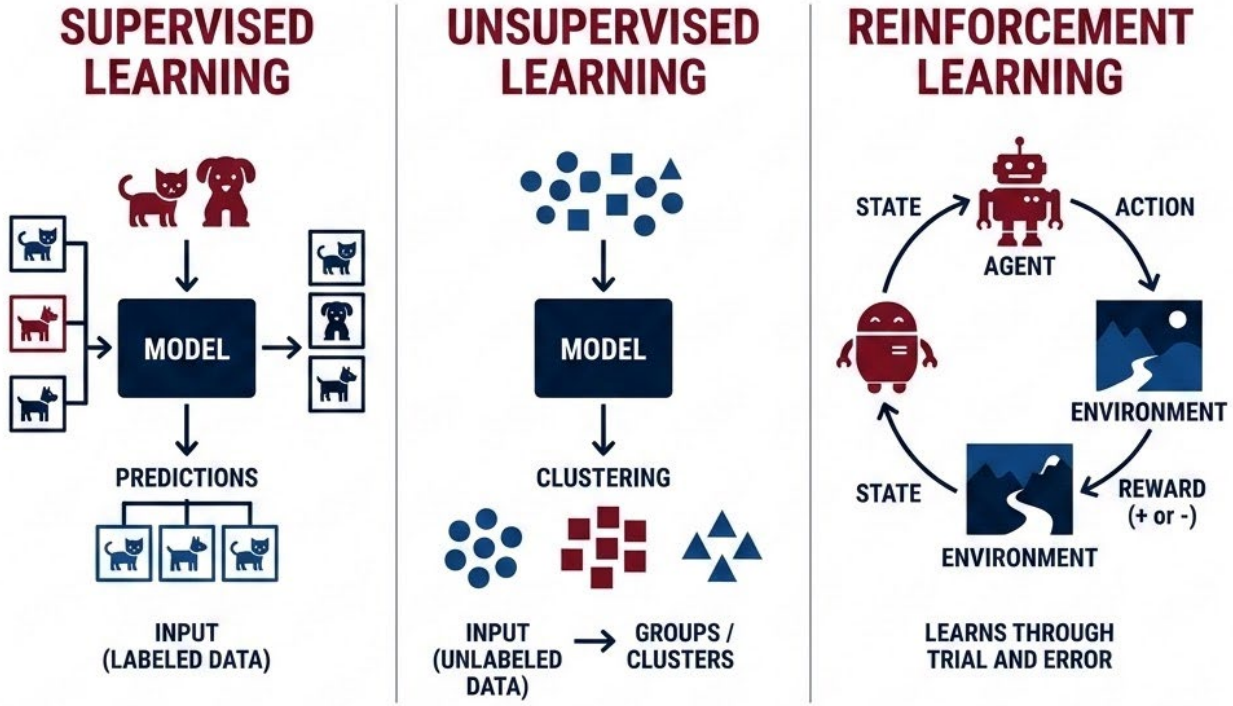
Long Live the Kings. Seattle, WA.

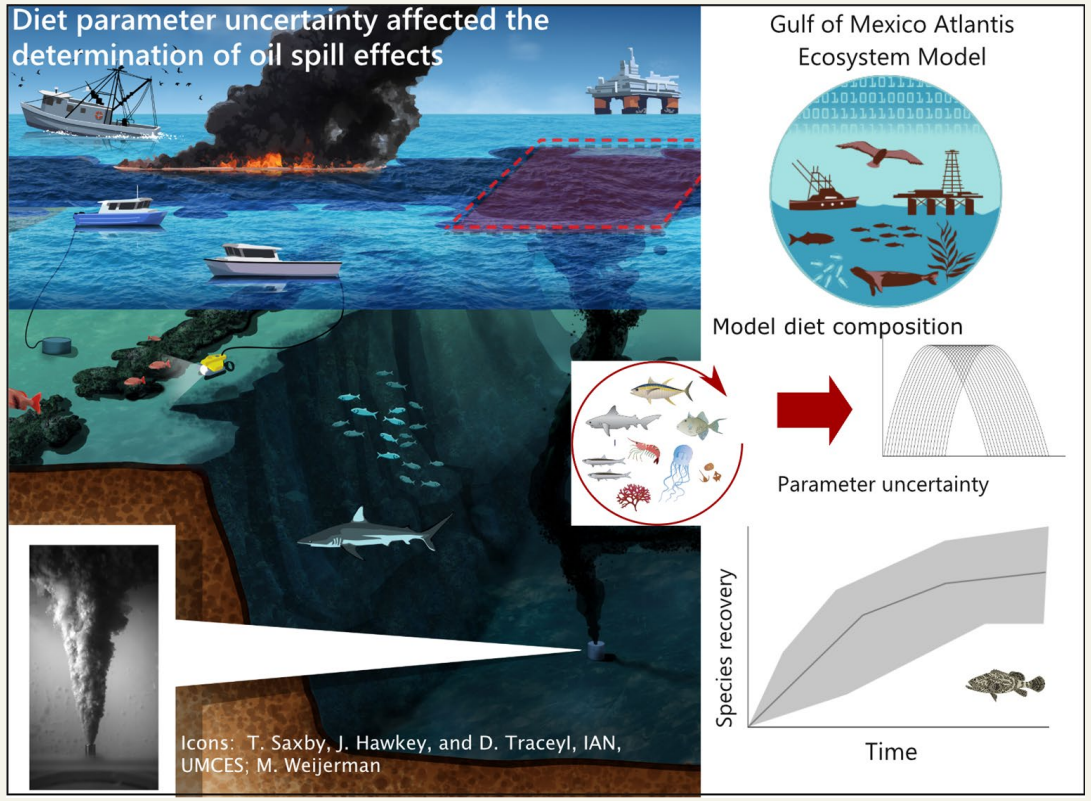

1950's
Artificial intelligence (AI)
Human intelligence exhibited by machines
1980's
Machine learning
AI systems that learn from historical data
2010's
Deep learning
Machine learning models that mimic human brain function
2020's
Generative AI (Gen AI)
Deep learning models (foundation models) that create original content

MAIN TYPES OF MACHINE LEARNING



Created with Google Gemini

Diet composition uncertainty determines impacts on fisheries following an oil spill

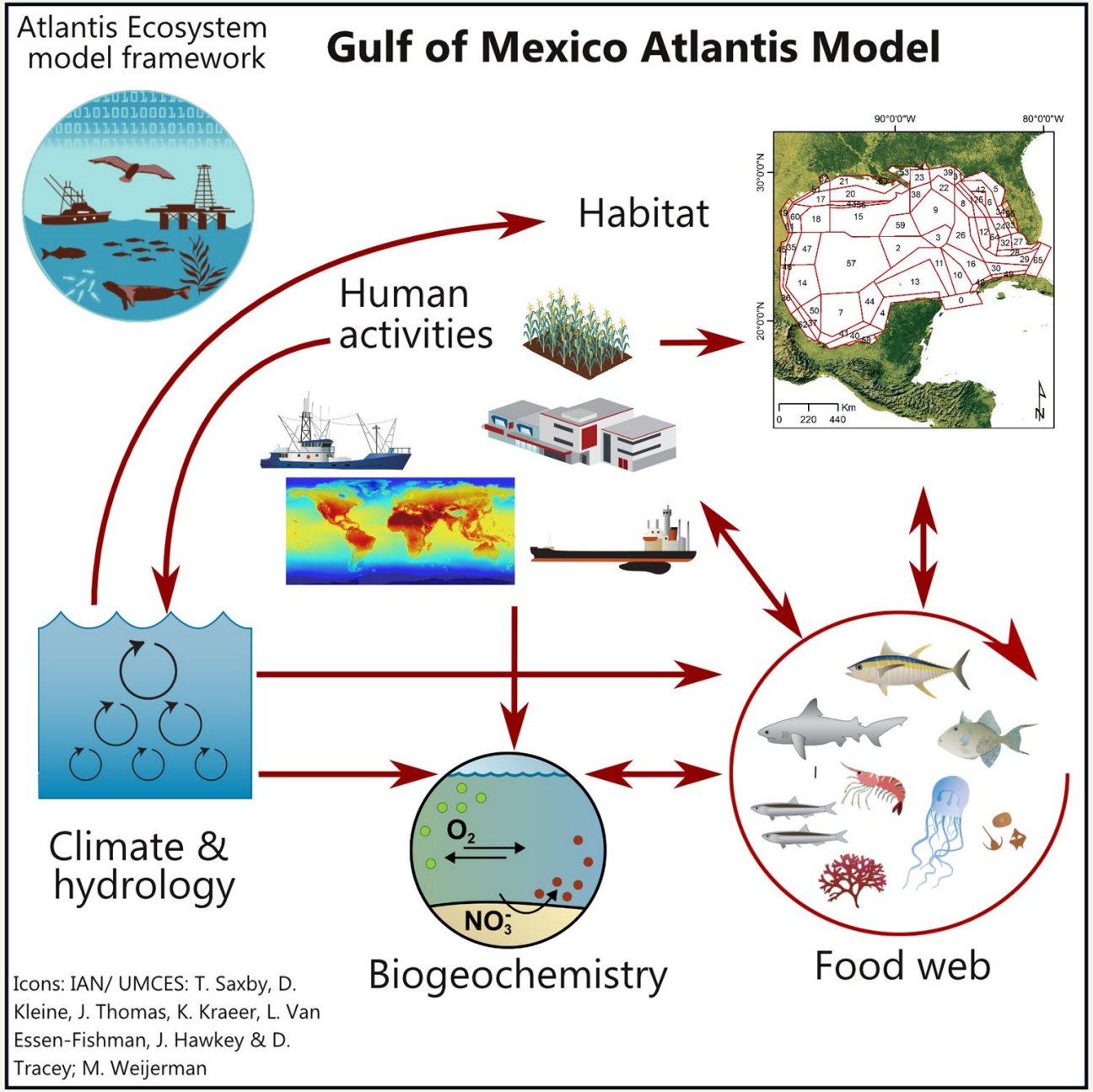


Morzaria-Luna, H, Ainsworth, CH, Tarnecki, JH and Grüss, A, 2018. Diet composition uncertainty determines impacts on fisheries following an oil spill. Ecosystem Services. https://doi.org/10.1016/j.ecoser.2018.05.002



Deep Water Horizon oil spill, 2010

- 20% US fish landings
- Sublethal effects
- Indirect food web effects



Ainsworth, C.H., Schirripa, M.J., Morzaria-Luna, H., 2015. An Atlantis ecosystem model for the Gulf of Mexico supporting Integrated Ecosystem Assessment, NOAA Technical Memorandum NMFS-SEFSG 676. NOAA. NFMS. SFSC, Miami. doi:10.7289/V5X63JVH

Ecosystem model trophic relationships are based on observed diet data



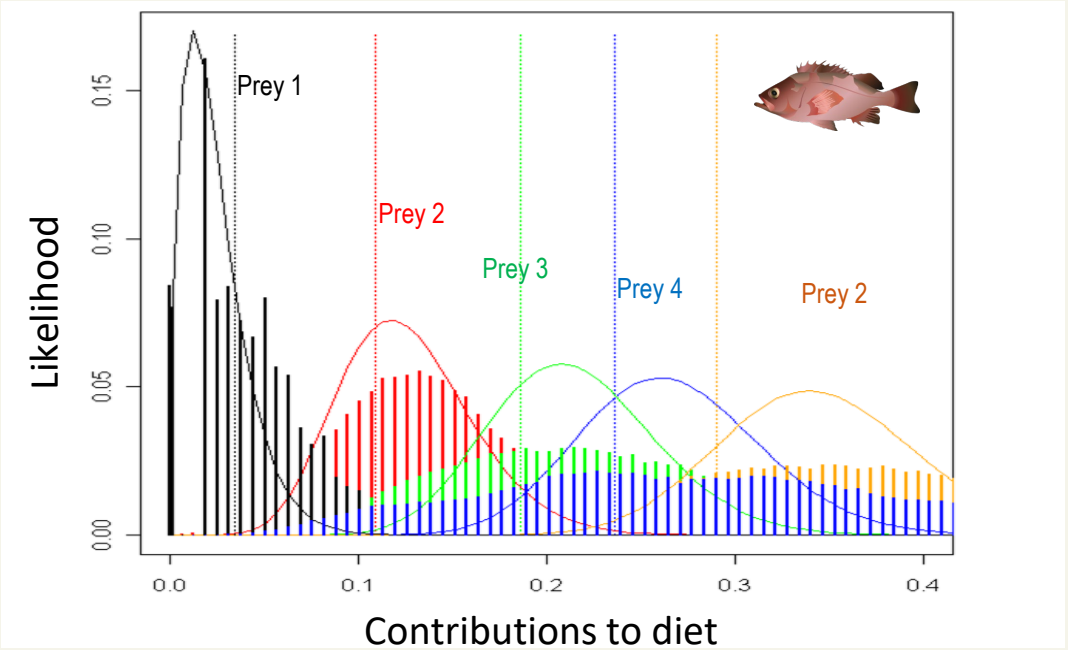


Gut content analysis





Statistical method to combine multiple data sources



Ainsworth, C. H., Kaplan, I. C., Levin, P. S., & Mangel, M. (2010). A statistical approach for estimating fish diet compositions from multiple data sources: Gulf of California case study. *Ecological Applications*, *20*(8), 2188-2202.

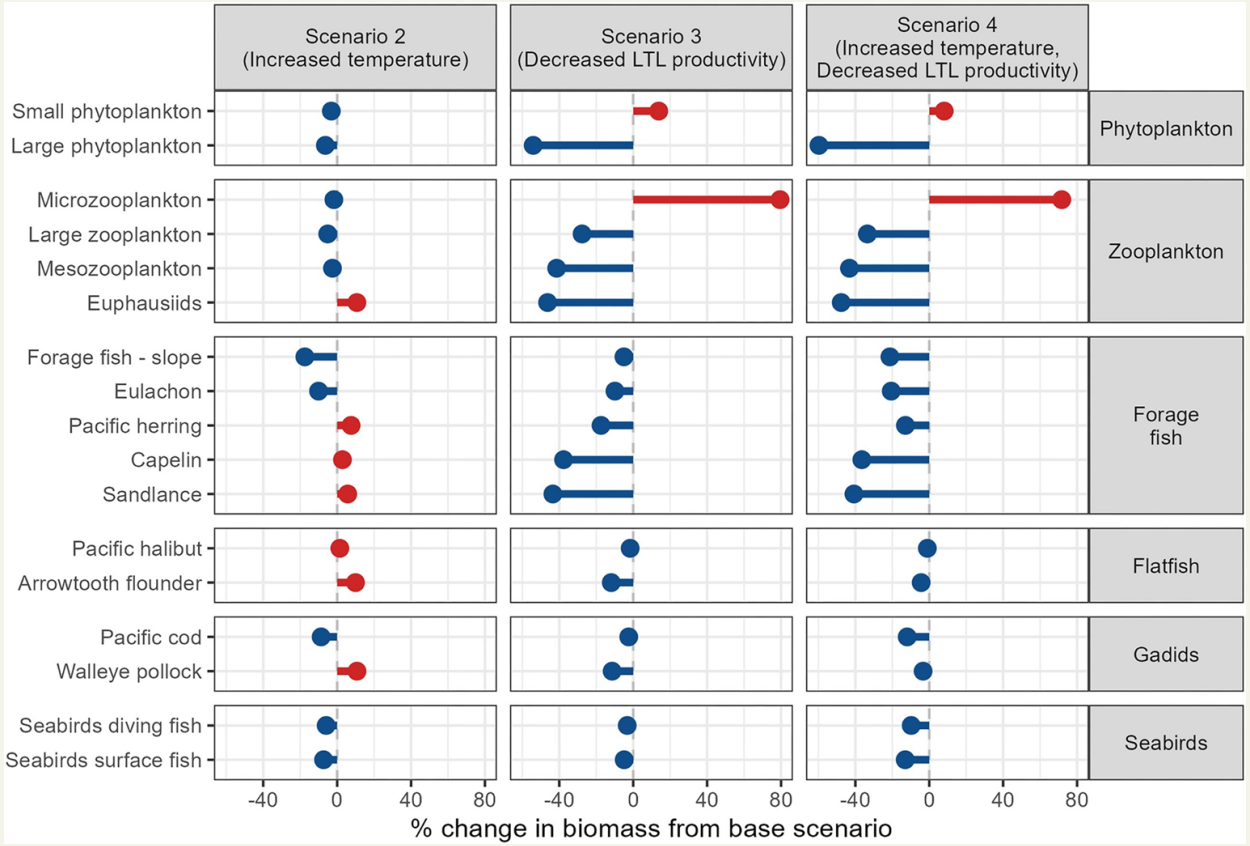
Masi, M. D., Ainsworth, C. H., & Chagaris, D. (2014). A probabilistic representation of fish diet compositions from multiple data sources: a Gulf of Mexico case study. *Ecological modelling*, *284*, 60-74.

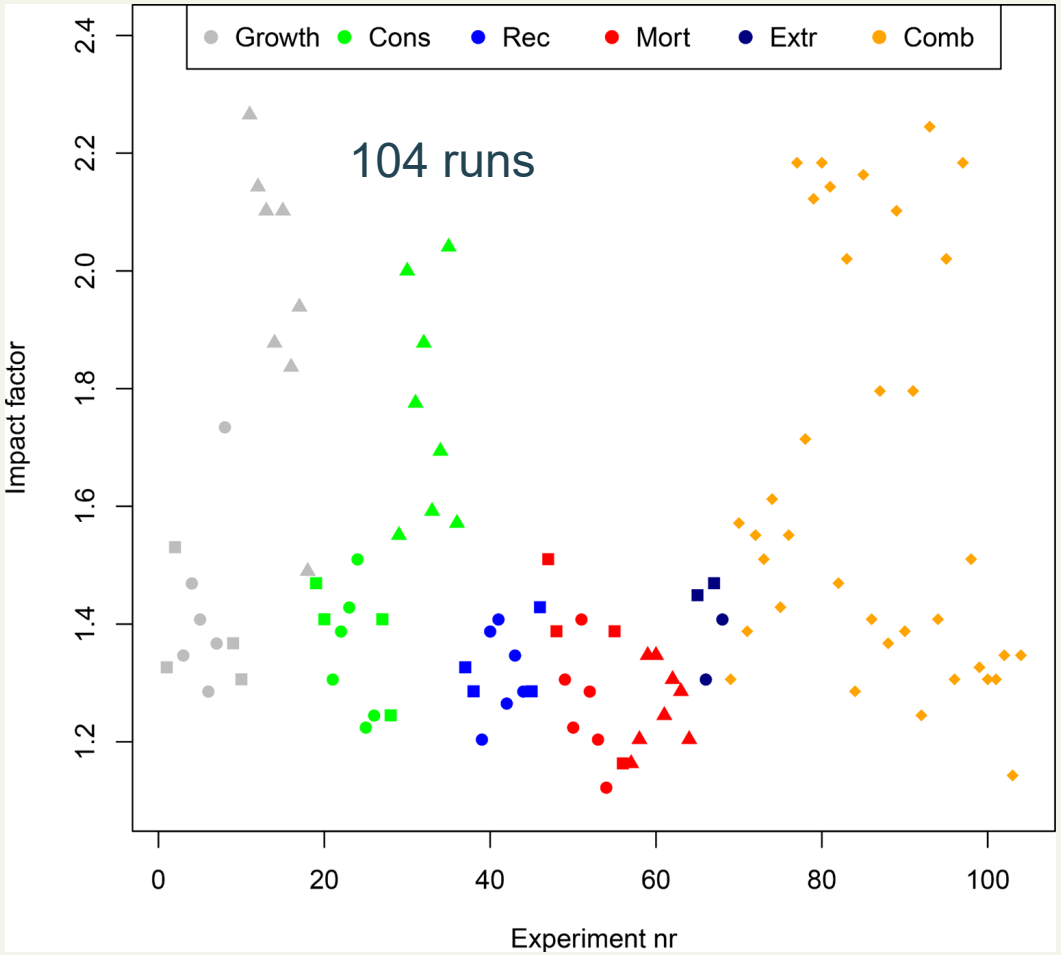
Tarnecki, J. H., Wallace, A. A., Simons, J. D., & Ainsworth, C. H. (2016). Progression of a Gulf of Mexico food web supporting Atlantis ecosystem model development. *Fisheries Research*, *179*, 237-250.

Estimates describe the likely diet contribution of a given prey item to a predator's diet and the uncertainty around this estimate

Uncertainty characterization has been limited for Atlantis

Bounded scenarios





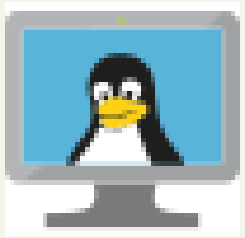
Rovellini et al. 2025. Linking climate stressors to ecological processes in the Gulf of Alaska

Hansen et al. 2019. Sensitivity of NoBA Atlantis to parameter perturbations of key species.

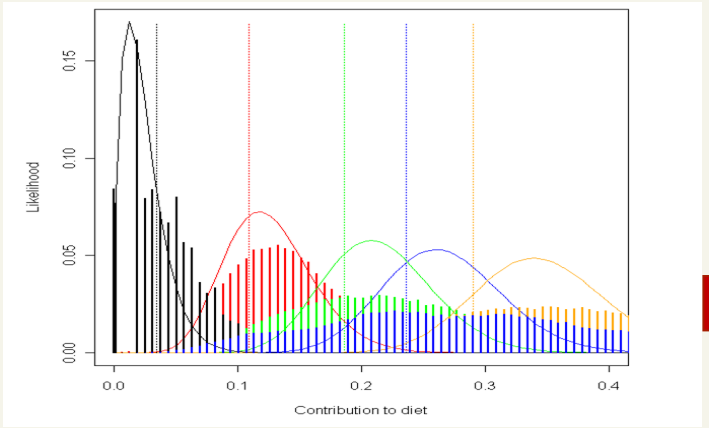
Uncertainty in model outcome may influence impact assessment - Uncertainty analysis of diet composition

Cloud computing



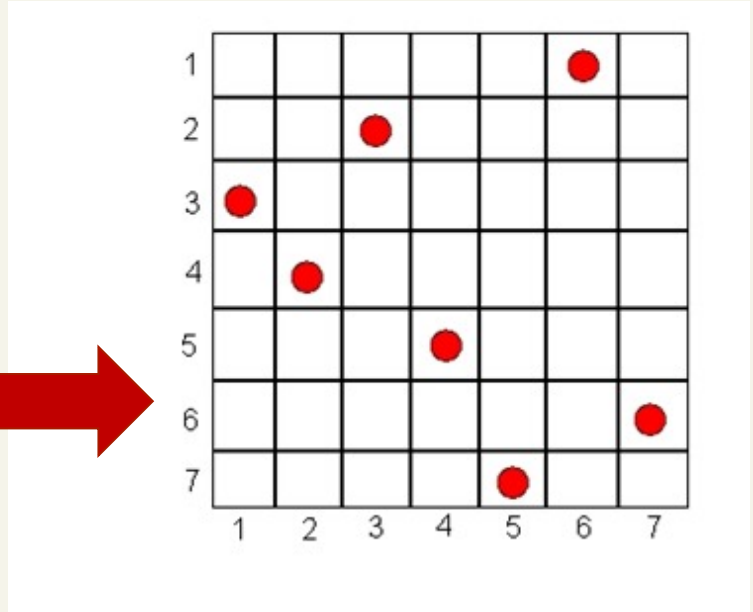


1 Bootstrapped data w/ fitted β distributions



Error ranges 10,000 values

2 Sample distribution

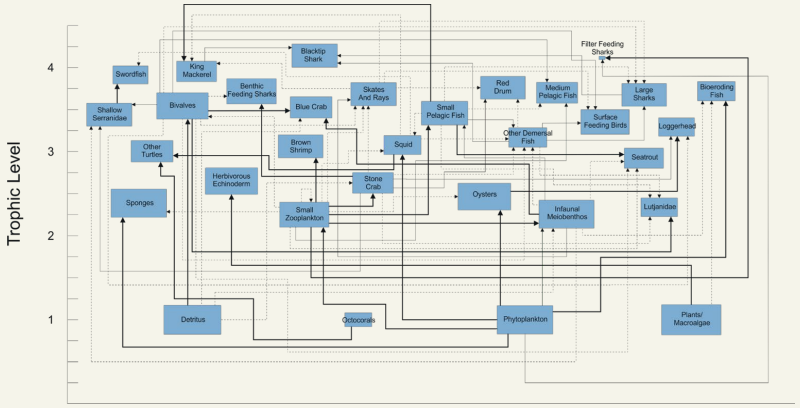


Latin Hypercube 1000 samples

Uncertainty analysis of diet composition

3

Availability matrix: Predator consumption potential and diet preference



1000 Alternate availability matrices

	A	B	C	D	E
A			■		
B	■			■	■
C	■	■			
D		■	■		
E				■	



1000 Atlantis 15yr simulations

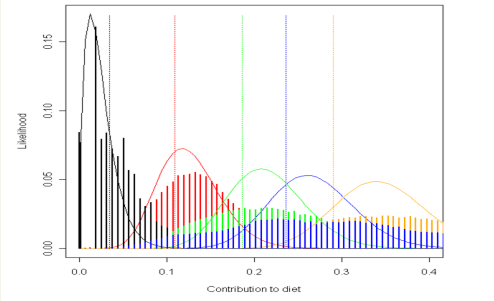
Scenario simulating oil spill from Deep Water Horizon (Ainsworth et al. In review; Dornberger et al. 2016)



Dornberger, L., Ainsworth, C., Gosnell, S., & Coleman, F. (2016). Developing a polycyclic aromatic hydrocarbon exposure dose-response model for fish health and growth. *Marine pollution bulletin*, *109*(1), 259-266.

Uncertainty analysis of diet composition

6 Examined full parameter distribution



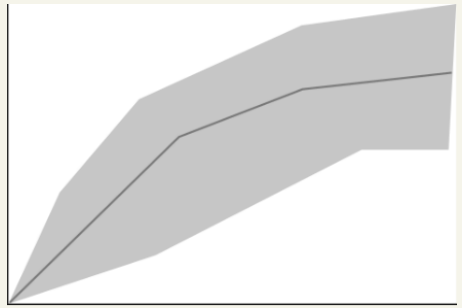
Bootstrapped data w/ fitted β distributions

	A	B	C	D	E
A			■		
B	■			■	■
C	■	■			
D		■	■		
E				■	

10, 0000 availability matrices

7 Statistical emulator or metamodel

Machine learning models



Biomass and catch
Sensitivity analysis

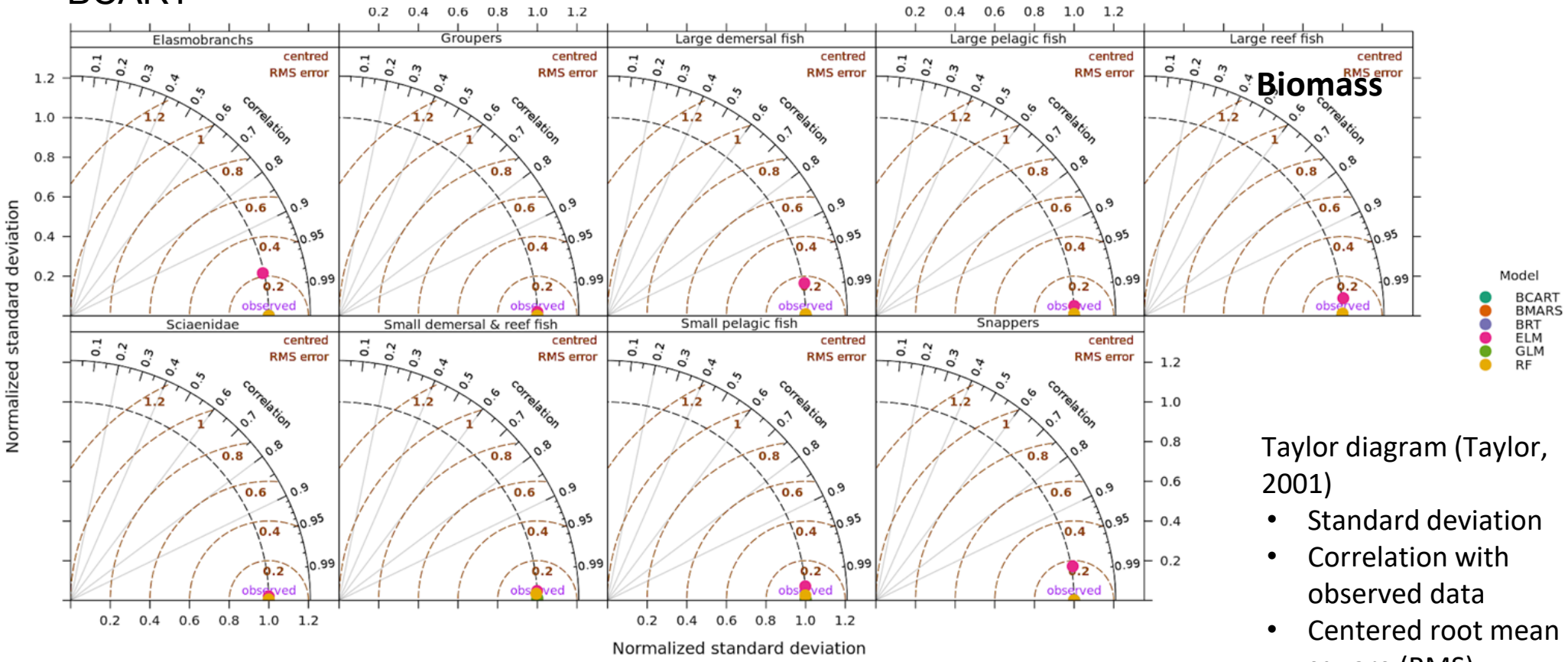
8



10, 000 Atlantis emulations

Emulator performance

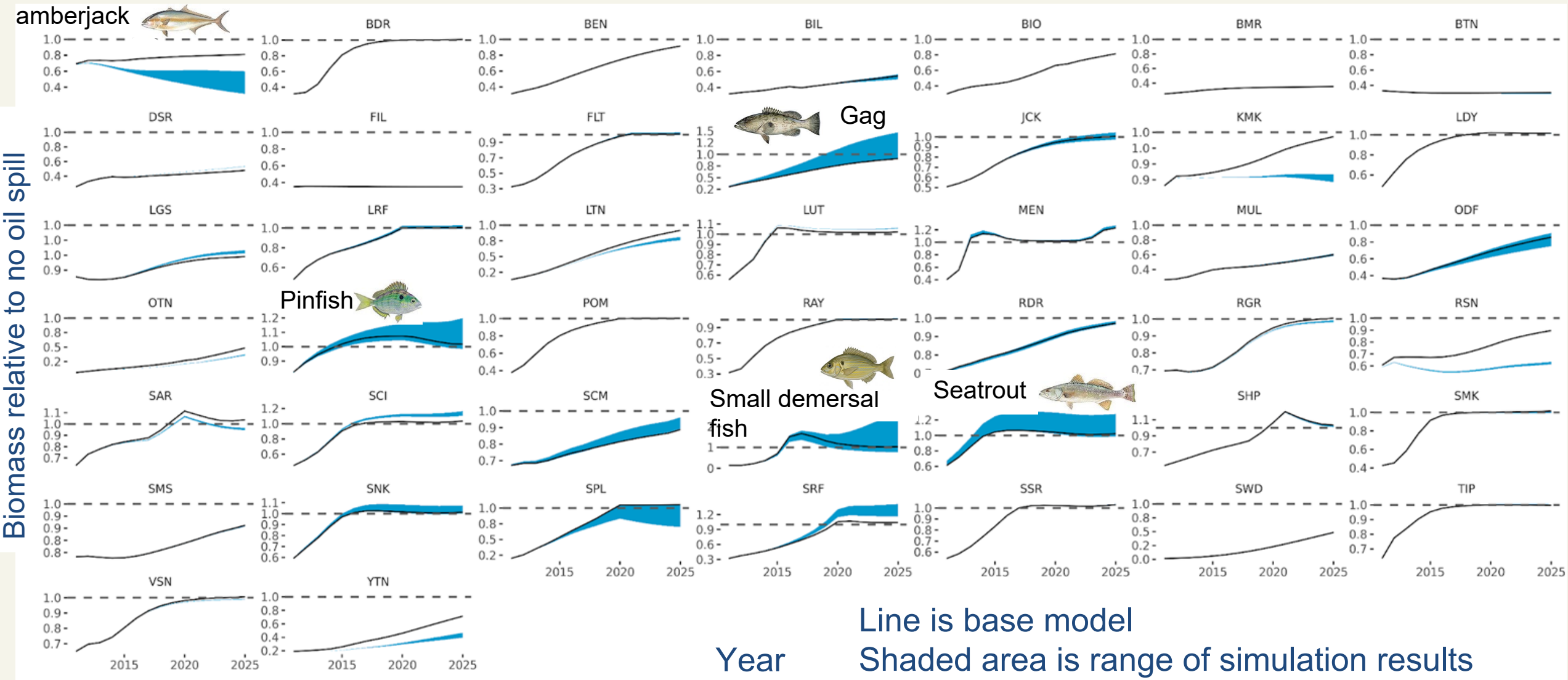
1. Generalized Linear Model, GLM
2. Bagged Multivariate Adaptive Regression Splines, BMARS
3. Bagged Classification and Regression Trees, BCART
4. Random Forest, RF
5. Boosted Regression Trees, BRT
6. Extreme Learning Machine Learning, ELM



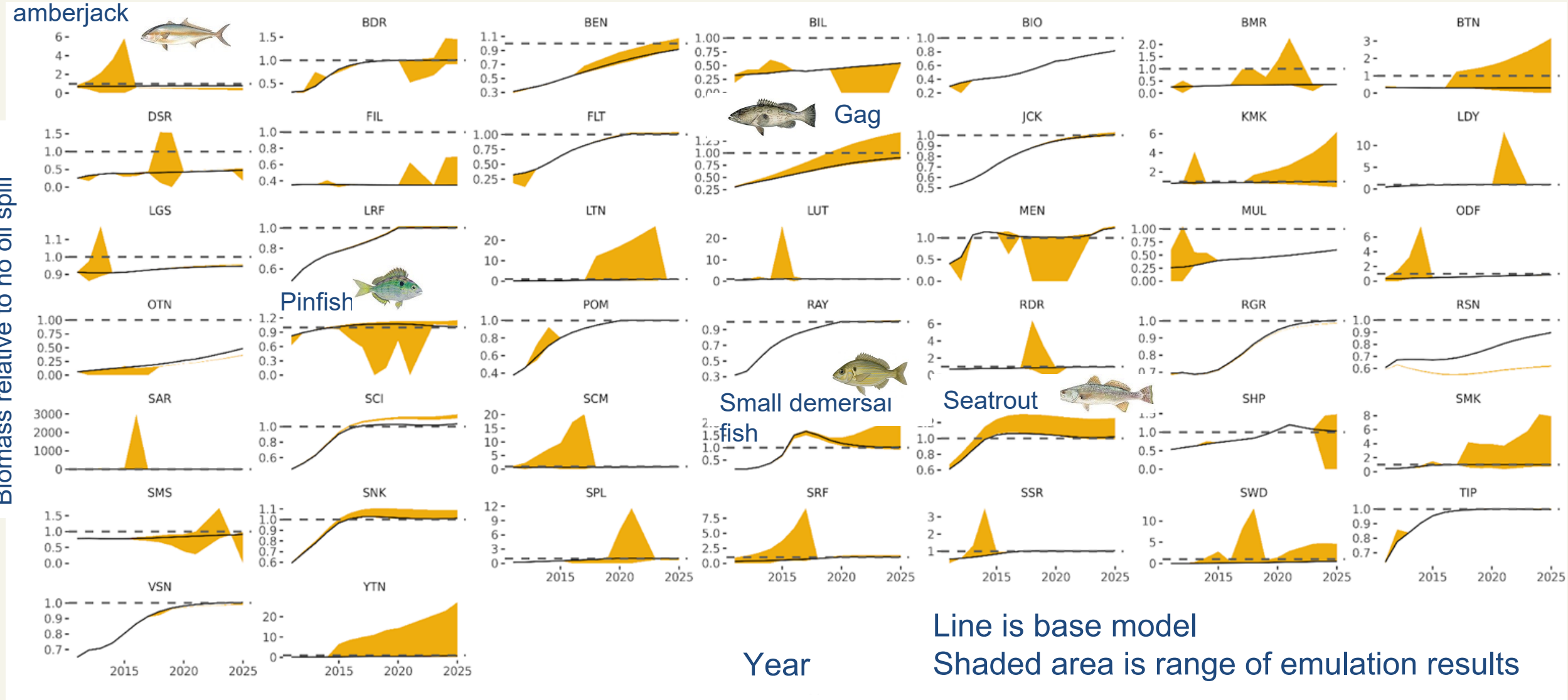
Taylor diagram (Taylor, 2001)

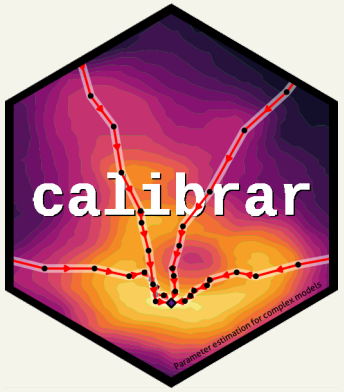
- Standard deviation
- Correlation with observed data
- Centered root mean square (RMS).

Simulated fish biomass trajectories



Emulated fish biomass trajectories





Training: Calibrating Atlantis using calibrar

Morell, A., Kaplan, I.C., Morzaria-Luna, H.M., Rovellini, A., Harvey, C., Porobic, J., Fulton, E.A., Oliveros-Ramos, R. From manual tuning to semi-automated calibration: a practical framework for calibrating Atlantis ecosystem models. *https://papers.ssrn.com/sol3/papers.cfm?abstract_id=5888414*

Presentation and code modified from the original publication by: Hem Nalini Morzaria-Luna, hmorzarialuna@lltk.org

Advantages of semi-automatization



OBJECTIVITY



QUANTITATIVE ASSESSMENT OF OUR MODELS



TIME GAIN



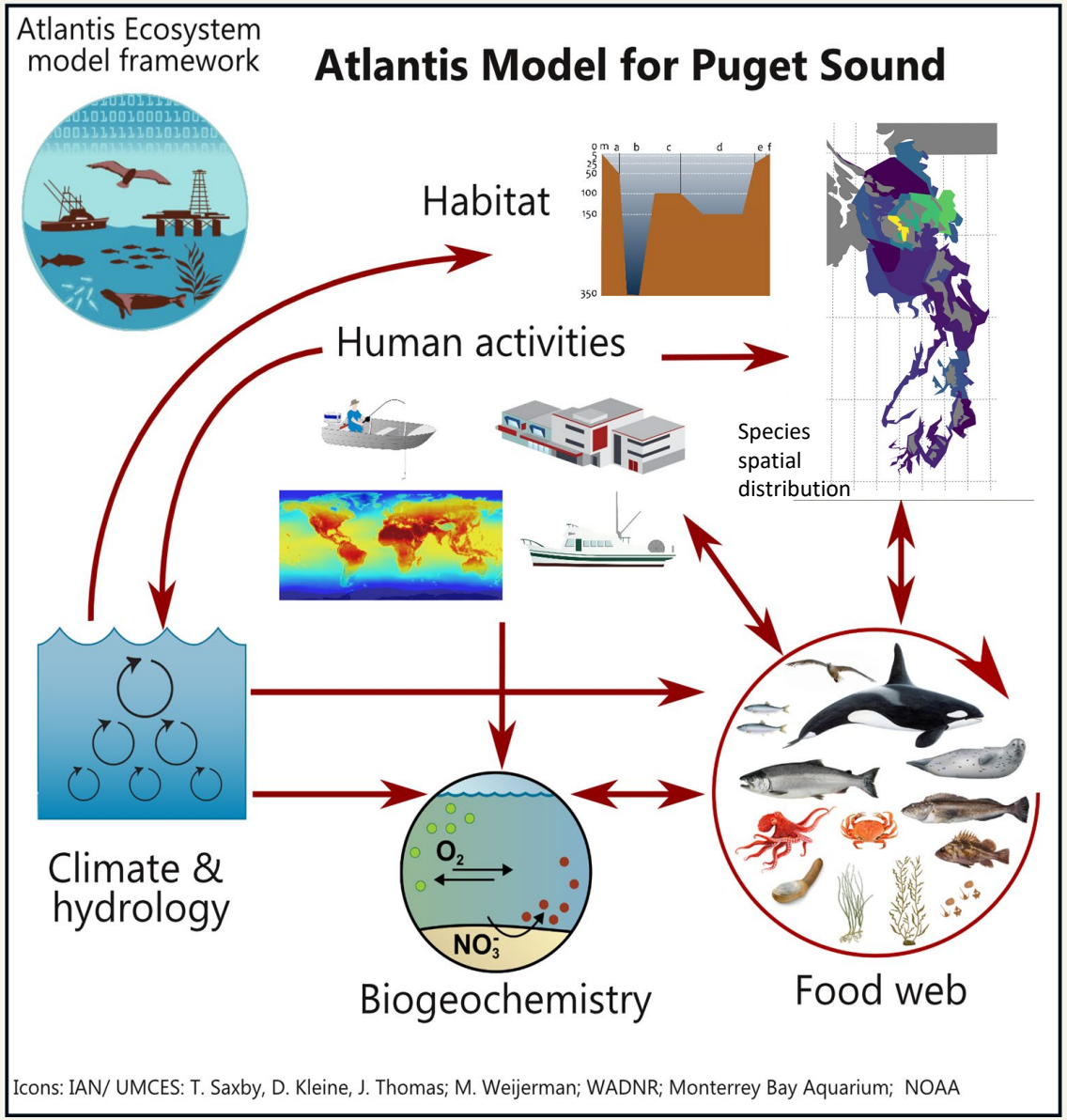
TRUST



BETTER ADJUSTMENT

Atlantis ecosystem modeling framework

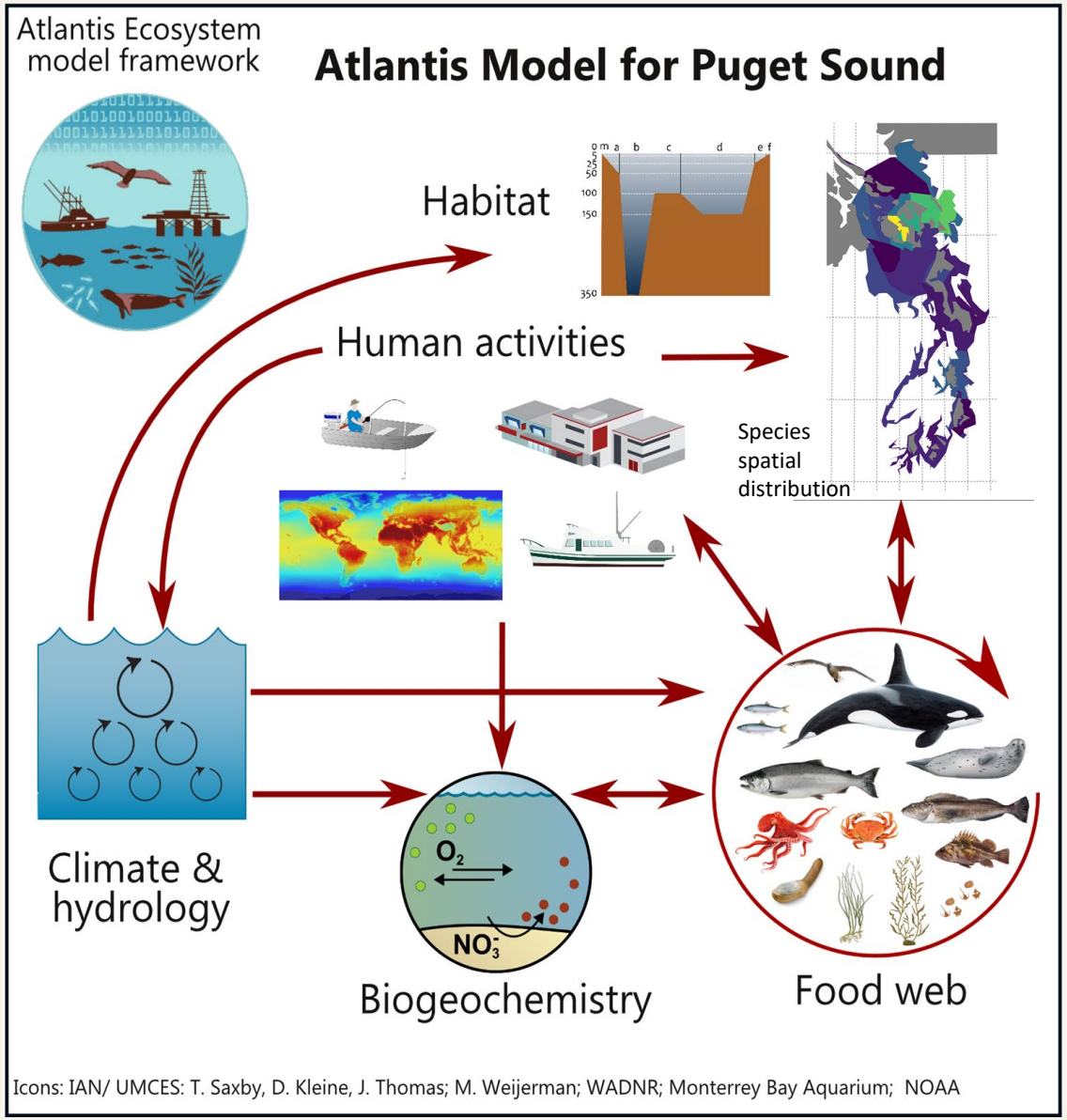
- Fully end-to-end marine ecosystem model
- Model species or functional groups by biomass pool or age class
- 3D, spatially explicit
- Irregular grid by habitat



Morzaria-Luna et al. 2022, Audzijonyte et al. 2019

Atlantis ecosystem modeling framework

- Each run is several hours/day
- The number of parameters is of the order 10^4 to 10^5
- Highly non-linear
- Calibration is highly time consuming

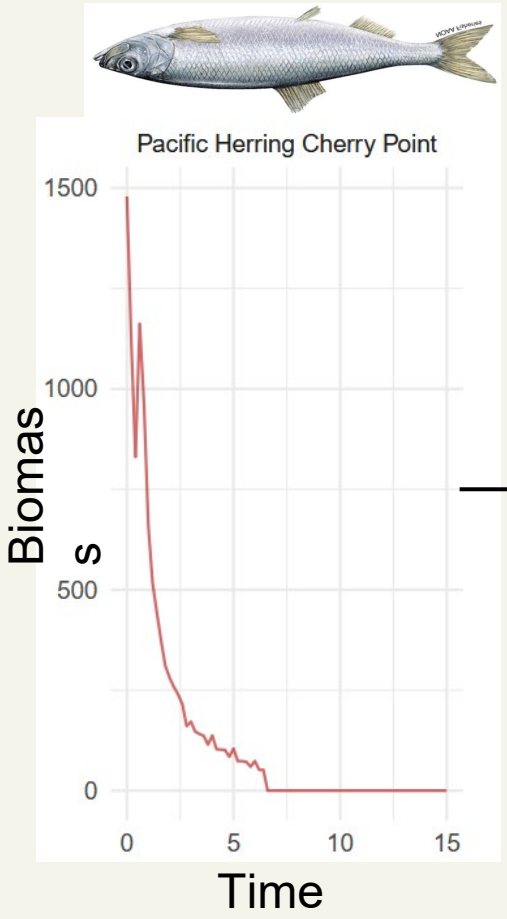


Morzaria-Luna et al. 2022, Audzijonyte et al. 2019

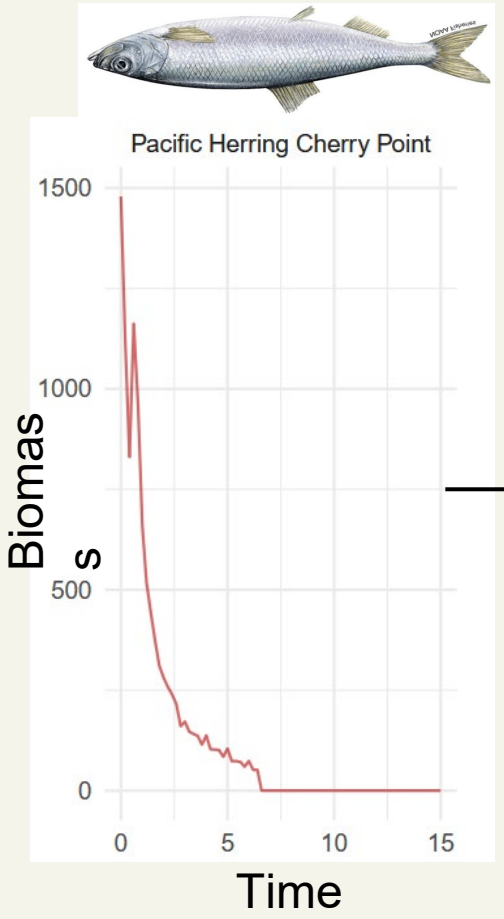
Common calibration practice

Manual tuning

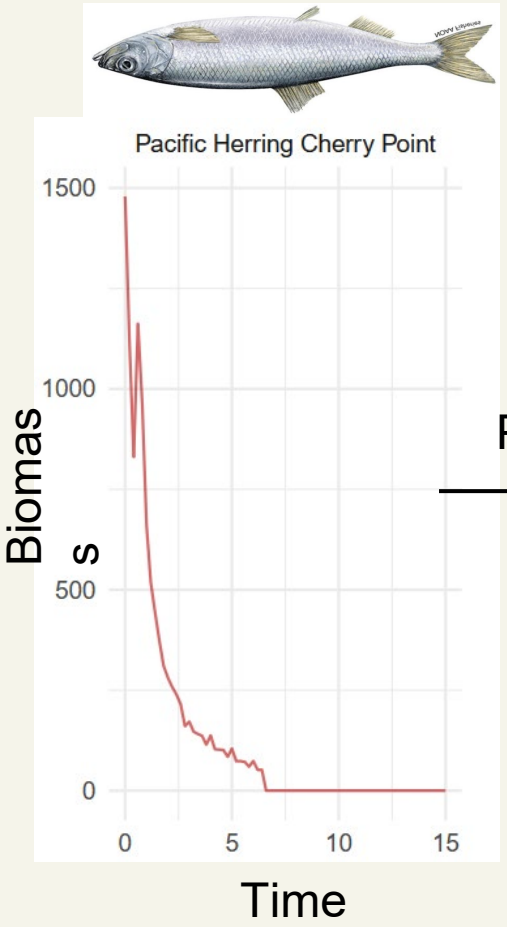
- Painful process…



Parameter change



Parameter change

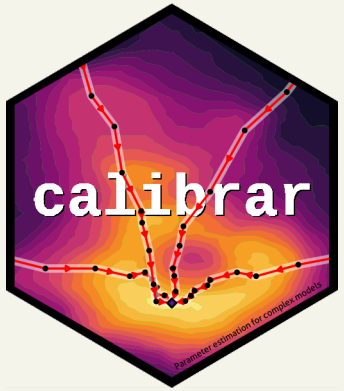


Parameter change

Modeler



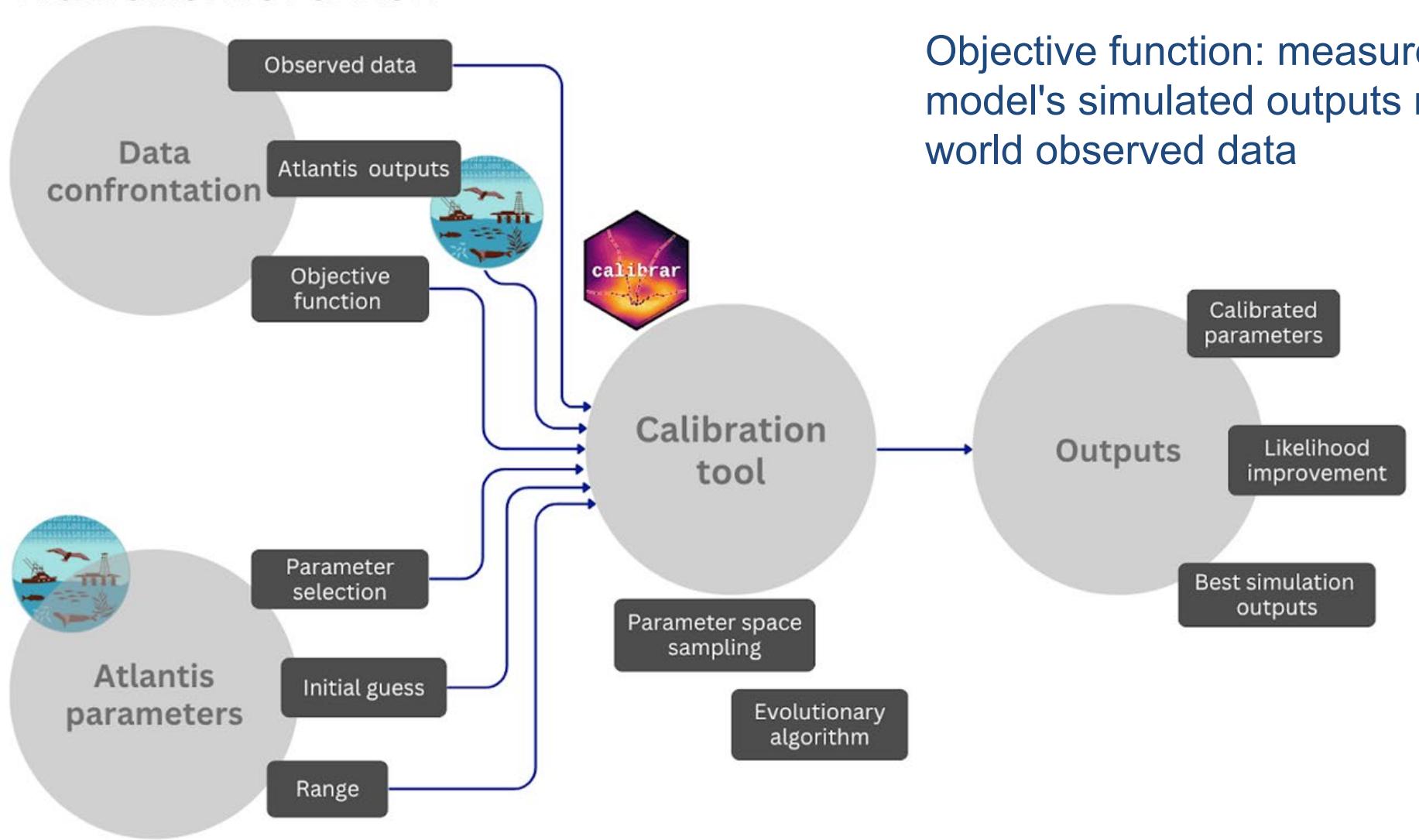
Automated parameter estimation for complex models



- Generic interface
- Generic functions to fit any type of models
- Allows the construction of the objective function without changes in the model's code

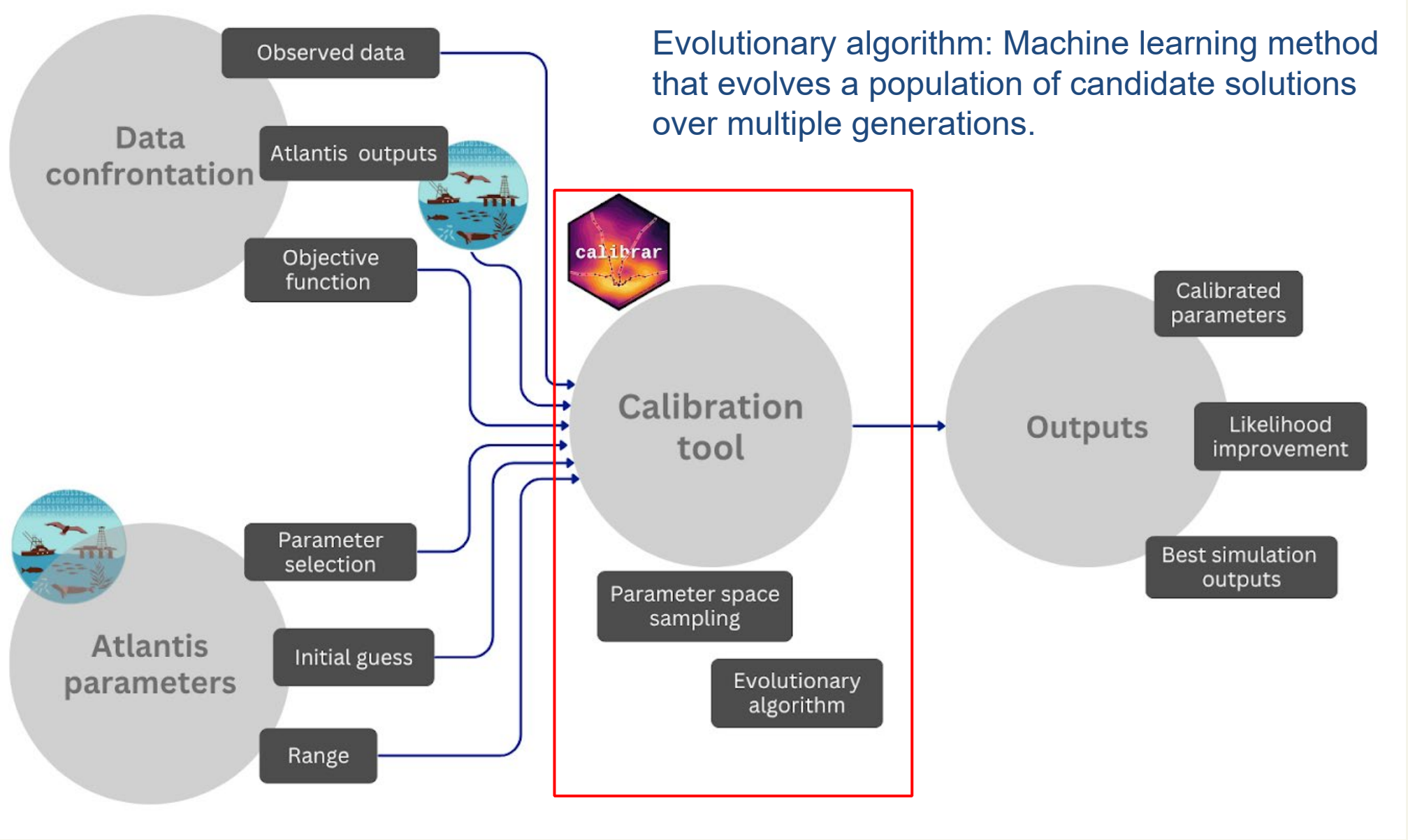
Oliveros-Ramos, R., Shin, Y.-J., 2025. calibrar: An R package for fitting complex ecological models. Methods in Ecology and Evolution 16, 507–519. https://doi.org/10.1111/2041-210X.14452

Framework overview



Objective function: measures how well a model's simulated outputs match real-world observed data

Framework overview



Evolutionary algorithm: Machine learning method that evolves a population of candidate solutions over multiple generations.

Resources

Github repositories:

- Calibrar package
https://github.com/roliveros-ramos/calibrar
- Package that connects Atlantis and calibrar:
https://github.com/amps/atlantiscalibration (in progress)

Calibrar documentation and papers:

- Calibrar vignettes: https://roliveros-ramos.github.io/calibrar/
- Calibrar paper: Oliveros-Ramos, R., Shin, Y.-J., 2025. calibrar: An R package for fitting complex ecological models. Methods in Ecology and Evolution 16, 507–519. https://doi.org/10.1111/2041-210X.14452
- Calibrar application to OSMOSE: Oliveros-Ramos, R., Verley, P., Echevin, V., Shin, Y.-J., 2017. A sequential approach to calibrate ecosystem models with multiple time series data. Progress in Oceanography 151, 227–244. https://doi.org/10.1016/j.pocean.2017.01.002

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