Evaluation of an automated approach for calibrating the NEMURO nutrient-phytoplankton-zooplankton food web model.

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Background

- ✓ **Calibration of complex ecological models with many potentially adjustable parameters is still an issue since it is usually impossible to estimate all parameters from experiments and observations.**
- ✓ **Many ecosystem models are manually adjusted to the observations by modelers.**
- ✓ **In those cases, we don't know if the adjustment is optimal.**

Why apply PEST

1. There are several methods to estimate optimal model parameters.

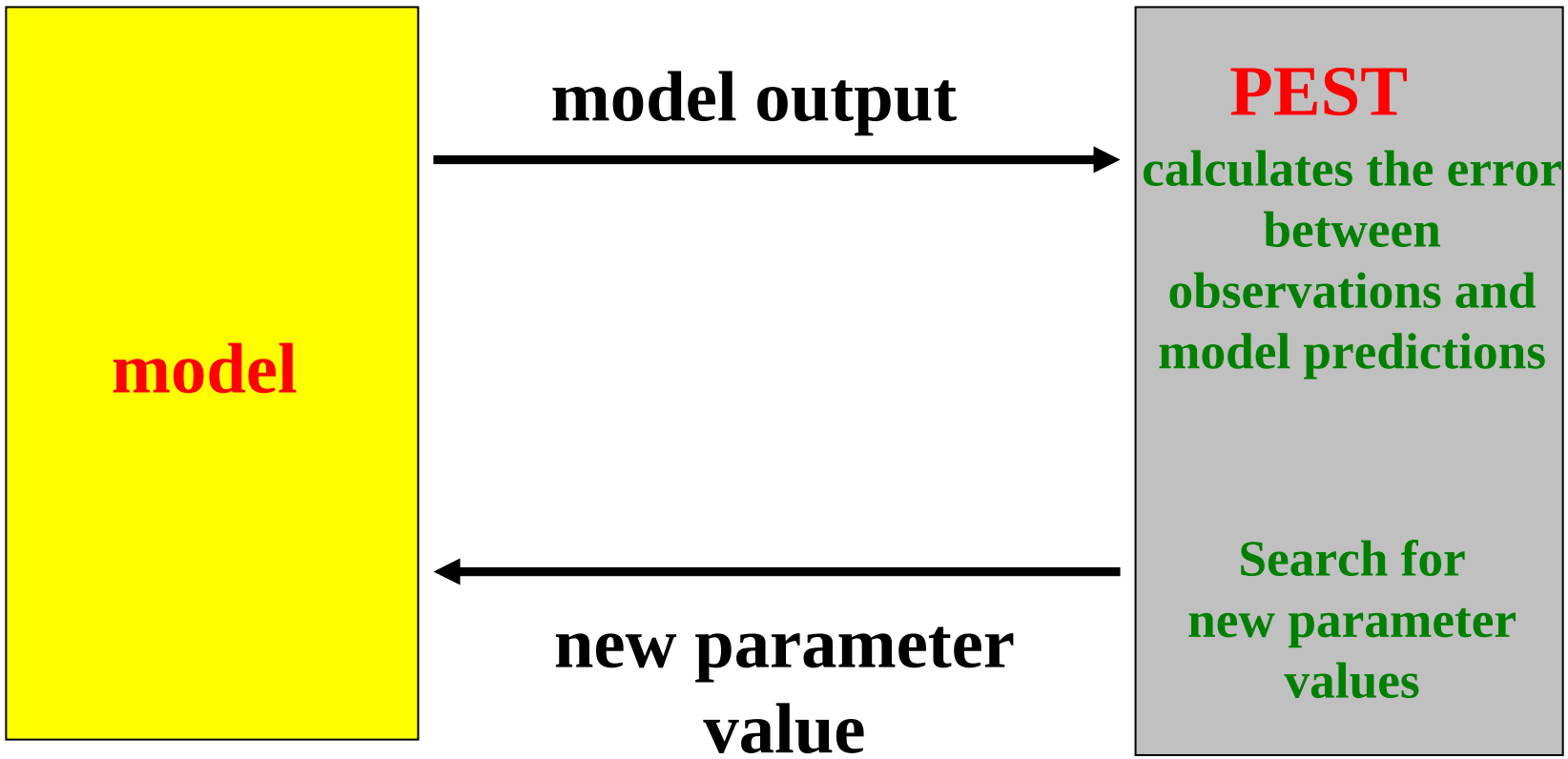
2. The adjoint method is one of the most popular methods. It estimates optimal model parameters by fitting the model results to observations, while conserving model dynamics.

3. However, it takes a lot of work to derive adjoint equations.

Model-Independent Parameter Estimation
PEST

Introduction of PEST

One big advantage of using PEST is no modification of the model source code is required.



Introduction of PEST

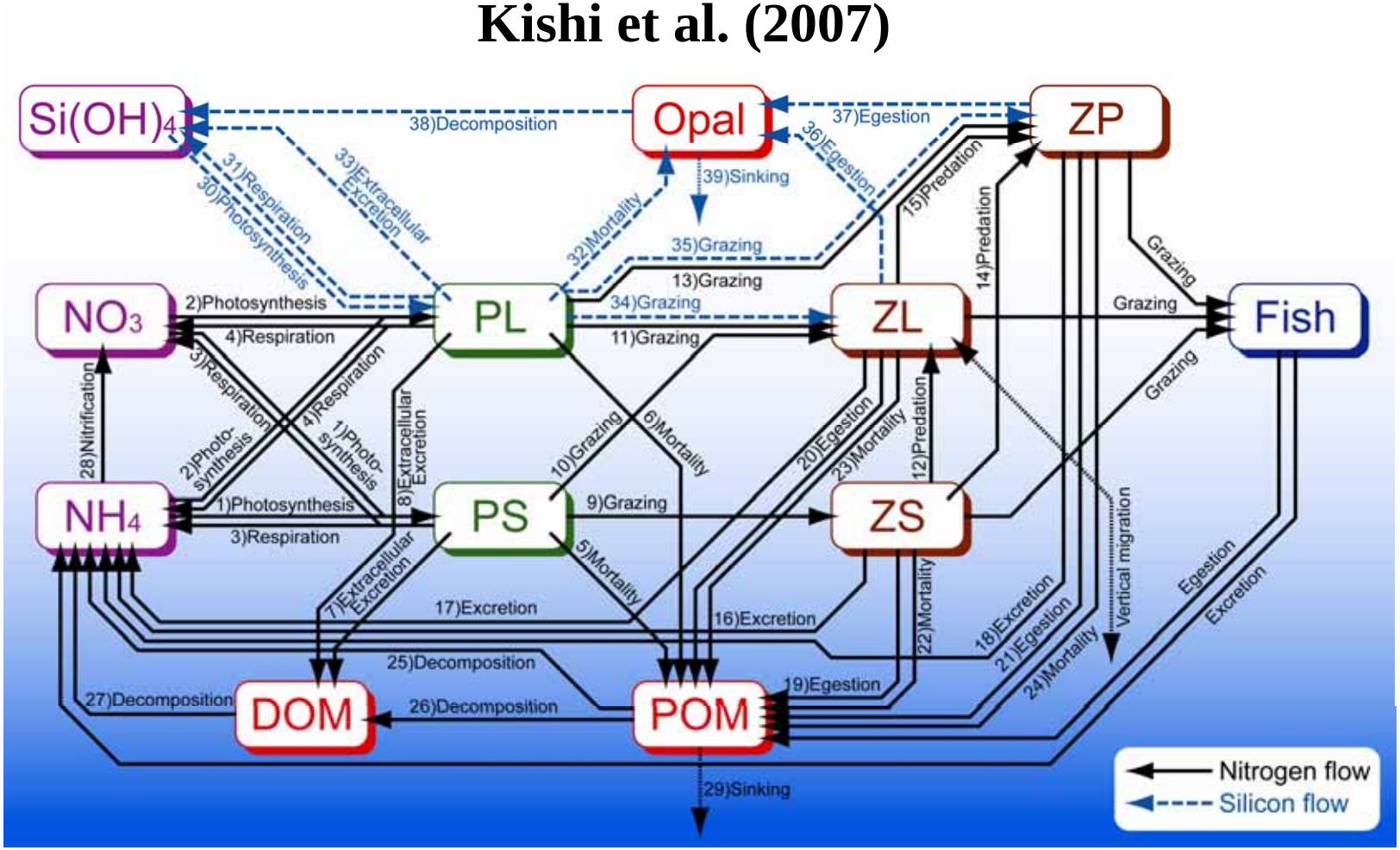
Gauss-Marquardt-Levenberg algorithm

1. **Minimize** the weighted sum of squared **deviations between predicted and observed values.**
2. **Linearize the relationship between model parameters and model-generated observations by** formulating it as **a Taylor expansion** about the currently best parameter set.
3. **Estimate the Jacobian matrix** (the matrix of partial derivatives of observations respect with parameters) using central differences.
4. **Determine the new parameter values using the Marquardt parameter** (denoted λ).
5. **Repeat the process**.
6. PEST stops searching when:
    1. objective function does not go lower over several iterations
    2. changes in parameters dictated by the update vector are very small
    3. the number of iterations or other internal calculations are triggered.

NEMURO

North Pacific Ecosystem Model for Understanding Regional Oceanography

Kishi et al. (2007)



Megrey et al. (2007)

Methods

1. Integrate the one box type NEMURO with an idealistic seasonal forcing at Oyashio site (western subarctic Pacific).

2. Model predictions were used as virtual observations and then PEST was used with arbitrary starting parameter values to determine if PEST could recover the original parameter values (Twin experiments).

Tuning parameters are the maximum grazing parameters of zooplankton.

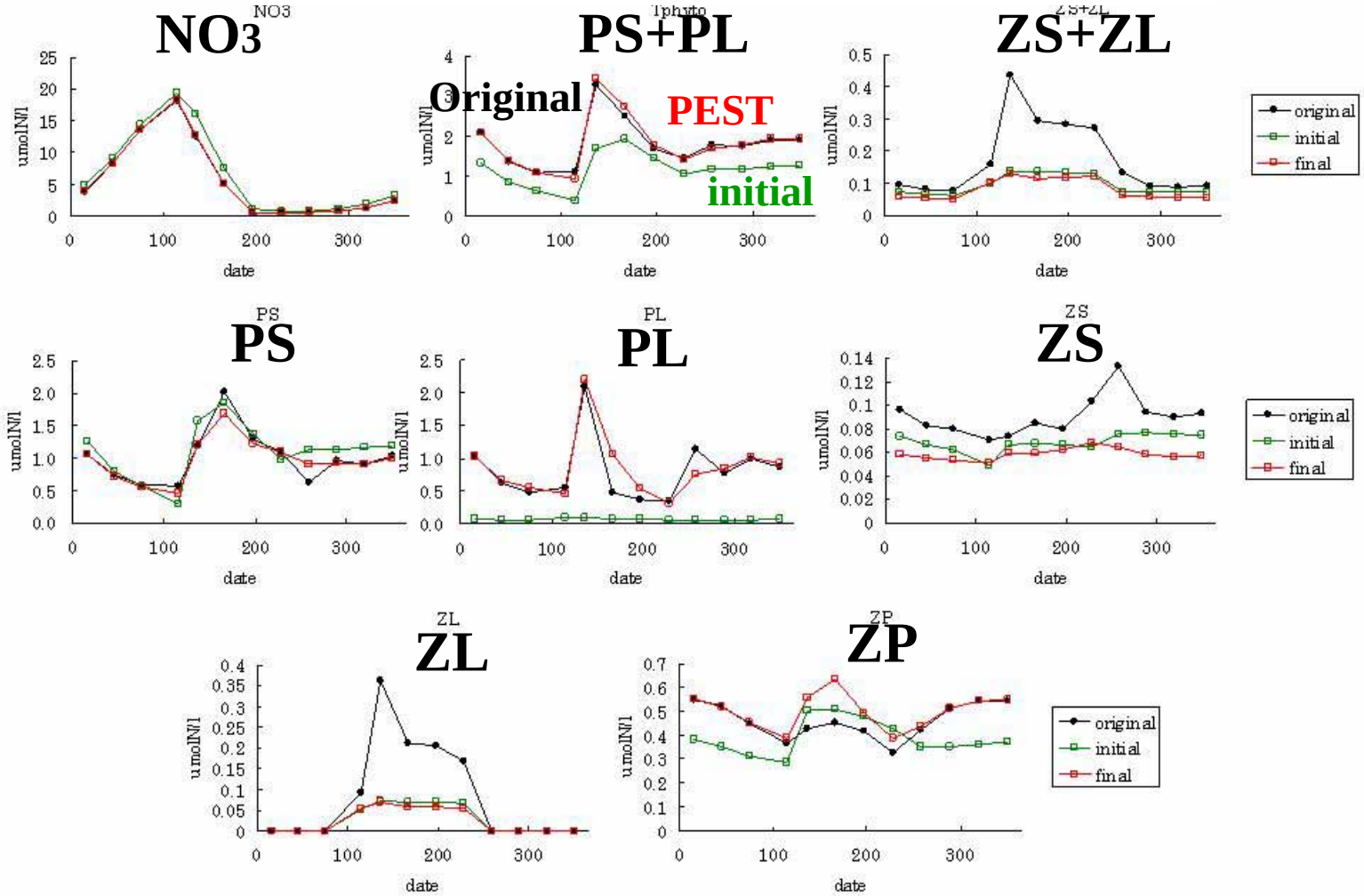
$$GraPL2ZLn = \mathrm{Max}\left[0, GR_{\max} L_{pl} * \exp(k_{GraL} TMP) * \left\{1 - \exp(\lambda_L (PL2ZL^* - PLn))\right\} * ZLn\right]$$

Evaluate model errors by examining the monthly biomass of each compartment.

Twin experiments

Experiment	Tuning parameters	Predicted variables	Ontogenetic migration
Case 1	Maximum grazing parameters of zooplankton	TNO_3, PS+PL, ZS+ZL, PS, PL, ZS, ZL, ZP	Included
Case 2	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Included
Case 2a	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Excluded
Case 3	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZP, ZL (only during spring – summer)	Included

Twin experiment Case1



Nutrient and phytoplankton biomass were reproduced correctly by PEST. However, the zooplankton biomass was not correctly reproduced by PEST. Especially, ZL and ZS+ZL values were not improved at all by PEST estimation.

PEST with ZL ontogenetic migration: case 1

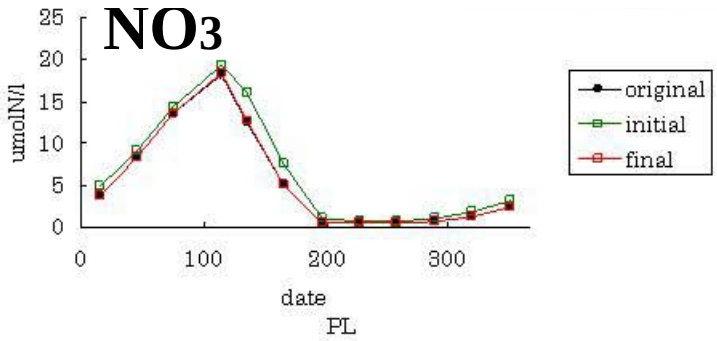
Parameters	Original values	Initial values	Estimated by PEST
GrmaxZS_PS	0.40	1.00	0.65
GrmaxZL_PS	0.10	1.00	0.27
GrmaxZL_PL	0.40	1.00	0.87
GrmaxZL_ZS	0.40	1.00	1.03
GrmaxZP_PL	0.20	1.00	0.17
GrmaxZP_ZS	0.20	1.00	0.61
GrmaxZP_ZL	0.20	1.00	1.01

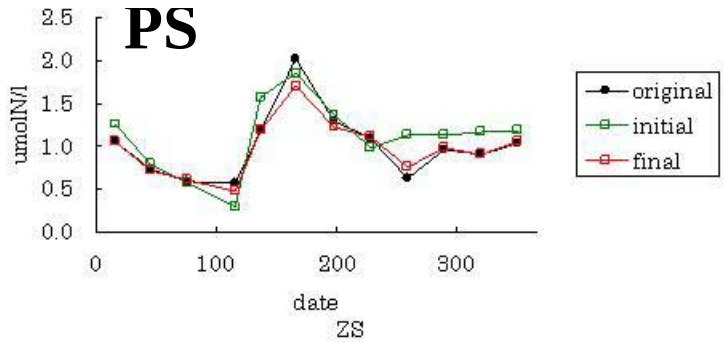
The maximum grazing parameters of zooplankton were estimated by PEST. However, PEST failed to find the original parameter values, especially ones related to ZL with ontogenetic migration.

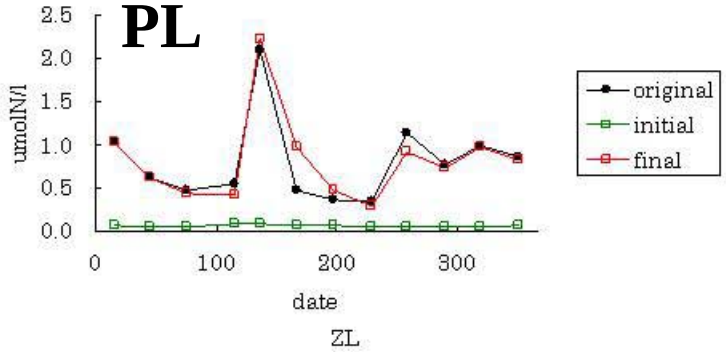
Twin experiments

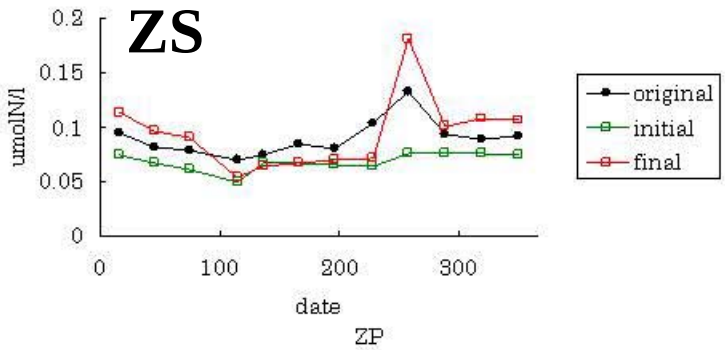
Experiment	Tuning parameters	Predicted variables	Ontogenetic migration
Case 1	Maximum grazing parameters of zooplankton	TNO_3, PS+PL, ZS+ZL, PS, PL, ZS, ZL, ZP	Included
Case 2	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Included
Case 2a	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Excluded
Case 3	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZP, ZL (only during spring – summer)	Included

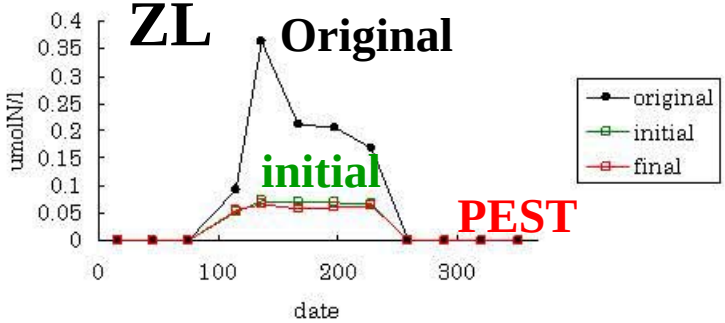
PEST with ZL ontogenetic migration (Case2)

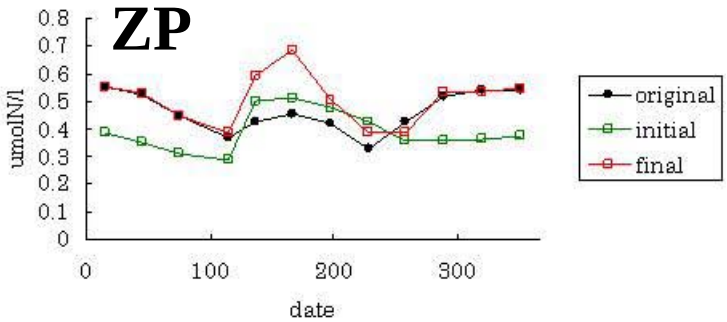












Nutrient and phytoplankton biomass were reproduced correctly by PEST. Since only individual values of zooplankton were evaluated by PEST, ZS and ZP values were improved while ZL values were not improved.

PEST with ZL ontogenetic migration: Case 2

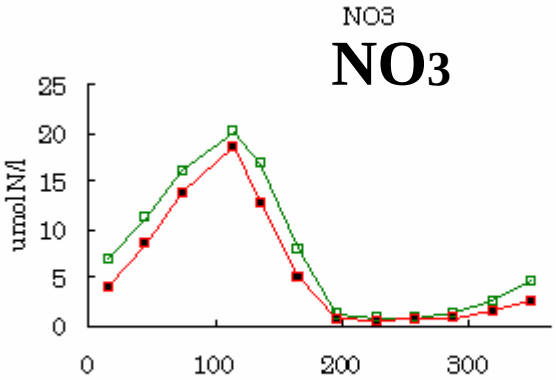
Parameters	Original values	Initial values	Estimated by PEST
GrmaxZS_PS	0.40	1.00	0.35
GrmaxZL_PS	0.10	1.00	0.54
GrmaxZL_PL	0.40	1.00	0.63
GrmaxZL_ZS	0.40	1.00	1.21
GrmaxZP_PL	0.20	1.00	0.22
GrmaxZP_ZS	0.20	1.00	0.15
GrmaxZP_ZL	0.20	1.00	0.97

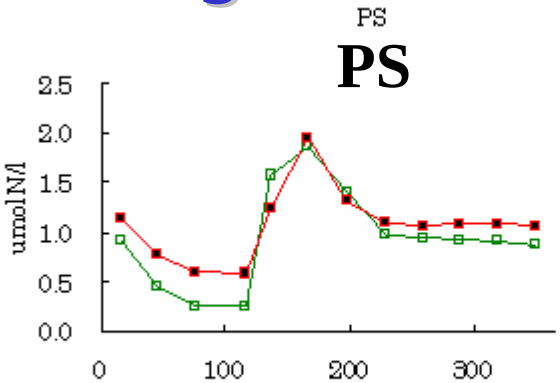
PEST failed to find the original parameter values, especially ones related to ZL with ontogenetic migration.

Twin experiments

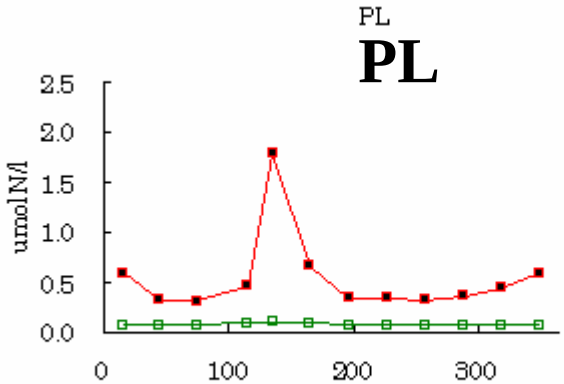
Experiment	Tuning parameters	Predicted variables	Ontogenetic migration
Case 1	Maximum grazing parameters of zooplankton	TNO_3, PS+PL, ZS+ZL, PS, PL, ZS, ZL, ZP	Included
Case 2	Maximum grazing parameters of zooplankton	TNO3, PS, PL, ZS, ZL, ZP	Included
Case 2a	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Excluded
Case 3	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZP, ZL (only during spring – summer)	Included

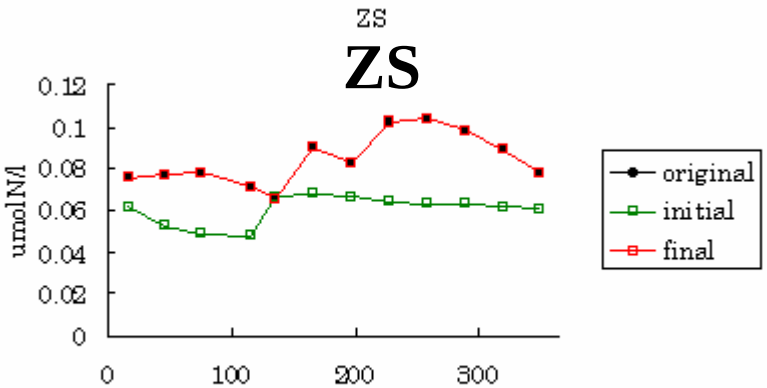
PEST without ZL ontogenetic migration(Case2a)

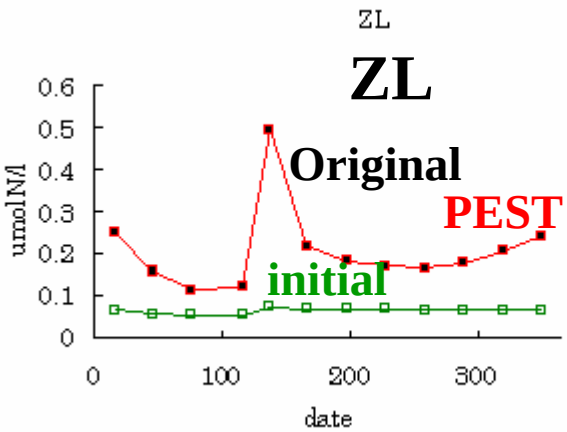


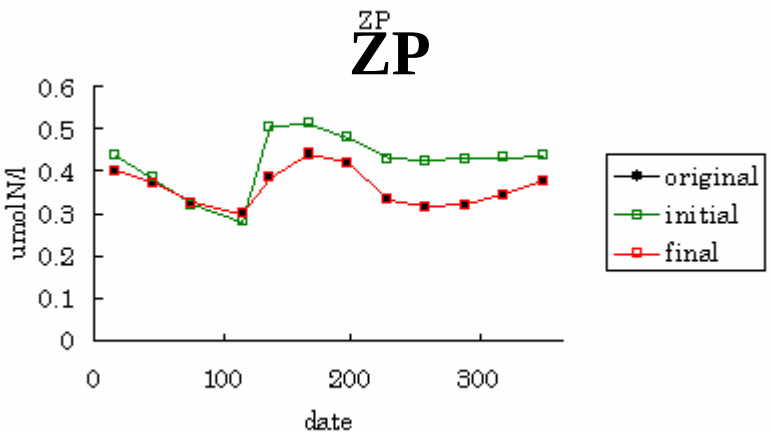


All variables were correctly reproduced by PEST. In this case, the ontogenetic migration of ZL was eliminated.









PEST with ZL ontogenetic migration: Case 2a

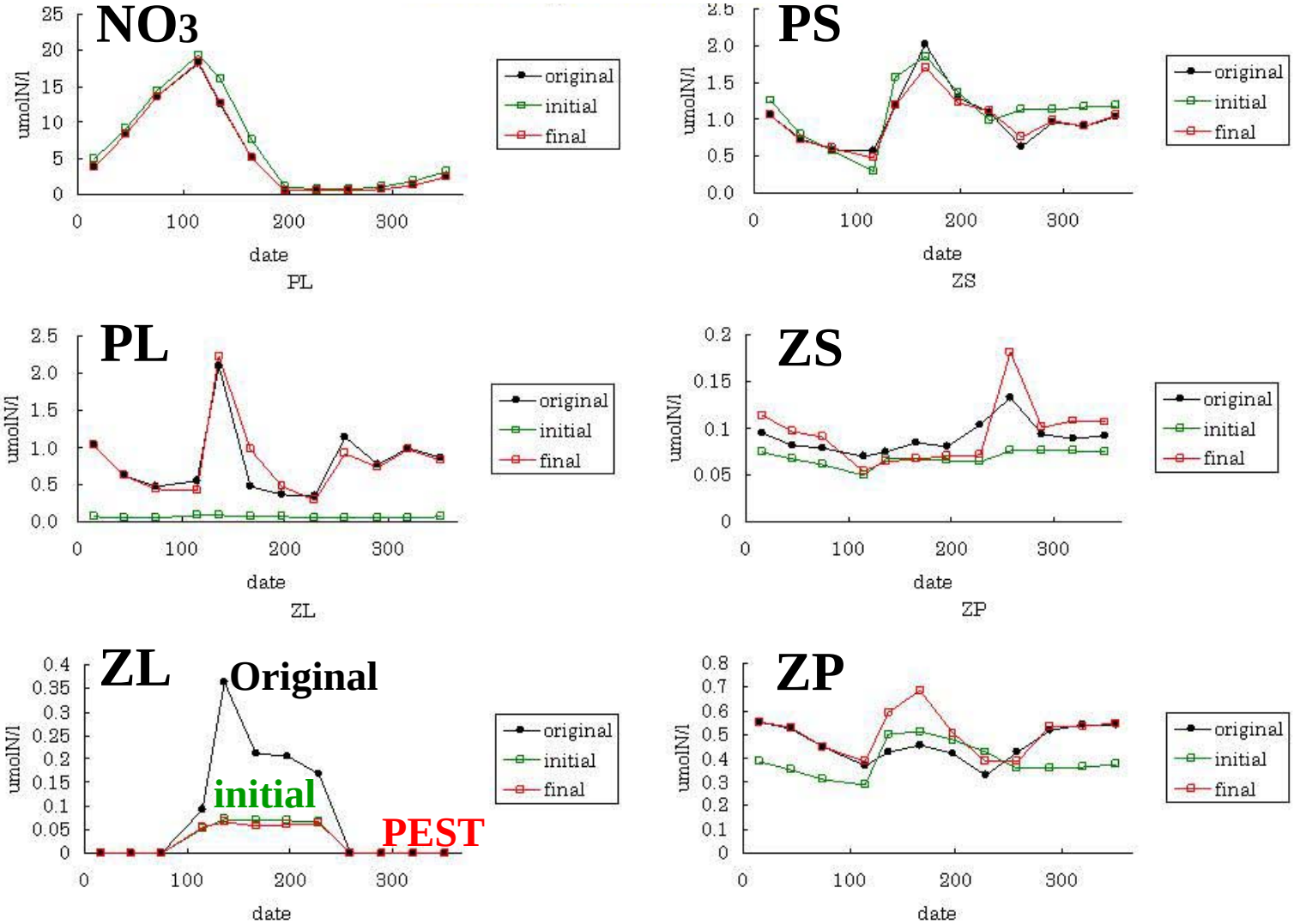
Parameters	Original values	Initial values	Estimated by PEST
GrmaxZS_PS	0.40	1.00	0.40
GrmaxZL_PS	0.10	1.00	0.10
GrmaxZL_PL	0.40	1.00	0.40
GrmaxZL_ZS	0.40	1.00	0.40
GrmaxZP_PL	0.20	1.00	0.20
GrmaxZP_ZS	0.20	1.00	0.20
GrmaxZP_ZL	0.20	1.00	0.20

PEST successfully estimated the original parameter values when the ontogenetic migration of ZL was eliminated.

Twin experiments

Experiment	Tuning parameters	Predicted variables	Ontogenetic migration
Case 1	Maximum grazing parameters of zooplankton	TNO_3, PS+PL, ZS+ZL, PS, PL, ZS, ZL, ZP	Included
Case 2	Maximum grazing parameters of zooplankton	TNO3, PS, PL, ZS, ZL, ZP	Included
Case 2a	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZL, ZP	Excluded
Case 3	Maximum grazing parameters of zooplankton	TNO_3, PS, PL, ZS, ZP, ZL (only during spring – summer)	Included

Twin experiment Case3



The results were very similar to that of Case 2. PEST stopped searching because detected changes in the update vectors were small.

Apply PEST to NEMURO

Results

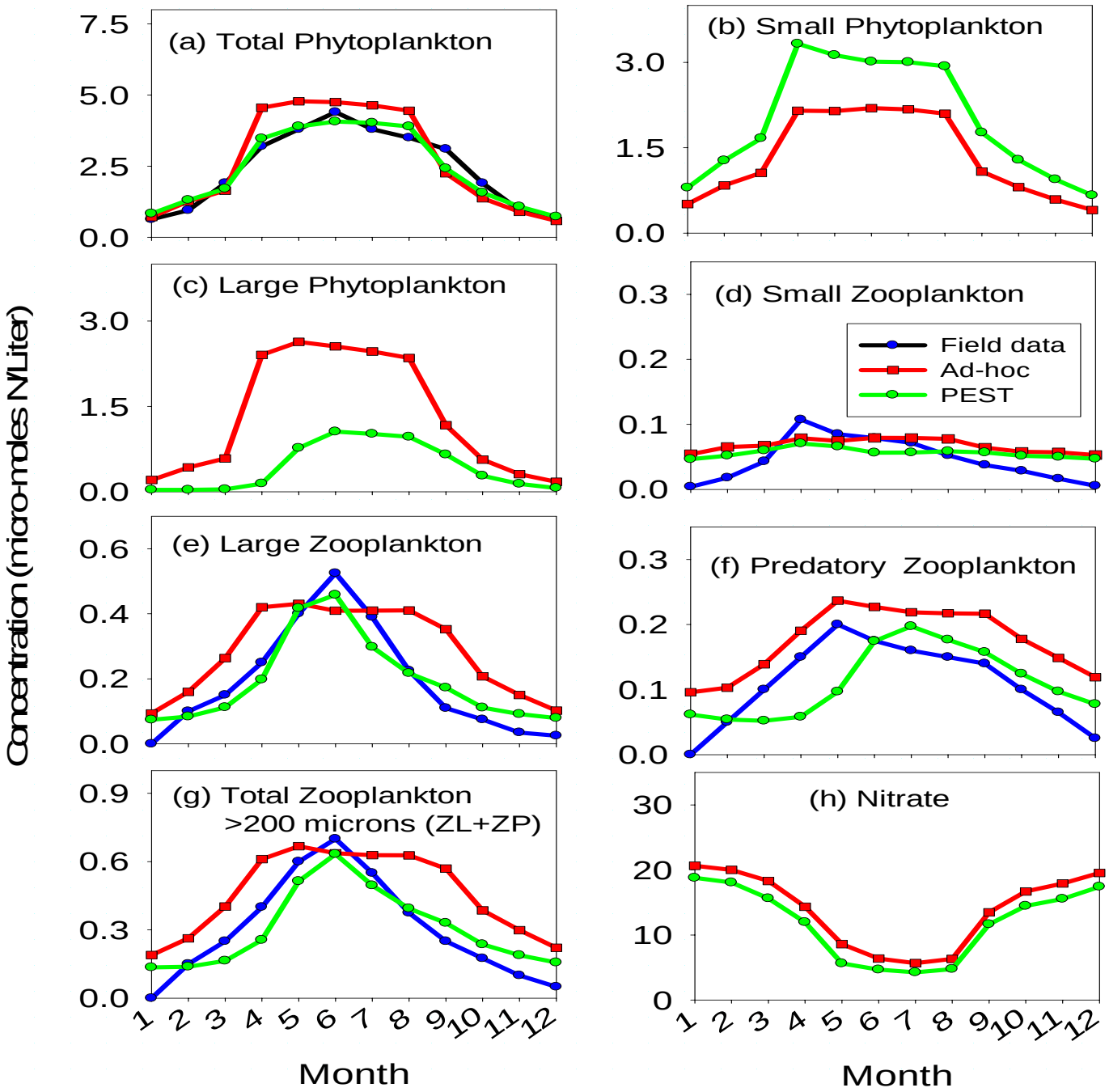
1. **PEST worked when the ontogenetic migration mechanism was excluded from the model.**
2. **PEST recaptured known values.**
3. **Automatic calibration depended on the quality of the data.**

Possible solutions

1. **Exclude ontogenetic migration.**
2. **Apply PEST separately to two stages (summer & winter).**
3. **Solve ZL biomass in the deep ocean.**

Example of fitting to observations Rose et al. (2007)

Parameter	Starting Values	Ad-Hoc	PEST (model as data)	PEST (field data)
Vmaxs PS max growth	0.4	0.49	0.49	0.56
Vmaxl PL max growth	0.8	0.71	0.71	0.25
Grmaxs PS => ZS	0.4	0.31	0.31	0.086*
Lams Ivlev function PS=>ZS	1.4	0.4	0.412	0.497
Morsz0 ZS mortality	0.677	0.877	0.886	0.943
Kmorzs temp coff. of ZS mortality	0.0693	0.1099	0.1099	0.0902



Rose et al. (2007)