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Parameter inversion of marine ecosystem dynamics model based on adjoint function

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ABSTRACT

In order to study the dynamic model of marine ecosystem and predict the response and impact service of marine ecosystem to climate change, this paper uses the method of adjoint assimilation function to divide a year into 72 processes and optimize the five key parameters VM, DZ, *E*, GM, and DP (referred to as KP). The correlation coefficients of VM, DZ, and *E* are 0.99, and so are DP and GM. The variation trend of VM, DZ, and *E* is negatively correlated with that of DP and GM, and the correlation coefficient is –0.99. Conclusion: it shows that in the numerical simulation of marine ecosystem dynamics, compared with only considering the spatial distribution of parameters or only considering the temporal distribution of parameters, the change trend of VM, DZ, and *E* is negatively correlated with that of DP and GM. Considering the spatial and temporal distribution of parameters is more reasonable, more physical significance and in line with the ecological mechanism.

Keywords: Adjoint assimilation; Ecosystem; Function; Spatial and temporal distribution

1. Introduction

However, due to the existence of the errors in the global mesoscale measurements and the seawater color, it can provide a basis for the study of the marine ecological system, even if there is an error in the measurement of the marine mesoscale and the sea water quality, it can promote the study of the marine ecosystem. Some key marine ecological variables and their vertical distributions and fluxes cannot be directly obtained from satellite observations. The numerical model of marine ecosystem dynamics can make up for the defects of observation data, provide important information that cannot be obtained by observation, and provide more complete temporal and spatial distribution of ecological variables, ER, the model is still insufficient in characterizing the dynamic process and interaction of the real ecosystem, and it is difficult to avoid the phenomenon that the simulation results deviate from the observation. The data assimilation method considers the model and observation as an organic whole, compared with the system analysis method only using physical model or observation results, the data assimilation method can obtain better results [1].

2. Literature review

Data assimilation methods are divided into two categories: sequential method and variational method. The former is mostly used for state and flux estimation, while the latter is mostly used for optimizing parameters, boundary conditions, and initial conditions. Compared with the atmospheric and oceanic models, the marine ecological model contains a large number of parameters, and slight changes in some parameters will lead to changes in the results of the overall ecosystem model [2]. Most of the parameters are obtained through numerical experiments, which are difficult to control due to the different complexity of the model,

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the different sea area studied, and the different amount of observed data. The optimization of model parameters by using existing observed data is becoming increasingly important in the numerical simulation of ecosystem dynamics, and data assimilation technology based on variational method has been widely applied in the past 20 y [3]. Among many parameter optimization techniques (gradient descent method, conjugate gradient method, simulated annealing method, micro genetic method, Newton method, and random search method), adjoint assimilation method, also known as the inverse method (essentially gradient descent method), is the most commonly used method. It takes the ocean dynamic model as the constraint condition, particularly, we use the method of Lagrange to control the difference between the objective function and the objective function in order to improve the accuracy of the objective function. On the other hand, parameters are not constant in time [4]. Especially in large-scale numerical simulation, the simulation time is long, and the ecological variables and ecological parameters also change in time, some scholars have begun to study the temporal variation of parameters [5]. Matter et al. [6] used polynomial chaos expansion method to optimize two parameters in a three-dimensional marine ecological model: the carbon/chlorophyll ratio of phytoplankton and the predation rate of zooplankton and obtained their values over time. Solidoro et al. [7] statistically analyzed the seasonal and spatial variations of water quality parameters of Venice lagoon, fan, and LV applied the adjoint assimilation method to the numerical simulation of marine ecosystem dynamics to study the spatial distribution of ecological parameters under the climate state background field of the climate coupled model foam. Wang et al. [4] applied the nitrogen, phytoplankton, zooplankton, detritus (NPZD) model to the Bohai Yellow Sea, and the experimental results showed that the ecological parameters changed with time in 1 y [8–12].

The innovation of this paper is based on the previous work, the adjoint assimilation method is used to study the spatiotemporal distribution of the parameters. Compared with the parameters only considering the spatial variation and the parameters considering only the time variation, it is verified that the spatiotemporal variation parameters are more reasonable in the numerical simulation of marine ecosystem [13–15].

3. Research methods

3.1. Ecological model and parameter setting

In this paper, a simple NPZD model based on nitrogen cycling is established on a global scale. Four state variables (CI, $I = P$, N, Z, and d) in the model can be expressed as follows:

$$\frac{\partial C_i}{\partial t} = \mathrm{phy}_i + \mathrm{Bio}_i \tag{1}$$

Among them, phy_{iis} is the change of state variable caused by physical mechanism (including convection and diffusion); bio_{iis} is the change of state variable caused by biological mechanism. The specific expression form of model equation is shown in fan and LV. The model parameters are shown in Table 1.

The calculation area of the ecological model is 0.5 ° e-359.5 ° e, 74.5 ° s-88.5 ° *n*, the horizontal resolution is 1 (°) × 1 (°). There are 14 vertical layers, and the depth (unit: m) is 5, 15, 25, 35, 46, 57, 70, 82, 96, 112, 129, 148, 171, and 197 (consistent with the background field). A grid is used and *Z* coordinate is used for discretization.

3.2. Adjoint method

In this paper, the adjoint method is used to optimize the ecological parameters. CF is defined as a cost function to describe the difference between the observed value $\bar{x}_{s,t}$ and the model simulation value $x_{s,t}(V)$ when the parameter *V* is used:

$$\mathrm{CF} = \frac{1}{2}\sum_{s,t} W_s \left(x_{s,t}\left(V\right) - \bar{x}_{s,t} \right)^2 \tag{2}$$

where $\bar{x}_{s,t}$ and $x_{s,t}(V)$ are surface phytoplankton observed and simulated respectively; *s* is the spatial index; *t* is the time index; W_s is the weight.

The process of parameter optimization is to reduce CF by adjusting the control parameters, and CF decreases along the negative direction of its gradient with respect to the parameters. Therefore, the gradient is used to determine

Table 1
Parameters and initial values in ecological model

Parameter	Description	Values
VM, d^{-1}	Maximum phytoplankton growth rate	0.80
KS, mmol × m^{-3}	Semi-satiety and constant of nutrient absorption	0.25
WP, m × d^{-1}	Sedimentation rate of phytoplankton	1.00
GM, d^{-1}	Maximum zooplankton predation rate	0.50
DZ, d^{-1}	Zooplankton mortality	0.05
G	Zooplankton assimilation rate	0.30
DP, d^{-1}	Phytoplankton mortality	0.10
E, d^{-1}	Rate of clastic remineralization	0.02
Q	Ratio of zooplankton excretion	0.40
WD, m × d^{-1}	Settling rate of debris	1.00

Table 2
Correlation coefficients of time varying parameters shown in Fig. 3

	E	DZ	DP	GM
VM	0.76	0.92	–0.91	–0.91
E		0.93	–0.94	–0.94
DZ			–0.99	–0.99
DP				–0.99

the direction of parameter optimization. Firstly, the initial guess value of control parameters is used to obtain the model value to calculate CF; secondly, the adjoint equation is derived by using the Lagrange multiplier method, and the inverse direction is obtained. Finally, the control parameters are adjusted according to $V_{k+1} = V_k + \alpha_k d_k$, k is the number of assimilation steps, d_k is the direction of adjustment of control parameters, $d_k = \frac{-V \cdot 5\%}{86,400} \cdot \frac{\vec{G}_k}{\left|\vec{G}_k\right|}$, and α_k are step factors, indicating the adjustment size of control parameters:

$$\alpha_k = 1 - 0.1^* \left(k-1\right), k = 1,2,3,\ldots,10 \quad (3)$$

$$\alpha_k = 0.1 - 0.01^* \left(k-10\right), k = 11,12,\ldots,19 \quad (4)$$

$$\alpha_k = 0.01 - 0.001^* \left(k-19\right), k = 20,21,\ldots,28 \quad (5)$$

Take the adjusted control parameters as the initial guess value and repeat the above steps until a convergence condition is met.

3.3. Spatial distribution of parameters

The specific implementation process of parameter spatial distribution: firstly, some grid points are selected as independent points in the study area. The values of parameters on independent points are independent, that is, they do not affect each other. The values of parameters on other grid points are obtained by linear interpolation from the values of independent points; secondly, the influence radius R is selected, and R represents the range of observation points that affect the values of independent points, i,j relationship between (j) and the other points (j) is determined by the independent point (j):

$$F_{i,j} = \sum_{ii,jj} \varphi_{i,j,ii,jj} \cdot E_{ii,jj} \quad (6)$$

$$\varphi_{i,j,ii,jj} = \frac{w_{i,j,ii,jj}}{\sum_{ii,jj} w_{i,j,ii,jj}} \quad (7)$$

$$w_{i,j,ii,jj} = \frac{R^2 - r^2_{i,j,ii,jj}}{R^2 + r^2_{i,j,ii,jj}} \quad (8)$$

where $\varphi_{i,j,ii,jj}$ is the interpolation coefficient; $w_{i,j,ii,jj}$ is the weight coefficient; $r_{i,j,ii,jj}$ is the distance between independent points and other grid points. The adjoint method is used to adjust $E_{ii,jj}$ and linear interpolation is used to obtain f_{ij}. The model is run with the adjusted parameter values, and the process is repeated 28 times.

4. Experimental results

Most of the work on parameter estimation is to reduce the error between simulation and observation by assimilating the observed data for a period of time. While making full use of these observations, the parameters are also reasonably estimated. Therefore, this paper will carry out practical experiments to optimize ecological parameters and reduce the error between observation and simulation values. The rationality and necessity of the spatial and temporal distribution of parameters are verified by comparative experiments.

4.1. Actual experiment

The study area a is defined as 17 ° *n*-45 ° *n*, 17 ° *n*-45 ° *n*, 173 ° e-142 ° *w* (located in the north Pacific) as study area a, which contains 1,334 grid points. Finally, the ecosystem near the Antarctic circumpolar current is iron limited, and the model in this paper does not consider iron limitation. Therefore, if the sea area near the Antarctic circumpolar current is chosen as the area to study the spatiotemporal variation of parameters, there may be errors caused by the model itself rather than by the optimization method. A year is divided into 72 processes, each of which has 5 d and a time step of 6 h, that is, each process needs to calculate 20 steps. Five KPS, VM, GM, DZ, DP, and *E*, which affect the ecological mechanism, are optimized to reduce the error between the simulated values and the observed values of phytoplankton. Other parameters are constant, and the values of KP in area *a* are changed in real space by setting independent points. The value of KP is obtained by linear interpolation of parameter values and constant parameter values in area *a*. Fig. 1 shows the spatial

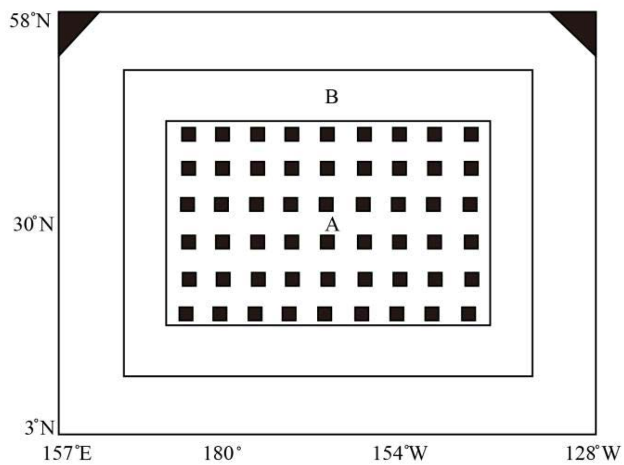

Fig. 1. Schematic diagram of the spatial distribution of parameters.

distribution of parameter a, and gray points indicate the grid points where independent points are located. The initial values of KP and other parameters are shown in Table 1.

Before assimilation, the minimum values of CF and mean absolute error (MAE) were about 3.9 and 0.007, respectively; after assimilation, the CF and MAE of each process decreased significantly, the maximum CF value was no more than 2.1, and the maximum MAE was no more than 0.003. The reduced cost function RCF was obtained by dividing the CF value after assimilation (cf28) by the CF value before assimilation (CF1), and the reduced cost function (RCF) was less than 0.12 for each process, and the ratio of MAE28 divided by MAE1 before assimilation was less than 0.3. After averaging the results of 72 processes (Fig. 2), RCF and MAE decreased rapidly in the first five steps of assimilation, and then reached stable values of 0.05 and 0.002, respectively. It shows that the adjoint assimilation method can not only optimize the parameters of spatial variation, but also optimize the parameters of temporal and spatial variation.

4.2. Comparative experiment and result analysis

Based on the above, the temporal and spatial distribution of the five key parameters is obtained in this paper, denoted as KP_k (i,j,t), k = 1,2,3,4, and 5; where, KP1, KP2, KP3, KP4, and KP5, respectively, represent VM, DZ, E, DP, GM, i, and j represent the spatial position of parameters, and t represents time. In this paper, we obtain KP (KPS) that changes only with space, KP (KPT) that changes only with time, constant KP (KPC), and another form of KP (KPST) that changes only with time through the following ways.

KPS: for each KP, the 72 plots of spatial variation are averaged in time. Therefore, the spatial distribution of 5 parameters in the study area is obtained, $\mathrm{KPS}(i,j)=\sum_t \mathrm{KP}_k(i,j,t)/1{,}334$, k = 1, 2, 3, 4, 5; KPS1, KPS2, KPS3, KPS4, KPS5 represent a two-dimensional array of VM, DZ, E, DP, and GM spatial distribution, respectively. The parameter values are reduced, that is, the assimilated value/initial value. For each parameter, there is only one spatial distribution, which does not change with time.

KPT: for each KP, the 72 scenes of its spatial variation are respectively in the $\mathrm{KPT}_k(t)=\sum_{i,j}\mathrm{KP}_k(i,j,t)/72$ h parameter, the author obtains a constant in each process. KPT1, KPT2, KPT3, KPT4, and KPT5 are one-dimensional time series representing the time distribution of VM, DZ, E, DP, and GM.

For each process, the parameter values in the study area are no longer spatial changes, but constants. For 1 y, there are 72 groups of constants (Fig. 3):

KPC: average $\mathrm{KPS}_k(i,j)$ in space (or $\mathrm{KPC}_k=\sum_{i,j}\mathrm{KPS}_k(i,j)/1{,}334=\sum_i \mathrm{KPT}_k(t)/72$ constants KPC1, KPC2, KPC3, KPC4, and KPC5 are obtained. The values of VM, DZ, E, DP, and GM are 0.5878, 0.4934, 0.0978, 0.0540, and 0.0241.

KPST: using $\mathrm{KPS}_k(i,j)$, $\mathrm{KPT}_k(t)$, KPC_k, another form of spatiotemporal distribution of parameters $\mathrm{KPSY}_k(i,j,t)$ = $\mathrm{KPS}_k(i,j)\cdot\mathrm{KPT}_k(t)/\mathrm{KPC}_k$ is constructed.

It can be seen from Fig. 3 that the five parameters show obvious spatial and temporal changes, and VM, DZ, and E decrease with the increase of GM and DP in both space and time. Therefore, they can be divided into two groups: (1) VM, DZ, and E have the same trend in most regions; DZ is the mortality rate of zooplankton. The larger the value is, the faster the zooplankton will decrease, and correspondingly, the more phytoplankton will be. E represents the mineralization rate of detritus. The larger the value is, the faster the detritus will be converted into nutrients, which is more conducive to the growth of phytoplankton. The smaller the value of GM is, the better the growth of phytoplankton is; DP is the mortality rate of phytoplankton, and the smaller the value is, the more conducive to the growth of phytoplankton. Therefore, the smaller the value of GM and DP is, the more conducive to the growth of phytoplankton biomass. The correlation coefficient between DP and GM is as high as 0.99, which shows that there is a

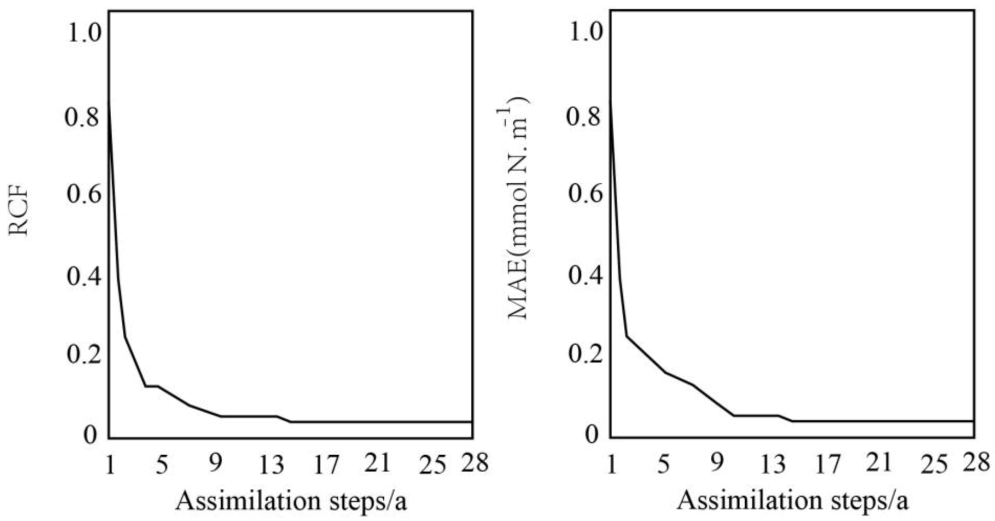

Fig. 2. 72 average process results.

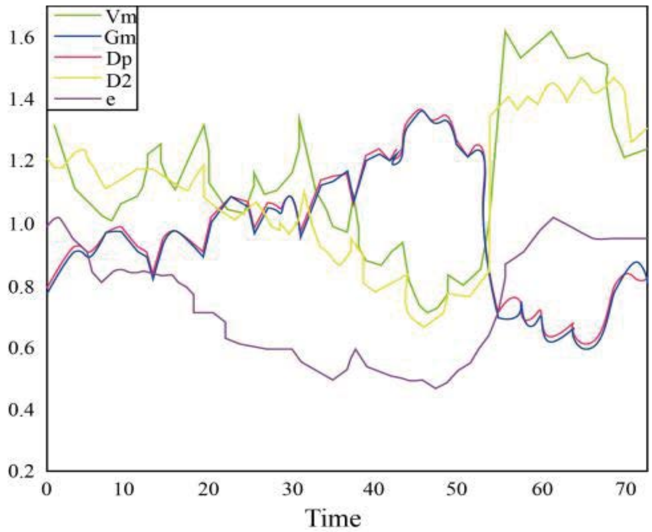

Fig. 3. KPT schematic diagram.

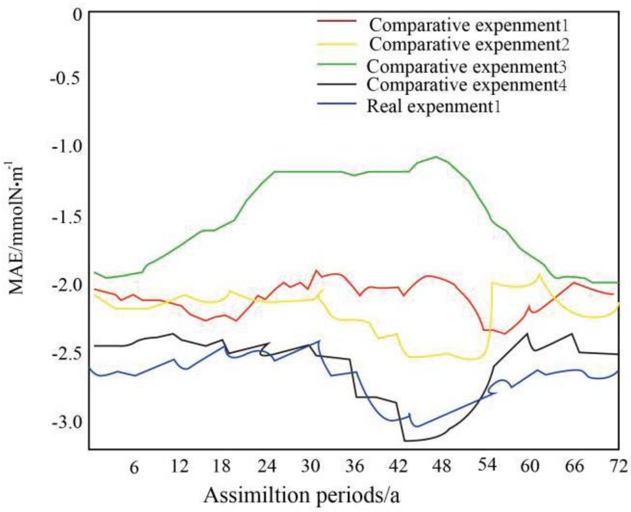

Fig. 4. Results of actual experiment and contrast experiment.

strong negative correlation between them, which verifies the above analysis.

Experimental results are compared with experimental results of KPM (1.0, 4.0) in the same model (Fig. 4), and the results are compared with those obtained in KPM (1.4) and 4.0 (KPM), respectively. The annual mean of MAE is about 0.0022 mmoln × m^{-3}; in contrast experiment 4, MAE obtained in each process is also less than 0.004 mmoln × m^{-3}, and MAE annual average value is about 0.0029 mmoln × m^{-3}, which is close to the actual experimental results. In contrast experiment 1, the method of only considering the spatial variation of KP is similar to fan and LV, and the annual average MAE obtained by this method is 0.008 mmoln × m^{-3}; in contrast experiment 2, the MAE annual average value is 0.008 mmoln × m^{-3}; in contrast experiment 2, the average MAE is 0.0029 mmoln × m^{-3}, in contrast experiment 3, KP is a constant and MAE is 0.04 mmoln × m^{-3}, which is 20 times of the results obtained by considering the temporal and spatial distribution of the parameters. On the other hand, any parameter KP is a three-dimensional array. It can be expressed by the product of a two-dimensional array representing spatial changes and a one-dimensional array representing time changes, namely KPST. In long-term numerical simulation, this method can reduce the number of variables in the program and improve the simulation efficiency.

5. Conclusion

In this paper, the spatial and temporal distribution of chlorophyll in the northern ocean is studied by using the spatial-temporal data assimilation method. For each parameter in KP, firstly, it is averaged in time and space to obtain the spatial distribution field (KPS) and time distribution sequence (KPT); secondly, the KPS is averaged in space (or KPT is averaged in time) to obtain a constant (KPC), KPS, KPT, and KPC are used to represent another kind of KP (KPST) with spatiotemporal variation. It is found that VM, DZ, and *E* have the same distribution characteristics and change trend in both time and space, so do DP and GM, while the change trend of VM, DZ, and *E* is negatively correlated with that of DP and GM. The correlation coefficient can reach –0.99. The correlation between the parameters in time and space is in accordance with the physical meaning and ecological mechanism, which provides a strong basis and reference for how to optimize the parameters in the future numerical simulation experiments, It is obvious that the experimental error is the smallest and the simulation accuracy is the highest when considering the spatial-temporal distribution of parameters. Compared with the results obtained when the parameters are constant, the MAE is reduced to 1,120. It is reasonable and necessary to consider the spatial-temporal distribution of parameters in the numerical simulation of marine ecosystem dynamics, and the adjoint assimilation method is an effective method to optimize the parameters of space-time variation, KPST, as a representation of KP spatio-temporal variation, reduces the number of variables in long-term numerical simulation.

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