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A perturbed biogeochemistry model ensemble evaluated against in situ and satellite observations

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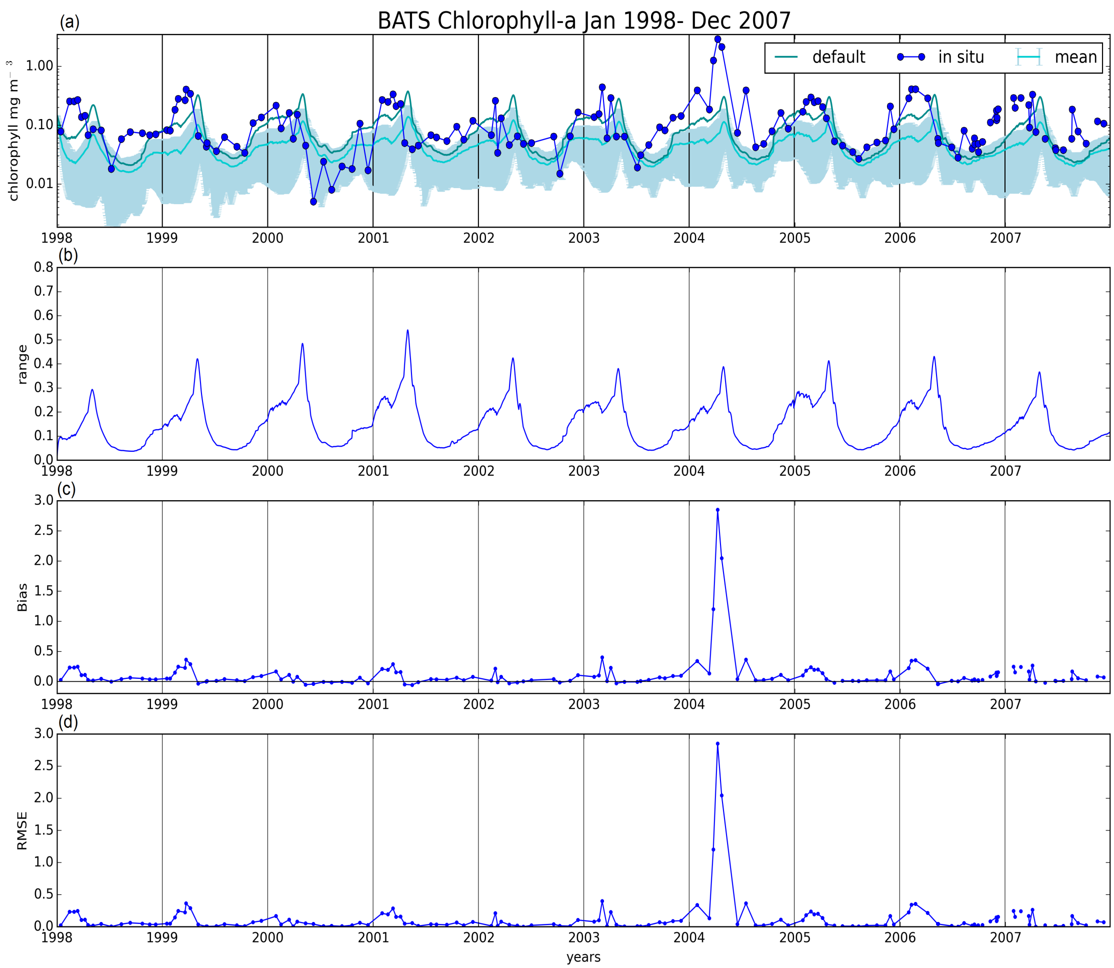

Figure S1. (a) In situ surface chlorophyll at station BATS overlain with the ensemble 75th and 25th percentile (blue shade), ensemble mean (cyan), and default run (dark cyan). Statistical metrics associated with the ensemble mean's surface chlorophyll such as range, bias, and RMSE are shown on (b), (c), and (d) respectively. Bias in this figure is (in situ – ensemble mean)

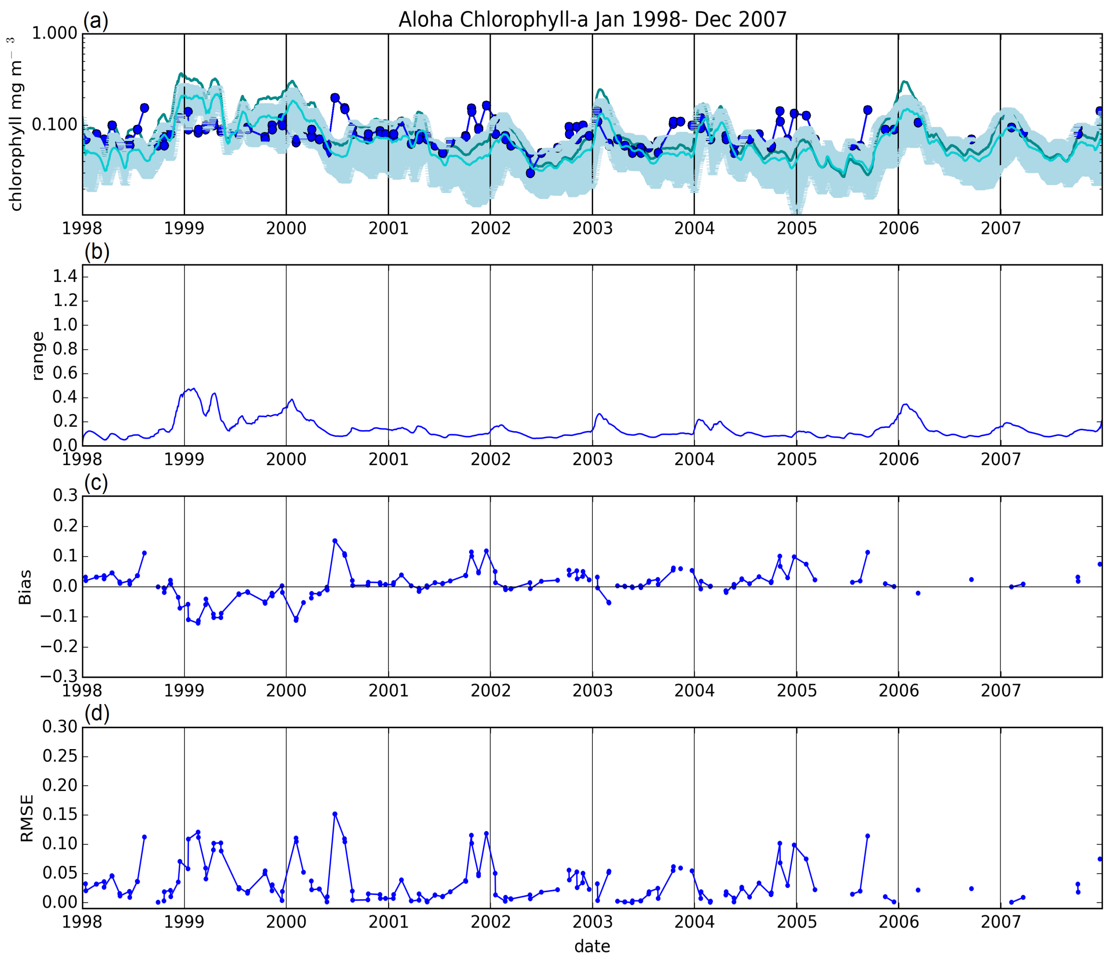

Figure S2. (a) In situ surface chlorophyll at station ALOHA overlain with the ensemble 75th and 25th percentile (blue shade), ensemble mean (cyan), and default run (dark cyan). Statistical metrics associated with the ensemble mean's surface chlorophyll such as range, bias, and RMSE are shown on (b), (c), and (d) respectively

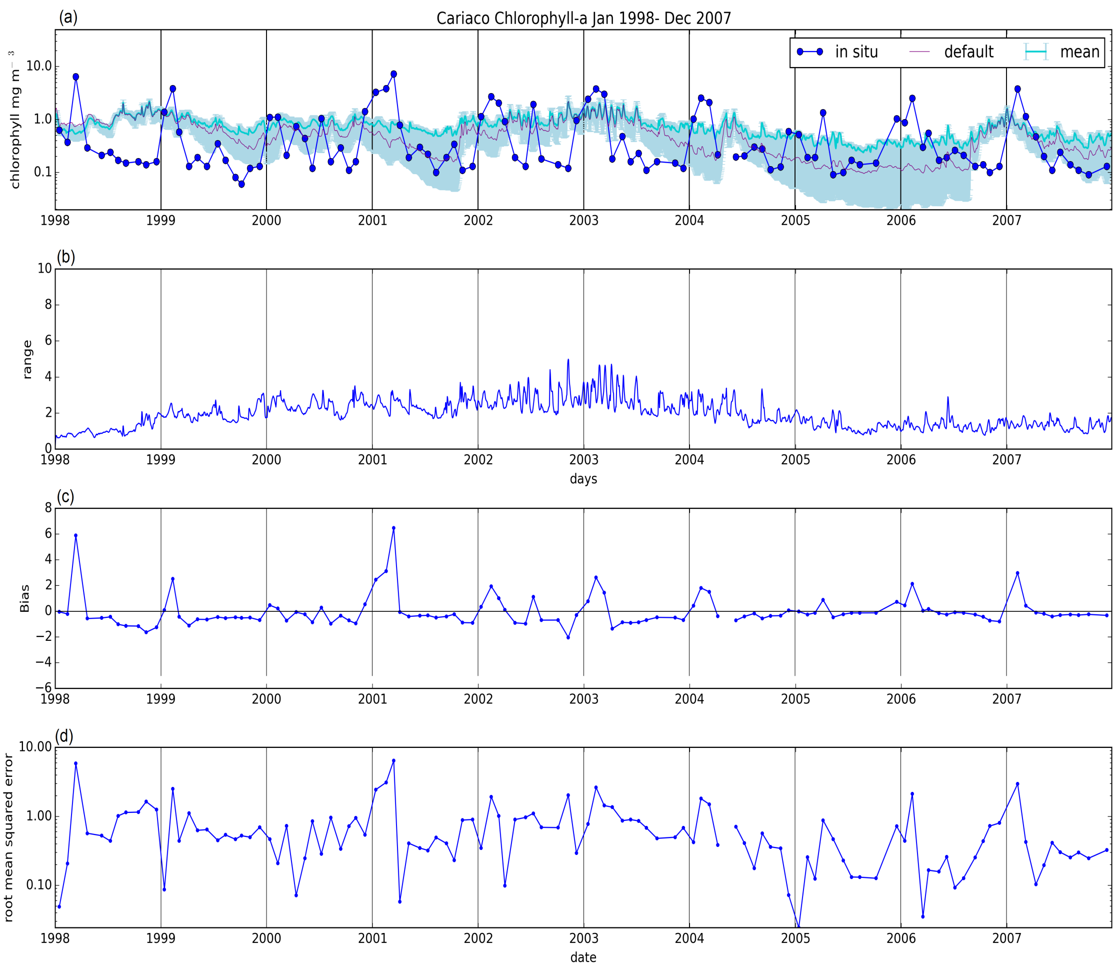

Figure S3. (a) In situ surface chlorophyll at station Cariaco overlain with the ensemble 75th and 25th percentile (blue shade), ensemble mean (cyan), and default run (violet). Statistical metrics associated with the ensemble mean's surface chlorophyll such as range, bias, and RMSE are shown on (b), (c), and (d) respectively. Bias in this figure is (in situ – ensemble mean)

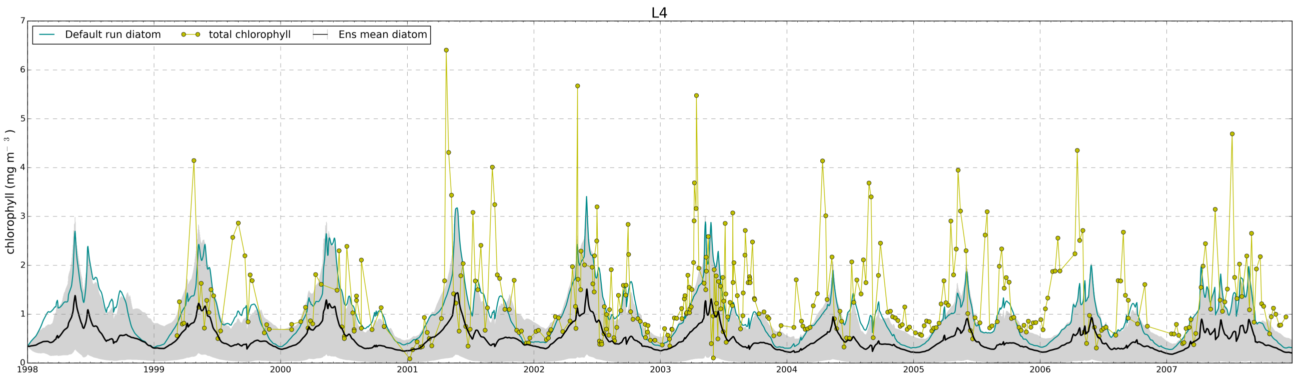

Figure S4. In situ surface total chlorophyll at station L4 (yellow) and the ensemble 90th and 10th (grey shade) percentile, ensemble mean (black), and default run (dark cyan) of diatom surface chlorophyll

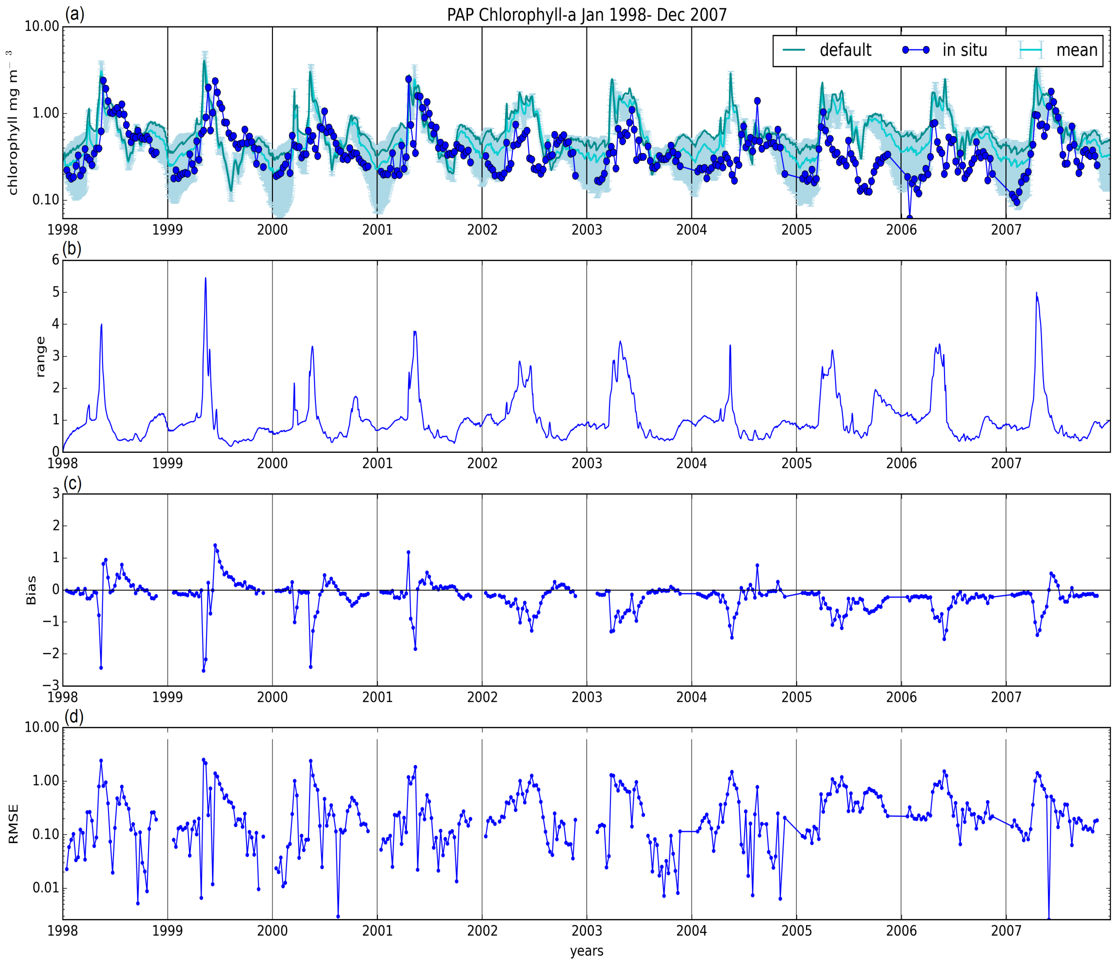

Figure S5. (a) SeaWIFs-derived surface chlorophyll-a at station PAP overlain with the ensemble 75th and 25th (blue shade), ensemble mean (cyan), and default run (dark cyan). Statistical metrics associated with the ensemble mean's surface chlorophyll such as range, bias, and RMSE are shown on (b), (c), and (d) respectively

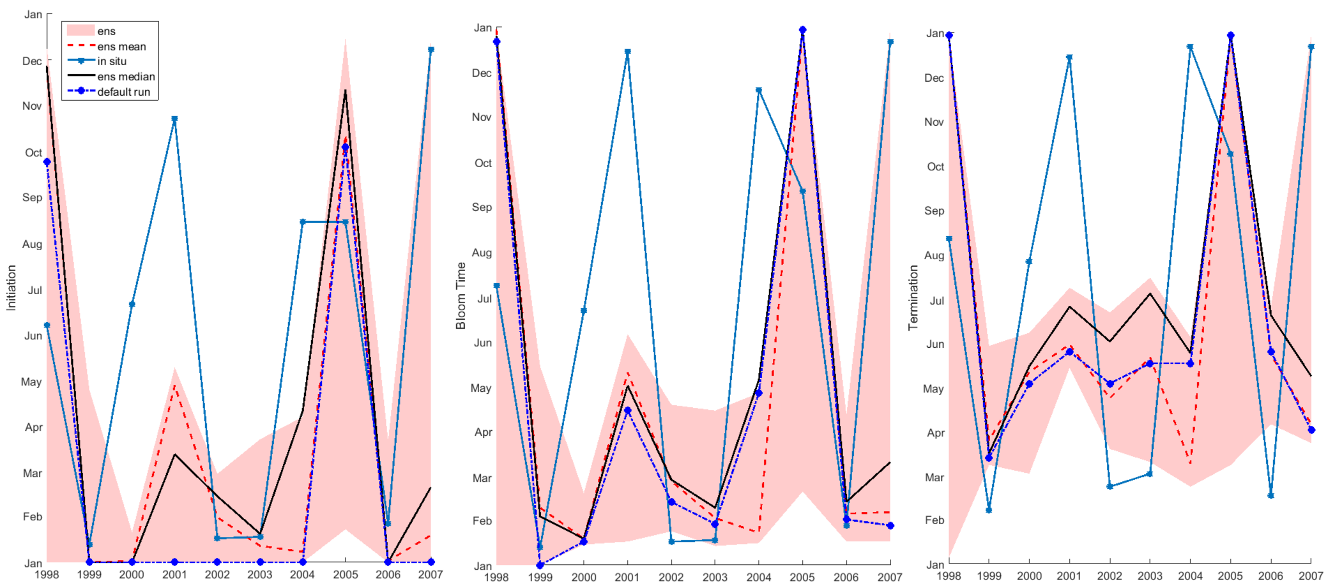

Figure S6. Initiation, bloom time, and termination at station ALOHA from 1998-2007. Some of the bloom time happening in January first because its the highest time is when the model started its simulation

S1 Spinning up the 1-D MEDUSA

As stated in the main manuscript, we have decided not to do any spin up runs to initialise the model. This is because the physical input parameters are available every 5 days, and regularly control the physical dynamics and therefore the biogeochemical tracers. Here we run the 1D MEDUSA using two different physical parameters and spinup period: (i) using the first year's physical parameters, repeated over 50 years and (ii) using the climatology (mean from 10 years of the physical parameter), repeated over 250 years. The initial condition for this run is taken from the in situ, similar to that in the full model run described section 2.5.2 of the main manuscript.

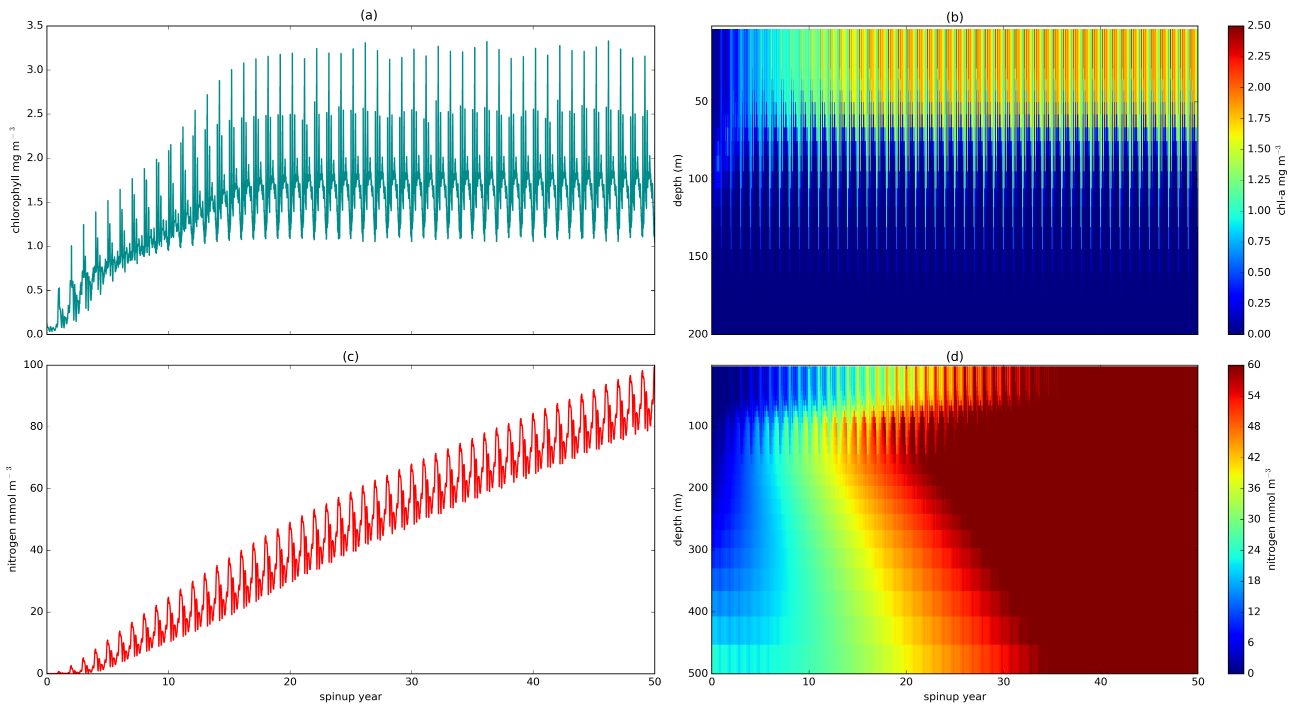

Figure S7. Spinning up 1-D MEDUSA using first year condition for 50 years. Chlorophyll surface and profile are shown on (a) and (b) respectively. Nitrogen surface and profile are shown on (c) and (d) respectively.

When repeating the first year's physical input for 50 years, the chlorophyll concentrations reached a repeating cycle after ∼16 years, but not the nitrogen. During the spinup period, surface chlorophyll concentration increases from 0.13 to 1.64 mg m^{-3} in the span of ∼15 years, then it reached a constant cycle for the rest of the spinup period, summarised in Fig. S7(a). Additionally, it's deep chlorophyll maxima vanished as the concentration increases (Fig. S7(b)). For surface nitrogen, on the other hand, the concentration increases throughout the spinup period, as shown in Fig. S7(c). This could be due to the mean vertical velocity is going upwards, making the nitrogen from the depth being upwelled to the surface, and therefore increasing the concentration. In terms of chlorophyll, the phytoplankton's maximum uptake rate has been reached and therefore the chlorophyll concentrations cannot increase.

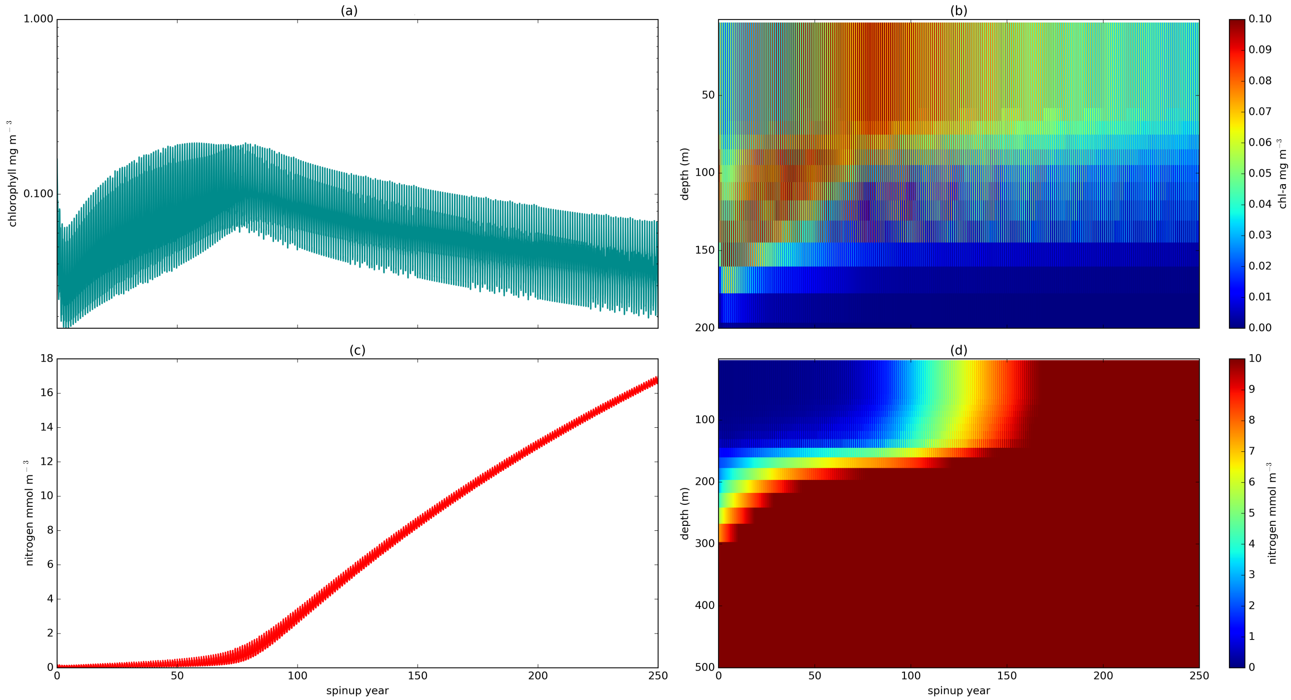

Figure S8. Spinning up 1-D MEDUSA using climatology of the physical input for 250 years. Chlorophyll surface and profile are shown on (a) and (b) respectively. Nitrogen surface and profile are shown on (c) and (d) respectively.

Another experiment has been carried out using the climatology of the physical input of the 10-year period (January 1998 - December 2007) and has been run for 250 years. In this spin up run, the surface chlorophyll decreases from 0.06 to 0.01 mg m^{-3} after four years, and starts to increase over $\sim$ 70 years to 0.2 mg m^{-3}. Then it starts to decline again for the rest of the time series, summarised in Fig. S8(a). When chlorophyll starts to decline, nitrogen increases drastically over the time series, (Fig. S8(c) and (d)). This might be caused by the decline of phytoplankton. The deep chlorophyll maxima also vanishes after $\sim$ 54 years.

From the two spinup runs, we decided not to initialise the model using the spinup run, as both runs show that nitrogen concentrations keep increasing. This is mainly due to the sum of the first 200m vertical velocity going upwards, making the nitrogen increases over the years, especially on the first spinup run.

S2 Station PAP using MEDUSA parameter

In this section, we will discuss how running the 1D MEDUSA in station PAP, using the original parameter would differ to that in the main manuscript. Similar to running the model using modified parameters, where maximum grazing and nutrient uptake rate have been changed, seasonality is still distinct with the highest mean surface chlorophyll occurring in May. However, all the in situ seasonal and inter-annual surface chlorophyll means are within the ensemble range, summarised in Fig S9(a) and (b). This results in a broader ensemble spread, as indicated by the NRR values, summarised in Table S1, that are mostly closer to reliable spreads. The NRR value for annual mean however is broader than the modified parameters. In terms of nitrogen, not of all the in situ observation have been captured by the ensemble range. The decline that has been observed between February to August is not captured and therefore making the in situ monthly means being overestimated by the ensemble and are outside the ensemble range. Instead, the nitrogen produced by ensemble only starts to decline between July to September. This in turns make the NRR value for nitrogen profile higher (1.33) than that running the model using the parameters described in Table 1 in the manuscript (1.25).

Table S1 summarised the statistical metrics when running the ensemble using MEDUSA parameters in station PAP. The RMSE of nitrogen is smaller in the default run, although the correlation coefficient is higher in the ensemble median, similar to the modified parameters run. Yet the RMSE and bias for the default run, ensemble mean, and median in nitrogen are generally higher compared to the modified parameters. Compared to the modified parameters, using MEDUSA parameters enhance the correlation coefficient for chlorophyll, both on the surface and over the depths, as well as reducing the RMSEs and bias. These improvements therefore making the NRR values for chlorophyll profile and surface closer to unity compared to using the modified parameter.

Table S1. Mean, correlation, RMSE, bias, and NRR for station PAP when the ensemble is run using MEDUSA parameters. The numbers in italic are statistical metrics from the ensemble run using the modified parameters (similar to Table 3 in the main manuscript).

Station PAP	nitrogen				chlorophyll				surface chlorophyll			
	r	RMSE	Bias	Mean	r	RMSE	Bias	Mean	r	RMSE	Bias	Mean
Ens mean	0.20	4.09	-3.08	8.99	0.50	**0.25**	0.08	0.32	0.48	0.32	0.04	0.40
	(±0.15)	(±1.82)	(±4.20)	(±4.27)	(±0.68)	(±0.41)	(±0.68)	(±0.75)	(±0.42)	(±0.70)	(±0.86)	(±0.86)
	0.23	*3.26*	*0.61*	*6.59*	*0.42*	*0.32*	*0.06*	*0.48*	*0.45*	*0.51*	*0.22*	*0.66*
Ens median	0.19	4.08	-2.16	8.90	0.60	0.26	0.110	0.29	0.54	**0.32**	0.09	0.36
	0.23	***3.16***	*0.54*	*6.38*	*0.49*	***0.29***	*0.003*	*0.42*	*0.54*	***0.46***	*0.15*	*0.60*
def run	0.19	**3.72**	-2.98	8.07	0.53	**0.25**	0.04	0.36	0.4	0.33	0.01	0.43
	0.21	*3.32*	*-0.20*	*5.64*	*0.28*	*0.40*	*0.18*	*0.59*	*0.36*	*0.57*	*0.30*	*0.74*
In situ				5.83				0.39				0.44
NRR			*1.25*	1.33			*1.20*	1.11			*1.29*	1.02

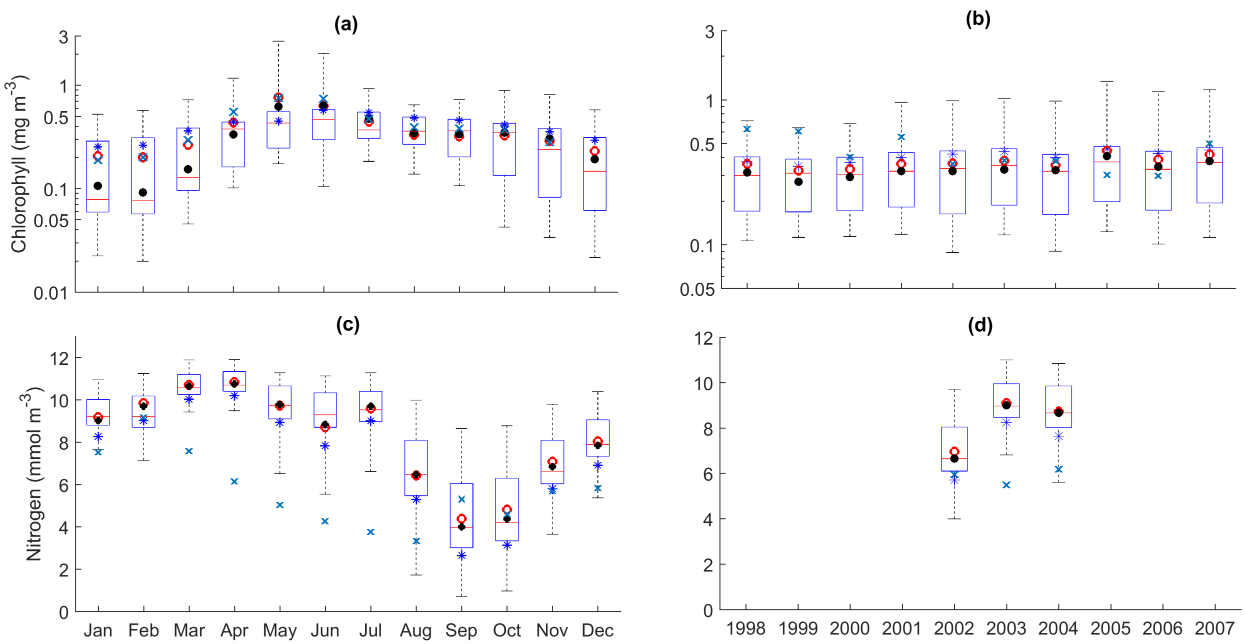

Figure S9. Seasonal and inter-annual mean of surface chlorophyll ((a) and (b)) and nitrogen ((c) and (d)) when running the ensemble MEDUSA using the original MEDUSA parameter.

In the original MEDUSA parameter, the maximum uptake is slightly lower (0.53 day^{-1}), and the grazing rate is twice higher (2.0 day^{-1}), compared to that in the modified parameter. This will cause lower phytoplankton abundance, and higher nitrogen concentrations as shown in Fig. S9 and from the 10-year mean shown in Table S1, especially in surface chlorophyll, where the mean is reduced to 60%, resulting in smaller bias. However, the effect of structural sensitivity is still quite similar to when using the modified parameter, where higher chlorophyll is produced when G_1 is applied. In terms of nitrogen, apart from applying G_1, low concentration is produced, when the functional form is combined with $\rho_2\xi_3, \rho_1\xi_2, \rho_3\xi_3$, and $\rho_1\xi_4$. These functional form combinations coincide with low RMSEs. However, higher nitrogen concentration > 9.5 mmol m^{-3}, is observed when the ensemble members contained G_2, unlike that in the modified parameter whereby high nitrogen is only produced when combining U_4 with G_2. In terms of surface chlorophyll, lower concentrations when using functional forms that contain U_4 and U_3 have not been observed. Instead, high chlorophyll concentrations and hence RMSE, both in the surface and profile, is produced when the functional forms that contain $\rho_2\xi_3$ and combine G_1 with $\rho_1\xi_2$. These are summarised in Fig. S10.

Indeed, using the MEDUSA parameters have improved the NRR values, RMSE, and correlation coefficients for surface chlorophyll and profile, but not nitrogen. The RMSE and bias for nitrogen are higher compared to using the modified parameters, as well as its NRR, indicating a narrow ensemble spread. Bias in chlorophyll is also higher than that in the original run using modified parameters. Nonetheless, G_2 still produced lower chlorophyll concentrations. The mortality functions that produced high chlorophyll and low nitrogen are also similar to that in the modified parameter.

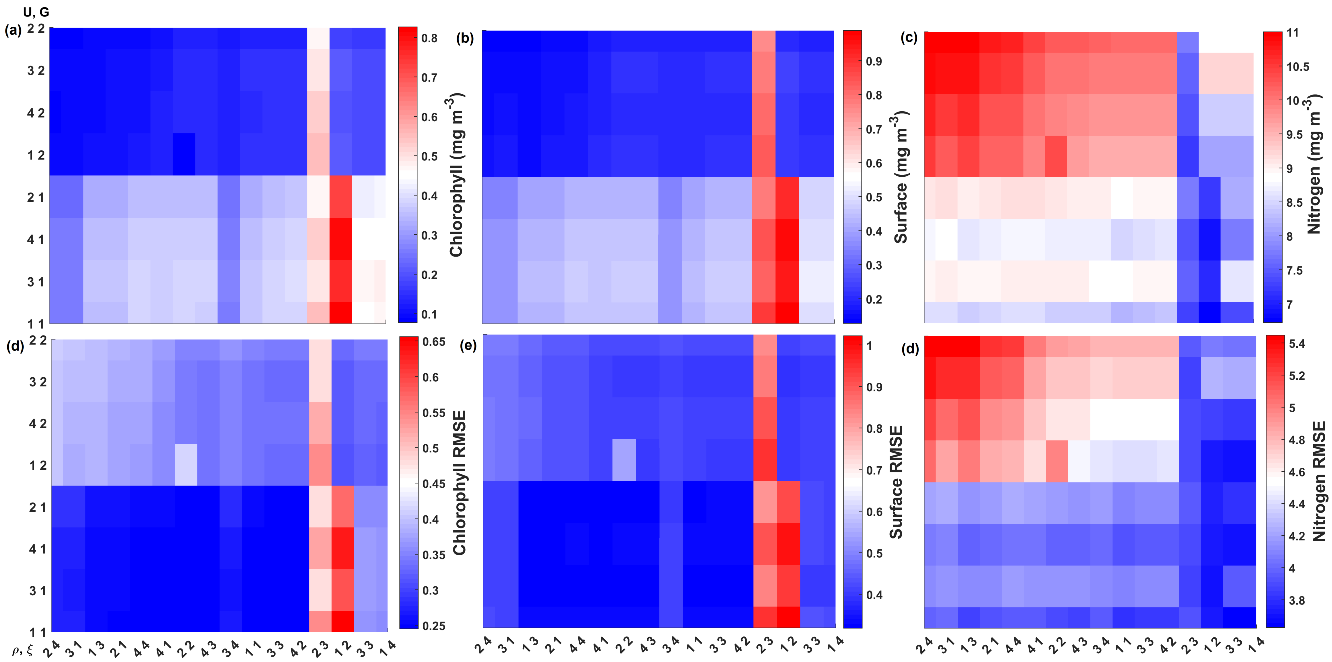

Figure S10. Mean chlorophyll profile (a), surface (b), and nitrogen (c), along with their RMSE ((d), (e), and (f) respectively) in station PAP when the ensemble is run using MEDUSA parameters. X-axis describe the combination of nutrient uptake (U) and grazing (G), and the y-axis describe the combination of phytoplankton (ρ) and zooplankton (ξ) mortality.

S3 Station PAP using in situ nitrogen as initial condition

The in situ nitrogen is only available from mid-2003 to mid-2005, and are not available at all depths (from 7-400 m) for every in situ measurements, therefore we initialised the nitrogen using test station data from 50°N 20°W. Here, we averaged all the available nitrogen at each depth and use it as the initial conditions. The ensemble is run using the modified parameters in 1D MEDUSA. The inter-annual and seasonal mean are shown in Fig. S11. In terms of chlorophyll, the satellite observation for seasonal and inter-annual mean are always within the ensemble range, as shown in Fig. S11(a) and (b) respectively. This results in the NRR being closer to unity in for annual mean (NRR= 1.05), and profiles (NRR= 1.07), although the surface chlorophyll is deemed too wide, summarised in Table S2. In terms of nitrogen, the inter-annual mean has an NRR value of 1.01, close to unity, as the in situ are always within the ensemble range, and there are only three data points available. However, in the seasonal means of nitrogen, shown on Fig. S11(c), during months of high concentrations, the ensemble underestimate this. Unlike using the MEDUSA parameters (Section S2), the ensemble have captured the decline of nitrogen between March to June. However in July, there is an increase of nitrogen and starts to decline from August to October, which has not been observed. This mismatch of pattern, therefore narrows the ensemble spread to 1.38.

Using the nitrogen input from the in situ data has enhanced the correlation coefficient in terms of nitrogen and reduced the RMSE compared to the original run and using MEDUSA parameters. The ensemble range for mean chlorophyll and nitrogen means are lower, especially for nitrogen, where the range for the means is now less than half of the original run, summarised in Table S2. This is expected as the in situ nitrogen, which is used as the initial condition, have lower nitrogen concentration, and therefore reducing the ensemble range. Similar to using the test station data as initial conditions, the RMSE is lower in the ensemble mean and median compared to the default run, as well as the correlation coefficient. This is also similar to the chlorophyll profile and surface, although in default run, the correlation is significantly lower than the one in Table 3 of the manuscript. This run also simulated lower chlorophyll means compared to the in situ, especially in the ensemble mean and median, as indicated by the negative bias. The NRR value for the chlorophyll profile is also reduced, from 1.20 to 1.07. Yet, the mean in situ chlorophyll is underestimated by the ensemble mean and median. These are summarised in Table S2.

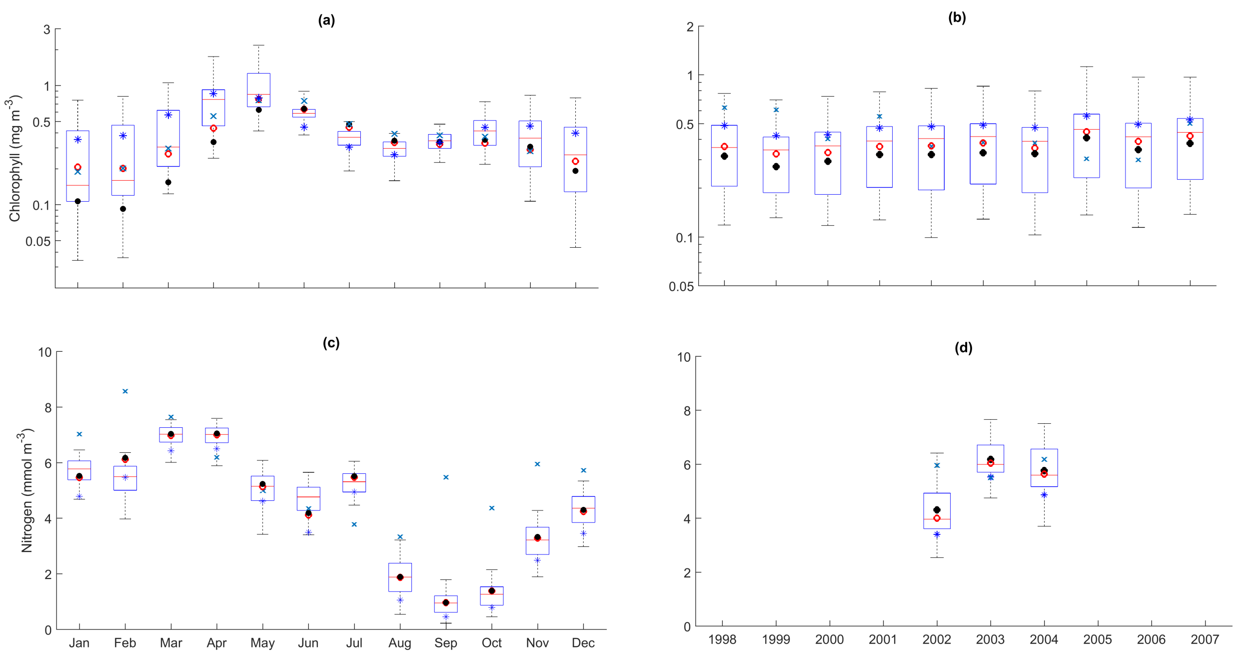

Figure S11. Seasonal and inter-annual mean of surface chlorophyll ((a) and (b)) and nitrogen ((c) and (d)) when running the ensemble MEDUSA using the in situ nitrogen.

Similar to that in section S2 and using the original run, G_2 still produced lower chlorophyll concentrations, and combining G_1 with $\rho_1\xi_2, \rho_3\xi_3$, and $\rho_1\xi_4$ produce high chlorophyll profile concentrations which coincide with high RMSE. This has also been observed in the surface, although the RMSE is slightly higher, with the addition of ensemble members that contain $\rho_2\xi_3$ and G_1 to have high chlorophyll concentrations > 0.6 mg m^{-3}. The opposite has been observed in nitrogen, where using functional form combinations mentioned above, produce lower nitrogen concentration. Unlike the original run, high nitrogen is not observed when combining U_4 and G_2, and overall, the ensemble produced lower chlorophyll with smaller range (see Table S2).

Table S2. Mean, correlation, RMSE, bias, and NRR for station PAP when the initial condition is the mean in situ nitrogen, using the modified parameters. The numbers in italic are the statistical metrics from the ensemble run using the modified parameters (similar to Table 3 in the main manuscript).

Station PAP	nitrogen				chlorophyll				surface chlorophyll			
	r	RMSE	Bias	Mean	r	RMSE	Bias	Mean	r	RMSE	Bias	Mean
Ens mean	0.26	2.77	-0.76	5.1	0.5	0.27	-0.08	0.29	0.44	0.32	-0.046	0.4
	(±0.06)	(±0.87)	(±1.85)	(±1.90)	(±0.57)	(±0.37)	(±0.50)	(±0.54)	(±0.31)	(±0.48)	(±0.60)	(±0.59)
	0.23	*3.26*	*0.61*	*6.59*	*0.42*	*0.32*	*0.06*	*0.48*	*0.45*	*0.51*	*0.22*	*0.66*
Ens median	0.26	**2.77**	-0.71	5.04	0.6	**0.26**	-0.11	0.32	0.47	**0.32**	-0.087	0.36
	0.23	***3.16***	*0.54*	*6.38*	*0.49*	***0.29***	*0.003*	*0.42*	*0.54*	***0.46***	*0.15*	*0.60*
def run	0.24	3.14	-1.37	4.44	0.16	0.34	0.043	0.44	0.11	0.45	0.037	0.48
	0.21	*3.32*	*-0.20*	*5.64*	*0.28*	*0.40*	*0.18*	*0.59*	*0.36*	*0.57*	*0.30*	*0.74*
In situ				5.83				0.39				0.44
NRR			*1.25*	1.38			*1.20*	1.07			*1.29*	0.9

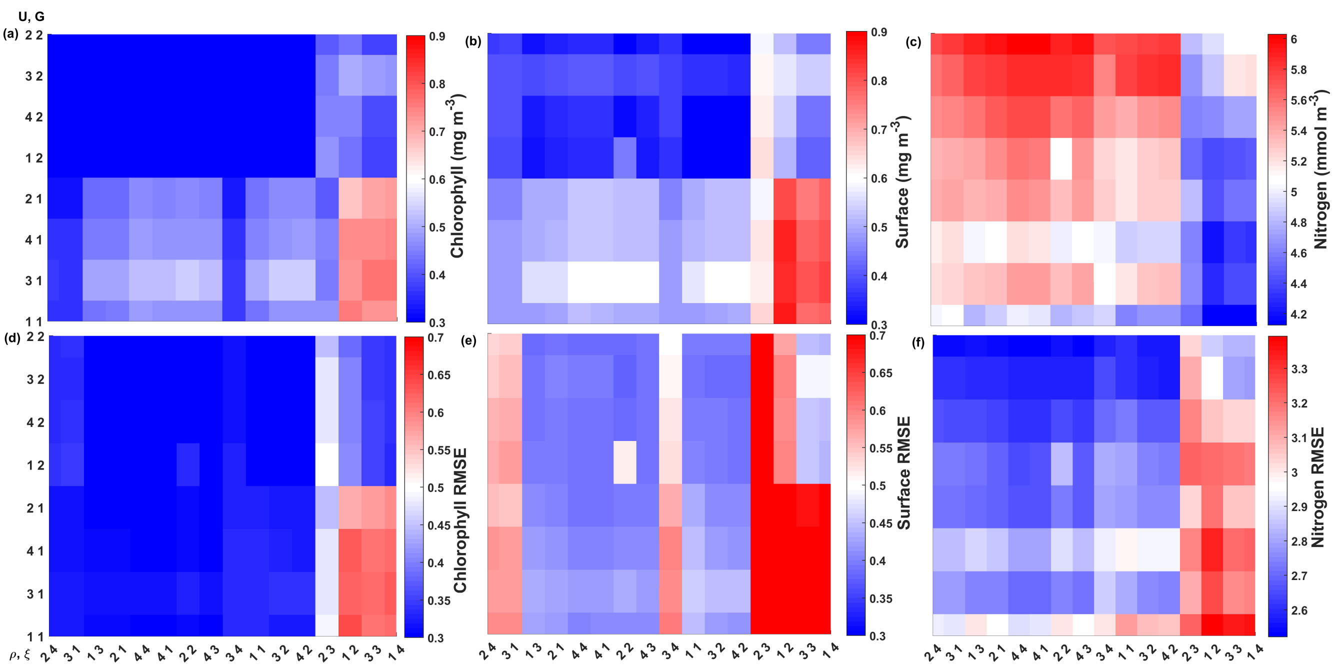

Figure S12. Mean chlorophyll profile (a), surface (b), and nitrogen (c), along with their RMSE ((d), (e), and (f) respectively) in station PAP when the ensemble is run using MEDUSA parameters. X-axis describe the combination of nutrient uptake (U) and grazing (G), and the y-axis describe the combination of phytoplankton (ρ) and zooplankton (ξ) mortality.

Overall, using the in situ nitrogen concentration as input data have improved the nitrogen and chlorophyll RMSE and correlation coefficient, as well as the chlorophyll profile's NRR, but makes the nitrogen and surface chlorophyll NRR too narrow and broad, respectively. All the range of mean nitrogen, chlorophyll profile, and surface have been reduced. The general effect of perturbing functional forms are still very similar to that in the original run, apart from nitrogen where using G_2 and U_4 does not produce high ($>$9 mmol m^{-3}) nitrogen concentration. The NRR for nitrogen is also considerably narrow compared to the original run.