Phytoplankton Functional Type Algorithm Theoretical Basis Document Ver.0 (2012.3.30)

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1. Introduction

This document describes algorithms that retrieve several Phytoplankton Functional Types (PFTs) as a satellite observation. PFTs may be defined in terms of a role of phytoplankton on biogeochemical cycles in the oceans or size of the phytoplankton cell which is an useful parameter in ecosystem analysis. In general, the agreement between functional- and taxonomic- or size-based classification, while far from universal, is adequate, therefore we use the term “phytoplankton functional types (PFTs)” to mean different groups of phytoplankton. This document provides (1) background of the algorithm (e.g. definition of PFTs), (2) in situ data used for the algorithm development, (3) algorithm equations, (4) operation procedure and (5) algorithm testing including uncertainty estimation.

2. Background of the algorithm

The PFT algorithms shown here are empirical algorithms. In the following, theoretical basis for ‘empirical-based algorithm’ is described.

Figure 1 shows in situ measurement of the total Chlorophyll-a concentration (TChla in [mg/m3]) against a percentage contribution of different PFTs [%] to TChla: a)Picoplankton, b) Nanoplankton, c) Microplankton, d) Pico-Eukaryote, e) Prymnesiophyte (Haptophyte), f) Diatom, g) Prokaryote, h) Green Algae, i) Dinoflagellates, j) Prochlorococcus sp. It is clear that there are well defined relationships between TChla and PFTs, which implies that a percentage contribution of PFTs to TChla can be estimated (or “inverted”) using TChla, if the relationships are quantified between them. TChla is a standard product of SGLI/ GCOM-C1, therefore it should be possible to derive the percentage contribution of PFTs to TChla. A practical issue in the estimation of PFTs by means of such approach is collection of in situ data to develop the empirical algorithms. It will be described in Section 3.

Relationships between TChla and PFTs observed in situ can be quantified by regression analysis. Non-linear regression was done by using Nelder-Mead method. However, the logistic function is applied here as a base function for the fitting, since ecological theory describes population dynamics by the equation; i.e. Y=A / [1-m * exp (-k*x)], where Y is a fractional contribution [0-1] of PFT to TChla, so that A=1, and m and k are fitting parameters. Finally, x is TChla if it is in linear or log space).

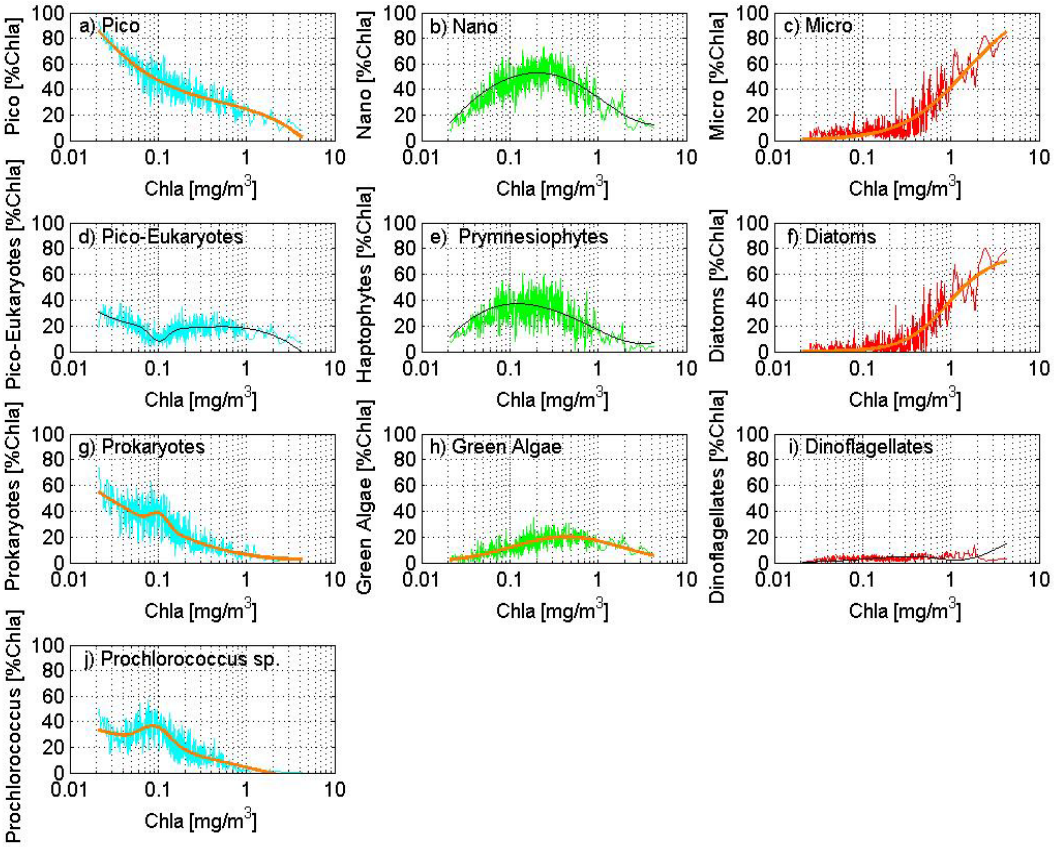

Figure 1. Observed relationship between TChla and PFTs.

3. In situ data set

The PFT algorithms are developed based on existing in situ data by seeking relationships between TChla and PFTs. Thus, the algorithms are empirical algorithms. To obtain PFTs from in situ observation, the following in situ data sets of HPLC are used: NERC AMT (Aiken et al., 2009), JAMSTEC BEAGLE (Barlow et al., 2007), NASA NOMAD and SeaBASS (Werdell and Bailey, 2005), University of Tokyo SEEDSII experiments (Suzuki et al., 2005), Fisheries Research Agency of Japan A-line cruise (Isada, 2009), Hokkaido University Oshoro-maru cruise (Howell et al., personal communication). These individual dataset was re-compiled to generate a global dataset which consists of 3966 data point after quality control. Fig. 2 shows spatial distribution of these dataset.

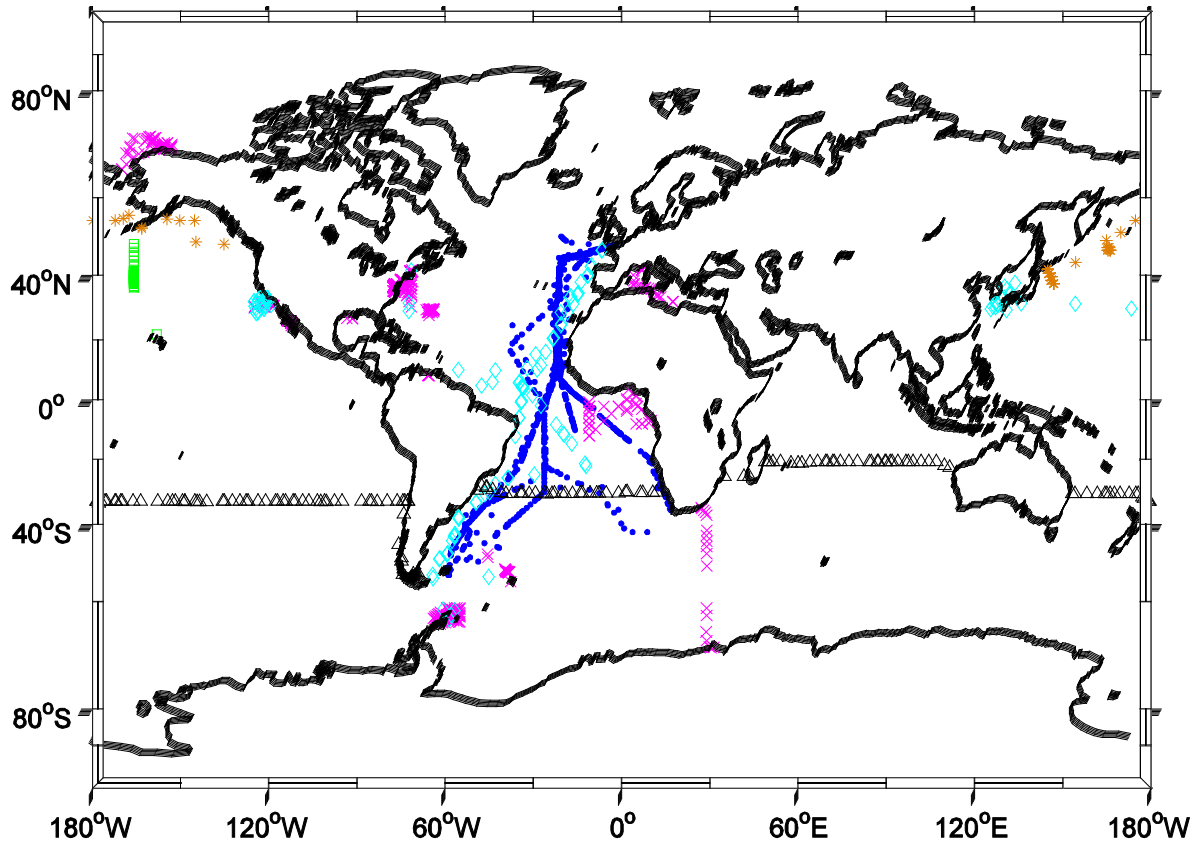

Figure 2. Distribution of phytoplankton pigment data used in this study; blue dot: the NERC AMT cruise (Aiken et al., 2009), black triangle: the JAMSTEC BEAGLE cruise (Barlow et al., 2007), cyan diamond: the NASA NOMAD (Werdell and Bailey, 2005), magenta cross: the NASA SeaBASS, brown star: the SEEDS II cruise (Suzuki et al., 2005) + A-line stations (Isada et al., 2009), green square: the HU Oshoro-maru cruise.

Quality control was undertaken by the procedure described by Hirata et al. 2008: A linear regression analysis of TChla vs accessory pigments was made to exclude 'outlier' data, which was defined as any data larger than 2x standard deviation around the regression line. This was repeated three times.

Within the quality controlled dataset, 70% were sub-sampled to find relationships between TChla and PFTs, and 30% were reserved for algorithm testing. The 30% dataset was obtained in such a way that 30% of individual dataset was sub-sampled using a random selection to ensure that each individual dataset evenly contribute to the 30% dataset.

PFTs were classified based on Diagnostic Pigment Analysis (Viddussi et al., 2001) which defines a suite of Diagnostic Pigments (DP) for specific PFTs that can be quantified towards

estimation of the relative abundance of a specific PFT (Table 1). The DPA was subsequently refined by Uitz et al. (2006) to scale DPs to TChla, permitting the application of DPA-based approaches to satellite-derived TChla. In addition, Hirata et al. (2008) used the refined DPA to separate pico-eukaryotes from nano-eukaryotes, and Brewin et al. (2010) developed a method to quantify the relationship, which is used in the present work. Here, DPA is further refined to account for ambiguity of the fucoxanthin (Fuco) signal. Fuco is defined as a DP for Diatoms by Vidussi et al. (2001). However, Fuco is also a precursor pigment of 19'-Hexanoyloxyfucoxanthin (Hex), the DP for prymnesiophytes (haptophytes), and can co-occur in this group. Fuco is also contained in the other heterokonts (e.g. chrysophytes, bolidophytes) and dinoflagellates, which are relatively abundant in coastal environments (Wright and Jeffrey, 2006). Thus, diatoms could be overestimated in DPA. Hirata et al. (2008) found a non-negligible proportion of Fuco within the oligotrophic gyres of the subtropical Atlantic, where small prokaryotes (predominantly Prochlorococcus sp. and Synechococcus sp.) and pico-eukaryotes (which can partly belong to the prymnesiophytes (haptophytes) so may also contain Hex) usually dominate the phytoplankton community (Zubkov et al., 1998; Tarran et al., 2006). In these oligotrophic waters, TChla is low (<0.25 mg m^{-3}, Aiken et al., 2009), therefore, it is more reasonable to assume that the background level of Fuco detected results from smaller prymnesiophytes (haptophytes) rather than diatoms which are more prevalent in eutrophic waters. Therefore, we calculated a baseline for the Fuco/Hex ratio, $(Fuco/Hex)_{baseline}$, using Fuco and Hex in the Chl-a range less than 0.25 mg m^{-3} in the original data set (denoted as $Fuco_{original}$ and $Hex_{original}$, respectively). The proportion of Fuco as a diatom biomarker is then corrected so that $Fuco_{corrected} = Fuco_{original} - (Fuco/Hex)_{baseline} \times Hex_{original}$.

The Fuco conversion is only significant in the lower Chl-a range (<0.5 mg m^{-3}) and is negligible for higher Chl-a values. Using these HPLC pigment signals, PSCs and PFTs are defined and classified as in Table 1.

Micro-, Nano- and Picophytoplakton are based on size-based classification, which may be defined, according to Sieburth et al. (1978), by microplankton >20 µm, nanoplankton 20–2 µm, picoplankton <2 µm in physical cell size. Although the DPA described above do not specify the size classes directly, outputs of the DPA are assumed to follow the size classification definition by Sieburth, since an agreement between taxonomic and size classification is generally accepted. However, a user must be aware this assumption in use of the present algorithms for micro-, nano- and picoplankton.

Table 1. Diagnostic Pigments and PSCs/PFTs

Size Classes/PFTs	Diagnostic Pigments	Estimation Formula
Microplankton (>20μm)[*1]	Fucoxanthin (Fuco), Peridinin (Perid)	1.41(Fuco+Perid) / ΣDP[*1]
Diatoms	Fuco	1.41Fuco / ΣDP[*2]
Dinoflagellates	Perid	1.41Perid / ΣDP[*2]
Nanoplankton (2-20μm)[*1]	19'-Hexanoyloxyfucoxanthin(Hex)	(X_n*1.27Hex+1.01Chlb +0.35But+0.60Allo)/ΣDP[*3]
	Chlorophyll-b (Chlb)	
	Butanoyloxyfucoxanthin (But)	
	Alloxanthin (Allo)	
Green algae	Chlb	1.01Chlb / ΣDP[*2]
Prymnesiophytes[*4]	Hex, But	
(Haptophytes)		
Picoplankton (0.2-2μm)[*1]	Zeaxanthin(Zea), Hex, Chlb	(0.86Zea+Y_p1.27Hex)/ΣDP[*3]
Prokaryotes	Zea	0.86Zea / ΣDP[*2]
Pico-eukaryotes[*5]	Hex, Chlb	
Prochlorococcus sp.	Divinyl Chlorophyll-a (DVChla)	0.74DVChla / Chla

[*1]Sieburth et al., (1978)

[*2]ΣDP= 1.41Fuco+1.41Perid+1.27Hex+0.6Allo+0.35But+1.01Chlb+0.86Zea=Chla (Uitz et al, 2006)

[*3]X_n indicates a proportion of nanoplankton contribution in Hex, respectively. Similarly Y_p indicates a proportion of picoplankton in Hex, respectively (Brewin et al., 2010)

[*4] Given that contributions of Allo to nanoplankton were only a few percent in our data set, haptophytes were approximated to Nano minus Green Algae

[*5] Pico-eukaryotes can be determined from picoplankton minus prokaryotes (see also Fig. 2 caption)

4. Algorithm Equations

The PFT algorithms use the following equations to estimate nine PFTs (i.e. Microplankton, Diatom, Nanoplankton, Green Algae, Prymnesiophyte, Picoplankton, Prokaryote, Pico-Eukaryote, Prochlorococcus sp.). The algorithms return a fraction [0-1] of a specified PFT relative to TChla [mg/m^3].

$$\text{Microplankton} = 1 / [\ 0.9117+\exp(-2.7330 * \log10(\text{TChla}) + 0.4003)\ ] \quad \text{Eq. (1)}$$

$$\text{Diatom} = 1 / [\ 1.3272 + \exp(-3.9828 * \log10(\text{TChla}) + 0.1953)\ ] \quad \text{Eq. (2)}$$

$$\text{Nanoplankton} = 1 - \text{Microplankton} - \text{Picoplankton} \quad \text{Eq. (3)}$$

$$\text{Green Algae} = (0.2490/\text{TChla}) * \exp(\ -1.2621 * (\ \log10(\text{TChla})-0.5523\ )^2 \quad \text{Eq. (4)}$$

$$\text{Prymnesiophyte} \fallingdotseq \text{Nano-Green Algae} \quad \text{Eq. (5)}$$

$$\text{Picoplankton} = - (1 / [0.1529+\exp(1.0306*\log10(\text{TChla}) - 1.5576)]) + 1.8597 + 2.9954 \quad \text{Eq.(6)}$$

$$\text{Prokaryotes} = (0.0067/0.6154/\text{TChla}) * \exp(\ -19.519 * (\log10(\text{TChla})+0.9643\ )^2 / 0.0067^2\ ) + 0.1027*[\log10(\text{TChla})]^2 - 0.1189*\log10(\text{TChla}) + 0.0626 \quad \text{Eq.(7)}$$

$$\text{Pico-Eukaryote} = \text{Picoplankton} - \text{Prokaryote}$$

$$\text{Prochlorococcus sp.} = (0.0099/0.6808/\text{TChla}) * \exp(\ -8.6276*(\log10(\text{TChla}) + 0.9668)^2 / 0.0099^2\ ) +0.0074*[\log10(\text{TChla})]^2 -0.1621*\log10(\text{TChla}) + 0.0436 \quad \text{Eq.(8)}$$

5. Operation Procedure

The PFT algorithms assume that total TChla are obtained in prior to their implementation.

Thus, it is important to note that (a) TChla must be obtained by any mean (e.g. GCOM-C1 Chlorophyll-a algorithm) prior to implementation of the present PFT algorithms. Without TChla, PFTs cannot be estimated. Once TChla is prepared, the following PFTs must be estimated first: Microplankton, Diatom, Green Algae, Picoplankton, Prokaryote and Prochlorococcus sp (these PFTs can be estimated in any order). Secondly, Nanoplankton (=1-Mircoplankton-Picoplankton) and Pico-eukaryote (=Picoplankton-Prokaryote) can be derived. Finally, Prymnesiophyte can be estimated from Nanoplankton-GreenAlgae. Figure 3 visually summarizes the operation flow.

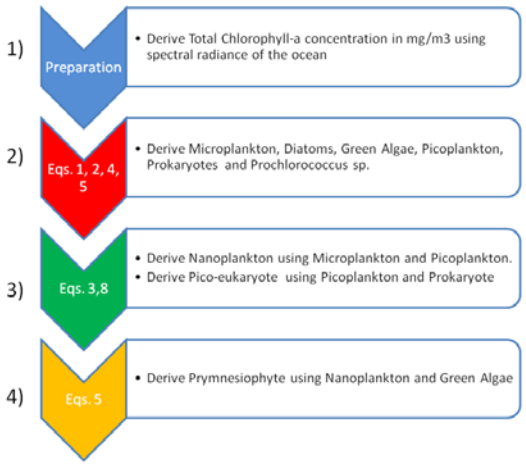

Figure 3. Flow chart of PFTs estimation. A step estimation is necessary to derive all nine PFTs.

6. Algorithm testing

Figure 4 shows residual between PFTs derived from the algorithms and in situ HPLC data used for the development of the algorithms. Ideally, the residual is zero, however, variable residual is found over the TChla range as well as over the PFTs. This residual may be assumed to represent uncertainty of the present algorithms, given that in situ data of PFTs for all location and time period is unavailable. Table 2 summarizes the mean and maximum residual for the nine PFTs.

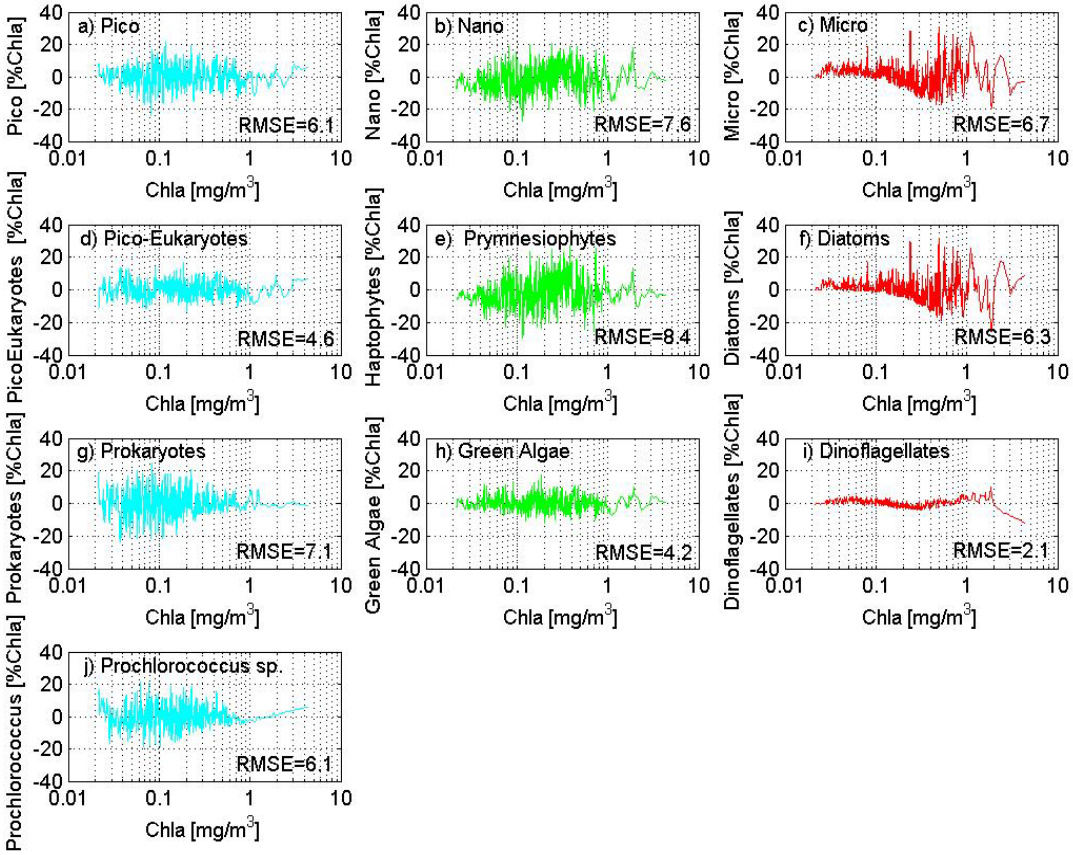

Figure 4. Residual between PFTs derived from in situ HPLC data and its best fit curve. Note that Dinoflagellate algorithm is not a deliverable.

Fig.5 shows PFTs derived from Eqs. 1-8 against another subset of NOMAD data (Werdell and Bailey, 2005) which was not used for algorithm development. Statistics are summarized in Table 3. Picoplankton is retrieved with the regression slope 1.00, although some scatters are found. While there is more scatter in Prochlorococcus sp. than Pico assembles, the regression slopes for both phytoplankton types are similarly good (1.0 for Pico and 0.982 for Prochlorococcus). Prokaryotes

and Pico-Eukaryotes have scatter (7.71%, 5.25%) and the regression slope is 0.864 and 0.801, respectively. Nanoplankton have relatively larger RMSE (8.55%) compared to other PFTs. However, Prymnesiophytes, which may be considered as nanoplankton fraction, has an increased RMSE and intercept (10.0 and -9.721, respectively) than Nanoplankton assembles. Microplankton and Diatoms show similar results. Note that Dinoflagellate algorithm is not a deliverable.

Since the algorithms were developed based on the global climatology of the PFTs derived from in situ observations, a check is need to ensure whether the temporal variation of PFTs is also retrieved from the present algorithms. Figure 6 shows power spectra of three phytoplankton types (Micro, Nano and Pico) for different ocean basins derived from the existing satellite data as an example. One of the significant variability of phytoplankton dynamics is known as seasonality (i.e. 365 day cycle). The seasonality is clearly seen in all basins under the present algorithms.

Table 2. Mean and Maximum Residual

PFTs	Residual [%]	Maximum Residual [%]
Microplankton	6.7	31.1
Diatom	6.3	31.8
Nanoplankton	7.6	27.6
Green Algae	4.2	17.8
Prymnesiophyte	8.4	29.5
Picoplankton	6.1	23.8
Prokaryote	7.1	25.2
PicoEukaryote	4.6	16.6
Prochlorococcus sp.	6.1	21.4

Table 3. Statistical results of the PFT algorithms against in situ data

	Slope	Intercept	RMSE
Micro	1.109	1.073	8.28
Diatom	1.115	1.732	7.98
Nano	1.168	3.055	8.55
Prymnesiophyte	1.218	-9.721	10.0
Green Algae	0.809	2.035	4.71
Pico	1.000	-8.093	7.12
Pico-Eukaryotes	0.801	2.564	5.25
Prokaryotes	0.864	3.712	7.71
Prochlorococcus sp.	0.982	0.353	6.25

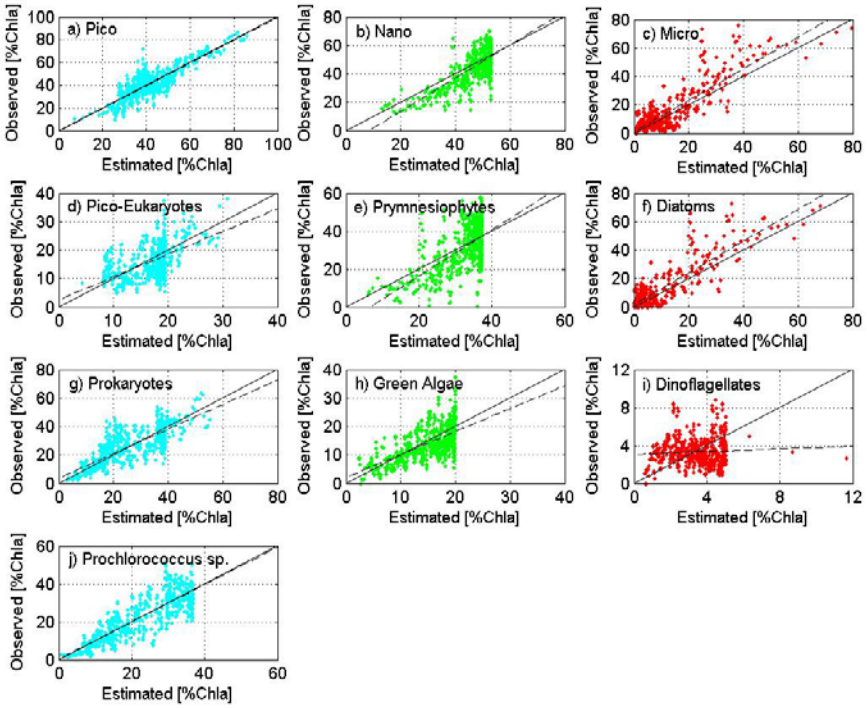

Figure 5. Comparison between in situ PFTs and those derived from the present PFT algorithms. Note that in situ data used for the algorithm evaluation is a subset of the original data set, which was not used for algorithm development.

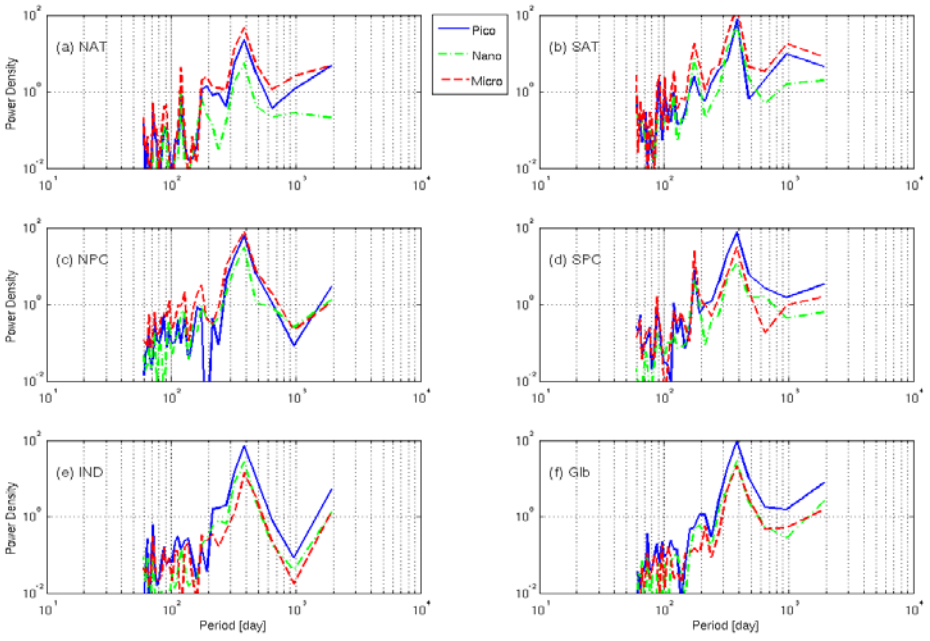

Figure 6. Power spectra for Pico, Nano and Microplankton for different ocean basins (NAT: North Atlantic, SAT: South Atlantic, NPC: North Pacific, SPC: South Pacific, IND: Indian Ocean, Glb: Global Oceans).

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