SCIENCE CHINA
Earth Sciences

• REVIEW •

September 2016 Vol.59 No.9: 1817–1826
doi: 10.1007/s11430-015-5432-6

Paleoclimate data assimilation: Its motivation, progress and prospects

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Received December 23, 2015; accepted May 3, 2016; published online July 15, 2016

Abstract Reconstructing past climate is beneficial for researchers to understand the mechanism of past climate change, recognize the context of modern climate change and predict scenarios of future climate change. Paleoclimate data assimilation (PDA), which was first introduced in 2000, is a promising approach and a significant issue in the context of past climate research. PDA has the same theoretical basis as the traditional data assimilation (DA) employed in the fields of atmosphere science, ocean science and land surface science. The main aim of PDA is to optimally estimate past climate states that are both consistent with the climate signal recorded in proxy and the dynamic understanding of the climate system through combining the physical laws and dynamic mechanisms of climate systems represented by climate models with climate signals recorded in proxies (e.g., tree rings, ice cores). After investigating the research status and latest advances of PDA abroad, in this paper, the background, concept and methodology of PAD are briefly introduced. Several special aspects and the development history of PAD are systematically summarized. The theoretical basis and typical cases associated with three frequently-used PAD methods (e.g., nudging, particle filter and ensemble square root filter) are analyzed and demonstrated. Finally, some underlying problems in current studies and key prospects in future research related to PDA are proposed to provide valuable thoughts on and a scientific basis for PDA research.

Keywords Climate reconstruction, Paleoclimate modeling, Proxies, Data assimilation

Citation: Fang M, Li X. 2016. Paleoclimate data assimilation: Its motivation, progress and prospects. Science China Earth Sciences, 59: 1817–1826, doi: 10.1007/s11430-015-5432-6

1. Introduction

Past climate changes can be inferred from proxy-based reconstructions (Jones et al., 1998; Yang et al., 2002; Mann et al., 2008, 2009; Zheng et al., 2013) and climate model simulations (Crowley, 2000; Otto-Blieser et al., 2001; Ammann et al., 2007; Jungclaus et al., 2010; Xiao et al., 2012). These two approaches have their own methodologies and provide two differentiated pragmatisms for past climate research. A proxy considers a "change scenario" of climate change over a certain period and coverage (PAGES 2k Consortium, 2013) because it serves as a "faithful recorder" of information of past climate change[1)]. Alternatively, climate models depend on the physical laws and dynamic mechanisms of the climate systems represented by them and thus provide continuous spatio-temporal variations of past climate. Therefore, we can study past climate change by using either of the above two approaches (Phipps et al., 2013). In

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1) NOAA Paleoclimatology Data Center compares proxies to a magnetic cassette tape recording, and in fact, the reconstruction and understanding of past climate change can be regarded as an action to play back the tape using appropriate methods. Therefore, the authors extend this definition of proxies to a faithful recorder of information of past climate change. http://www.ncdc.noaa.gov/paleo/slides/slideset/12/.

fact, these two approaches can be regarded as two complementary strategies in paleoclimatology because (1) cross-validation of the results from the two approaches is beneficial for identifying some deficiencies of climate models and thus improving the modeling performances of climate models, and (2) it can help researchers to better recognize and understand the mechanisms of past climate change by combining the "real condition" of past climate change constrained by proxies with variability laws of the climate system represented by climate models (Phipps et al., 2013).

However, we should note that the above two approaches are not perfect, although many cases associated with them have been reported. First, there are some limitations in understanding some of the physical processes in the climate system and in mathematically describing those physical processes due to the following reasons: (1) the climate system is a complex, nonlinear and gigantic system, and (2) some complex physical processes in the climate system have not yet been clearly identified and understood by researchers. Moreover, very slight variations in the parameterization, coupling, discretization, initialization and boundary conditions of climate models may give rise to simulations that obviously deviate from instrumental observations (Gillett, 2005; Kalnay, 2003; Widmann et al., 2010; Phipps et al., 2013; Fang and Li, 2016). Second, variations in climate system are commonly influenced by the internal variability of the climate system and climate forcings; internal variability is quasi-random and is an intrinsic factor, whereas a climate forcing is an external factor (Kalnay, 2003; Phipps et al., 2013). Simulating the temporal evolution of "quasi-random" variations in the climate system relying solely on climate models, however, is impossible due to the chaotic nature of the climate system (Widmann et al., 2010). Additionally, the response of the climate system to external forcings is an extremely complex process; thus, accurate simulation of this complex process is extremely difficult. Third, the spatial distribution of existing proxies is sparse around the globe (Mann et al., 2008, 2009). A proxy is a point-observation, and it is generally defined as a random variable; hence, it inevitably contains observational error. Observational error can be decomposed into two parts, namely, representative error and instrumental error (Li, 2014). Estimation of representative error is very difficult because quantifying the representative space of climate information derived from a proxy obtained at a sampling site is a quietly complicated question; this difficulty always affects researchers in analyzing and explaining the proxy-based climate variations within a certain spatial coverage because they are unable to accurately determine the spatial uncertainty of these proxy-based reconstructions. Lastly, proxy-based reconstruction of past climate generally relies on a stationary relationship between climate variables and proxy indexes (Franke et al., 2010; Bhend et al., 2012). This stationary relationship is constructed based on statistical methods (e.g., regression methods) using instrumental data over a relatively short period (from approximately 1850 to the present day). Proxy-based reconstruction is a frequently used method in paleoclimatology; nonetheless, it has been substantially debated by some researchers (Christiansen et al., 2009; Rutherford et al., 2010; Smerdon, 2011; McShane and Wyner, 2011; Wahl and Ammann, 2011). For instance, von Storch et al. (2004) noted that many proxy-based reconstructions are not consistent with model simulations (Crowley, 2000; Gerber et al., 2003; Bauer et al., 2003; Goosse et al., 2004); these inconsistencies have led some researchers to question the credibility of proxy-based reconstructions using regression methods. Phipps et al. (2013) and Steiger et al. (2014) also argued that a statistical relationship is one that varies with the variations of the sample data (e.g., the count of samples, time-length of samples, etc.); thus, the statistical relationship is, in fact, dynamic rather than stationary. Therefore, it is largely subject to incredulity when one uses a statistical relationship to reconstruct past climate over the past 1000 years or longer.

2. Concept, characteristics, methods and applications of PDA

2.1 Concept

Data assimilation (DA), an optimization method originating in atmospheric and oceanic science, allows us to combine optimal information from observations with models of the earth system and thus optimally estimate geophysical fields of interest (Wang, 1999). We can quantitatively estimate uncertainties of observations and simulations, and can also use observations to effectively constrain model trajectories through DA. Updated results of DA are consistent with both the information contained in observations and the physical mechanisms represented by the models. Furthermore, these updated results are always better than observations and simulations alone (Talagrand, 1997; Bouttier and Courtier, 1999; Robinson and Lermusiaux, 2000; Li et al., 2007; Li, 2014).

In the context of past climate research, DA is a promising way to obtain better estimates of past climate states because DA is a mathematical framework that (1) can combine information recorded in proxies with the physical understanding of the climate system represented by climate models and (2) can skillfully address errors contained in both proxy data and simulation results. The basic idea behind PDA is to constrain a climate model trajectory using proxy data and an observation operator (e.g., a forward model), and hence optimally estimate past climate. Estimated climate variation using DA is generally consistent with both climate signals recorded in proxies and the physical laws and dynamic mechanisms represented by climate models. We can also quantitatively estimate uncertainties of proxies and simulations (Widmann et al., 2010; Hakim et al., 2013). Therefore, as Edwards et al. (2013) has stated, PDA is a best-of-both-worlds method for estimating time slices in the past.

Since von Storch et al. (2000) first introduced the DA concept into the paleoclimatology field, various DA methods had been used continuously in paleoclimate research, such as nudging (von Storch et al., 2000), Bayesian estimation (Hargreaves and Annan, 2002), forcing singular vectors (FSV) (Barkmeijer et al., 2003), ensemble square root filter (EnSRF) (Pendergrass, 2009; Pendergrass et al., 2012; Bhend et al., 2012), particle filter (PF) (Dubinkina et al., 2011; Gossess et al., 2012), etc. Nudging and FSV are based on the same theoretical basis. The basic idea of those two methods is to add an artificial forcing-term to forecast equations to drive the forecasting results forward based on available observations. The difference between these two methods is how the artificial forcing-term is constructed. EnSRF is a variant of ensemble Kalman filter (EnKF) (Evensen, 1994, 2003); EnKF and PF, two typical ensemble methods in DA, are commonly developed based on the Bayesian estimation rule. Moreover, although variational DA methods have been used in the Twentieth Century Reanalysis Project (Whitaker et al., 2004; Compo et al., 2006, 2011), such as NCEP/NCAR and ERA40, they are not suitable for reconstruction of past climate with a much sparser set of observations for longer analyses, whereas the EnKF has performed well under these circumstances (Widmann et al., 2010). Bhend et al. (2012) also clearly showed that variational DA methods are not suitable for reconstructing past climate with a much smaller number of observations or climate proxies.

Processes involved in PDA can be summarized in Figure 1. The NOAA Paleoclimatology Data Center provides initial conditions and forcings for running climate model simulations. Assimilation operations will be activated after the model has reached an equilibrium status via a "spin-up" period. Observations in the assimilation phase can be divided into two categories: the first type is proxy-based reconstruction of climate variables of interest, such as temperature, precipitation and runoff[2)]; this type of observation is defined as product data. The second alternative is original proxy data, such as tree-ring width, tree-ring density and stable oxygen isotope ratios recorded in ice cores, lake sediments, and ocean sediments. A relatively simple observation operator, for example, a transformation matrix, can implement assimilation if one uses the first type of observation. For assimilating the second type of observation, it must rely on a forward model that maps climate variables from state space to observation space. Climate variables of interest are updated in the assimilation phase; these updated values are defined as "analysis values". At the end of the entire period of interest, we can obtain a series of optimal estimations of climate states over a certain area for a given period of time through recursively activating the DA operation.

2.2 Characteristics of PDA

Although the theories of PDA and DA in the fields of atmosphere science, ocean science and land surface science stem from the same theoretical foundations, PDA has some special characteristics. For clarity, we have summarized these special characteristics as follows:

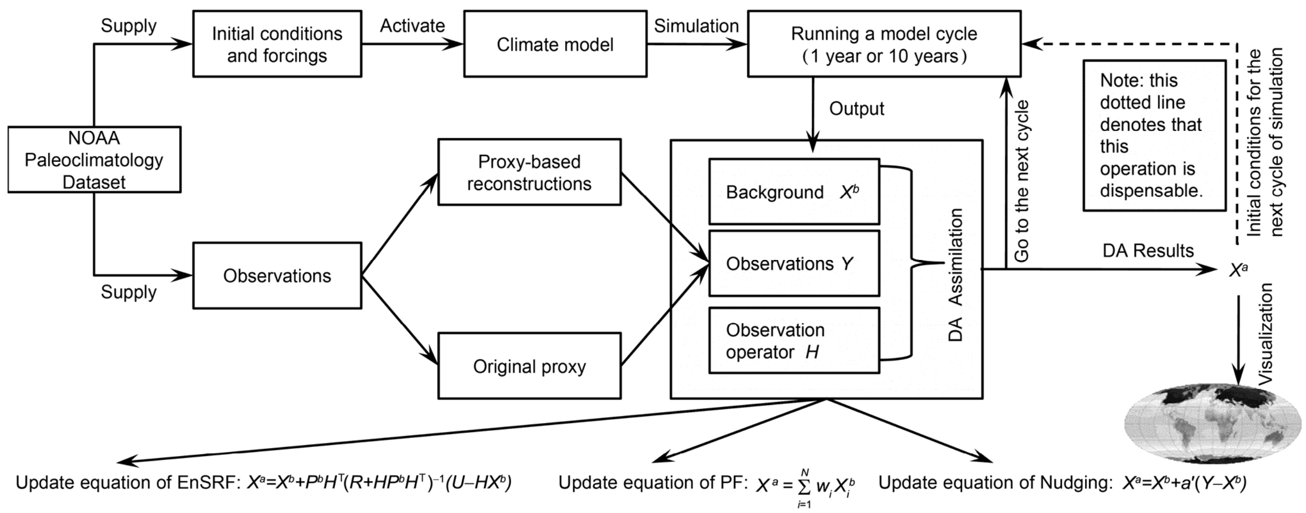

Figure 1 The process diagram of PDA. X^a, analysis ensemble; X^b, background ensemble; P^b, background error covariance matrix; R, observations error covariance matrix; H, observation operator; Y, observations; a', relaxation factor of Nudging; N, the amount of particles; w_i, weight of the ith particle; X_i^b, background of the ith simulation; $(\ )^T$, matrix transpose; $(\ )^{-1}$, matrix inversion. The temporal resolution of states is same to that of observations.

2) We express this as "the first type is proxy-based reconstruction of climate variables of interest, such as temperature, precipitation and runoff"; however, only the proxy-based temperature products have been considered in PDA studies; proxy-based precipitation and runoff have not yet been used in PDA, but their potential as PDA observations still exists; therefore, the authors list them in this paper.

(1) PDA observations (e.g., proxies and proxy-based reconstructions) are time-averaged and continuous in time, whereas DA observations in the fields of atmosphere science, ocean science and land surface science (e.g., *in-situ* observations, remote sensing data) are usually instantaneous and discontinuous in time. Prior to the instrumentally observed epoch, direct observations of climate variables are generally not available; therefore, proxy data are the primary sources of observations used in PDA. Compared with the modern observational network, these proxy data are insufficient and sparse in space. In addition, proxy data always represent the average state of the climate over a period of time, i.e., they are time-averaged (Dirren and Hakim, 2005; Steiger et al., 2014) and time-continuous. For example, information recorded in each ring of a tree-ring proxy represents the average conditions of temperature and precipitation in that year. Furthermore, temporal resolutions of existing proxies are usually 1, 10 or even 100 yr (Saltzman, 2002; Yu et al., 2007). Limited by the time-averaged nature and temporal resolutions of proxies, time-intervals of PDA are usually 1 or 10 yr currently; these time intervals are far greater than the time steps and predictability of climate models (Lorenz, 1963, 1969, 1982; Kalnay, 2003; Reichler and Roads, 2003; Bhend et al., 2012).

(2) Long-term integration is a notable feature in PDA. The target of PDA is to reconstruct interannual, decadal or centennial climate change over hundreds of years or longer, whereas DA in the fields of atmosphere science, ocean science and land surface science mainly focuses on the prediction of the atmosphere, ocean and land surface conditions over a short period of time in the future (e.g., in the next 6 h, 24 h, 3 d, 1 week, or 1 month). Therefore, PDA has a notably higher requirement in computing performance and is more time consuming than DA in the fields of atmosphere science, ocean science and land surface science.

(3) In the context of climate research with long-term integration, initial conditions have minor impacts, if any, on the results because the effects of initial conditions will gradually attenuate in time due to the chaotic nature of the atmosphere (Chou, 1983). Huntely et al. (2010) had conducted a PDA experiment and found that no difference can be found between the DA results with a DA time-interval of 100 model time-steps and the results without DA; that is, the effects of initial conditions are lost long before the end of the simulation cycle (integration of 100 model time-steps); therefore, updating the initial conditions using PDA with longer DA time-intervals (far greater than 100 model time-steps) becomes dispensable. Some PDA studies with coupled climate models and pseudo-proxies conducted by Bhend et al. (2012), Annan et al. (2012) and Steiger et al. (2014) have demonstrated that in the context of PDA using time-averaged observations, little to no improvements of past climate estimations can be obtained by the analysis using the initial conditions to generate the following year's background estimate.

Influenced by these special aspects of PDA, we could not arbitrarily apply the DA methods that are appropriately used in the fields of atmosphere science, ocean science and land surface science to PDA (Widmann et al., 2010; Hakim et al., 2013); instead, we were required to improve or revise current DA methods to the special aspects of PDA to study interannual, decadal and even centennial climate variability over large spatial and temporal scales.

2.3 Introduction of three PDA methods

2.3.1 Nudging

Nudging is a sequential DA method that uses a dynamic relaxation to adjust a model toward observations through adding an artificial forcing-term to the governing equations of the model (Kistler, 1974; Hoke and Anthes, 1976). Briefly, the artificial forcing-term is proportional to the difference between the observations and the equivalent quantity computed by the integration of the state equations. The effects of nudging include the following: (1) model forecasts will approximate to the available observations, and (2) dynamical coordination among various variables in the model can be guaranteed. In addition, the adjusted model forecasts in this cycle of simulation serve as the initial conditions in the next cycle of simulation to improve the prediction skill of the model.

The DA method that von Storch et al. (2000) first introduced into paleoclimatology is nudging. von Storch et al. (2000) compared DA results with proxy-based reconstructions and GCM simulations to demonstrate the applicability and superiority of DA in paleoclimatology. Compared with variational methods and ensemble methods, the nudging method shows some advantages, including simplicity, effectiveness and easy implementation. The advantages of nudging can be attributed to the following: (1) nudging does not require a linear model operator as in the case of Kalman filter, and (2) nudging does not require an adjoint model as in the case of the three-dimensional variational method; thus, nudging is more suitable for DA with complex, nonlinear and practical models, for example, coupled climate system models (Widmann et al., 2010). The nudging method, however, also has two obvious disadvantages, namely, (1) it cannot assimilate the observations that models cannot forecast. It requires first converting the observations into forecasted variables before assimilating this type of observation. In addition, (2) the assignment of the relaxation factor in the forcing-term lacks a theoretical basis because it is generally determined based on experiences and variables of interest.

2.3.2 Particle filter

The particle filter method (PF) proposed by Gordon et al. (1993) is a Bayes estimation algorithm based on the Monte Carlo method that performs the posterior probability density function (PDF) via a number of weighted random particles in state space (Li and Bai, 2010). The estimated posterior PDF will be equal to the real posterior PDF if the number of particles used is as high as possible. The PF is suitable for state estimation problems of nonlinear and non-Gaussian systems because it can obtain approximately optimal numerical solutions using optimal filter based on a physical model rather than based on an approximate model produced by linearizing the physical model (Pan, 2006).

The application experience of the PF in PDA can be roughly divided into two stages. Prior to 2011, a simplified or degenerated PF was used in paleoclimate research (Goosse et al., 2006a, 2006b, 2008, 2009, 2010; Crespin et al., 2009; Widmann et al., 2010). In those studies, although the critical processes of standard-PF, such as prediction, updating and resampling, were also performed in the simplified-PF or the degenerated-PF, the greatest difference between the simplified-PF or the degenerated-PF and the standard-PF is that the updated states in this period were represented by only the particle with a state closest to that of the observations. This particle is regarded as the optimal particle in this period. In addition, the resampling process in the simplified-PF or the degenerated-PF is very simple because the states of the optimal particle in this cycle of simulation are directly treated as the initial conditions of the next cycle of simulation. The standard-PF always shows particle degeneracy and particle impoverishment; therefore, it is easy to consider that these problems may become more serious in the simplified-PF or the degenerated PF; theoretically, this may further lead to the DA skill becoming even worse. However, several PDA studies (Goosse et al., 2006a, 2006b, 2008, 2009, 2010; Crespin et al., 2009; Widmann et al., 2010) have shown that although the simplified-PF or degenerated-PF is simple, a satisfactory skill level still can be achieved in PDA studies using those two methods, even with fewer numbers of particles (e.g., only 11 particles were used in Widmann et al., 2010), under the constraint of high-quality proxies. This result confirmed the availability and superiority of DA in paleoclimatology. Moreover, to solve the serious degeneracy and impoverishment associated with the simplified-PF, Dubinkina et al. (2011) used an advanced-PF with residual resampling to improve reconstructions of past climate change. Dubinkina et al. (2011) showed that the advanced-PF demonstrated a significant improvement in performance compared to the simplified-PF. Annan and Hargreaves (2012) confirmed this conclusion once again based on a supplementary experiment of Dubinkina et al. (2011). Dubinkina et al. (2011), Annan and Hargreaves (2012) created a new situation of PF in PDA, which led to a number of PDA studies (Goosse et al., 2012; Loutre, 2012; Dubinkia and Goosse, 2013; Mathiot et al., 2013; Mairesse et al., 2013; Klein et al., 2014).

2.3.3 *Ensemble square root filter*

Ensemble square root filter (EnSRF) is a deterministic DA algorithm that does not rely on the perturbation of observations and was first proposed by Whitaker and Hamill (2002) based on ensemble Kalman filter (EnKF) (Evensen, 1994, 2003). The key concept of EnKF is to use the Monte-Carlo method to compute the background error covariance; this allows us to use the ensemble simulation method to solve the background error covariance issue, which makes it difficult to estimate and forecast in practice; thus, EnKF can be applied to the DA experiments with non-linear models and can also reduce the calculated amount in DA.

Dirren and Hakim (2005) improved the EnSRF for assimilating time-averaged observations instead of instantaneous observations and then implemented a PDA experiment with the Lorenz98 model to demonstrate the effectiveness of the proposed method in PDA. The study conducted by Huntley and Hakim (2010), which employed EnSRF, indicated that in PDA, no significant differences were found for assimilating with a lower number of proxies with better spatial distribution or assimilating with a greater number of proxies with random spatial distribution. This result revealed that the DA skill does not increase with the number of proxies used; meanwhile, the spatial distribution of proxies also plays an important role in DA. This fact can serve as a theoretical guide for selecting potential sites of proxies prior to proxy collection. Two PDA experiments conducted by Pendergrass et al. (2012), which also employed EnSRF, showed that the greater the difference between the temporal resolution of the model variables and that of the proxies, the worse the DA skill, and vice versa. Therefore, in PDA, choosing the proxy with the most appropriate temporal resolution from a large number of existing proxies according to the objectives is a necessary prerequisite to improve the DA skill. Steiger et al. (2014) compared the results generated from a PDA experiment using EnSRF with those reconstructed by using principal component analysis (PCA), which is a traditional method for reconstructing the temperature field. Their study showed that the PDA results were superior to those of PCA and that, in particular, more significant correlations can be found between the PDA results and the real temperature fields in regions with sparse proxy data.

2.3.4 *Development history of PDA*

In this section, we summarize and review the development history of PDA. In general, PDA has already experienced three development stages from 2000 to the present.

The first stage was from 2000 to 2005. In this stage, DA was tentatively introduced into the paleoclimate community. Nudging and FSV, two DA methods with relatively simple theories, played dominant roles in PDA in this stage. The theoretical basis of the two methods was developed in the 1970s (Kistler, 1974; Hoke and Anthes, 1976); thus, these two DA methods were gradually replaced by some more advanced DA methods within the context of atmosphere, ocean, and land surface DA. The two DA methods, although simple, successfully introduced the concept of DA to paleoclimatology; the study conducted by von Storch et al. (2000) is also considered a pioneering contribution to the field of PDA.

The second stage was from 2006 to 2010. In this stage, some advanced DA methods, such as EnSRF and PF, were introduced into the field of PDA. Some PDA numerical experiments of EnSRF were conducted using conceptual climate models rather than coupled climate system models; we should note that PDA experiments using coupled climate system models are more meaningful and practical than those using conceptual climate models. Moreover, although PF was applied to several PDA studies with a coupled climate system model (LOVECLIM) (Goosse et al., 2006a, 2006b, 2008, 2009, 2010), the PF method in those studies was a simplified-PF rather than the standard-PF. Overall, in this stage, the applicability of advanced DA methods in PDA was preliminarily explored and verified. Typical studies effectively addressed some scientific problems to a certain extent, and those studies were also beneficial to the PDA improvement in the next stage.

The third stage was from 2011 to the present. In this stage, substantive improvements of PF in PDA included the following: (1) the PF algorithm used in PDA was standard-PF, (2) the model operators employed in PDA were coupled climate system models, and (3) the resampling methods of PF were more efficient. These improvements commonly improved the estimation skill of PDA. In addition, in this stage, the application directions of PDA became more diverse than those of PDA in the first and second stages. Compared with the prosperous development of PF in PDA, EnSRF did not receive significant attention in this stage. It should be noted, however, that EnSRF is a variant of EnKF and that EnKF always shows better convergence and stability than PF in DA (Zhou et al., 2006; Han and Li, 2008); thus, EnSRF is a good choice if a PDA experiment is limited by computing resources, but we still want to achieve convergence and stability as much as possible. Moreover, the notable nature of PDA is the long-term integration (hundreds and even thousands of years) with an ensemble of many simulations, which always requires a large amount of computing resources. From this point of view, similar to PF, we believe that EnSRF will attract more attention in the PDA community in the future.

3. Underlying problems with PDA

Although the remarkable achievements of PDA can be observed in both theory and application during the last dozen years, in contrast to the complete architecture of DA in atmospheric, oceanic and land surface science, at present, some underlying problems of PDA can still be easily identified.

(1) The spatial distribution of existing proxies is uneven and sparse, and an obvious diversity can also be easily observed among existing proxies. These features are extremely apparent in typical proxy datasets produced by Mann et al. (2008, 2009) (Figure 2). The spatial distribution of observations has a significant influence on the estimation skill of DA. In general, for some regions that are located far away from observations, such as the southern hemisphere and marine realms, updated DA results in those regions always show little to no improvement because long-range “spurious correlations” must be considered in DA. Covariance localization and observation localization (Houtekamer and Mitchell, 2001; Annan and Hargreaves, 2012; Anderson and Lei, 2013; Han et al., 2015) are two feasible solutions for addressing the problem of long-range “spurious correlation” in DA; however, they can also lead to some non-optimized model states. In addition, a DA algorithm that can effectively incorporate proxies of various temporal resolutions and types into the same assimilation process is still in the development stages. Moreover, accurately quantifying some proxies with qualitative characteristics (e.g., historical documents) (Zhang and Jiang, 2004; Su et al., 2014) so that those qualitative proxies can be integrated into the numerical calculation of DA is a very difficult endeavor.

(2) Forward models of proxies are difficult to construct or lack explicit expression. To date, PDA observations have solely been proxy-based temperature reconstructions, i.e., product data reconstructions. The observation operator in this type of DA is only a simple transformation matrix because the quantity of observations is the same as that of the model used for the simulation. This assimilation strategy is known as indirect DA (Li, 2014). In the field of DA, in fact, assimilating original observations (direct DA) is more respected by researchers than assimilating product data (e.g., proxy-based reconstructions) because additional uncertainties may be brought into the products during the reconstruction process using proxies and statistical methods. Therefore, assimilating original observations should be the focus of the next phase of PDA. In addition, a crucial issue to directly assimilate original observations is that we must rely on forward models of various proxies. In view of the current situation, however, some problems associated with forward models of various proxies are still apparent, including the following: (1) many forward models are difficult to construct or lack explicit expression, and (2) the credibility and applicability of some forward models have not yet been tested. At present, only tree-ring proxies have a relatively mature forward model (Vaganov, 2006), and its applicability in PDA has already been validated (Breitenmoser et al., 2014). A forward model of stable isotope $\delta^{18}O$ in precipitation has been proposed in some studies (Sturm et al., 2005; Fischer, 2006; Zhang et al., 2009); however, so far, its applicability in PDA has not yet been verified. Forward models related to other types of proxies are still in the research stage, or require improvement. Overall, the lack of appropriate forward models is a bottleneck restricting the further

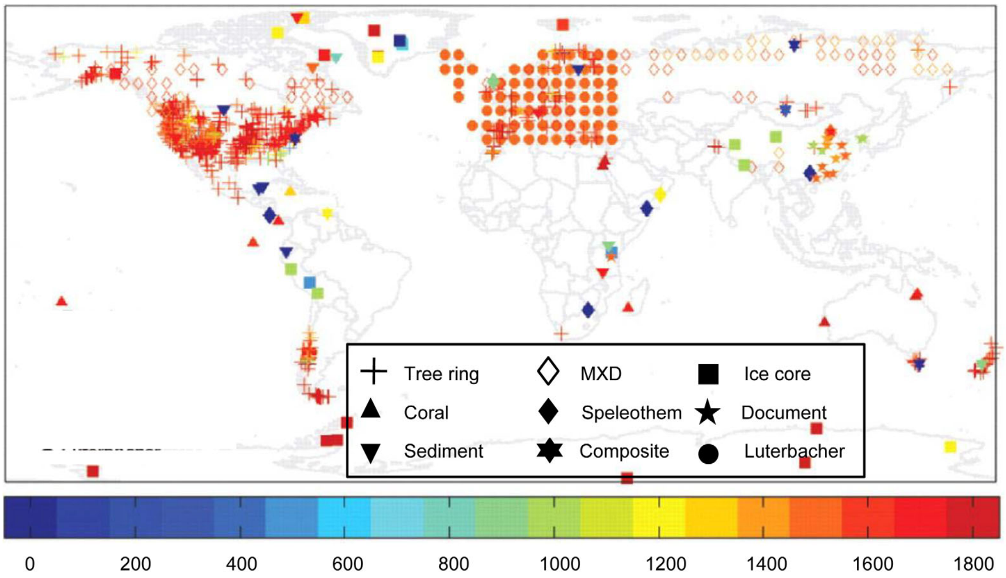

Figure 2 The spatial distribution of existing proxies screened from the NOAA Paleoclimatology Dataset (Mann et al., 2008). Nine different proxy types are denoted with different symbols as shown in the map. Beginning dates of proxy records are represented by color scale. "Luterbacher" denotes surface temperature reconstructions based on a composite of proxy, historical, and early instrumental data (Luterbacher et al., 2004). MXD: tree-ring maximum latewood density.

development of PDA (Widmann et al., 2010; Bhend et al., 2012; Steiger et al., 2014).

(3) Uncertainties of initial conditions and forcings are significantly greater in PDA than in DA for modern climate research. In modern climate research, initial conditions and forcings are obtained from instrumental data, which generally show higher accuracy and lower uncertainty; however, initial conditions and forcings of paleoclimate research are solely derived from proxy-based reconstructions, which generally exhibit lower accuracy and higher uncertainty. Smerdon et al. (2011b) and Smerdon (2012) reported that signal-to-noise ratios (SNRs) of proxies on the order of 0.25–0.5 (by standard deviation) are representative of the actual noise level of real-world conditions. The SNR of pseudo-proxies in PDA experiments conducted by Steiger et al. (2014) was also set to 0.5. Therefore, the uncertainties of initial conditions and forcings in PDA are obviously greater than those of DA for modern climate research; thus, the expected skill of past climate estimations may not be guaranteed.

(4) Verification of PDA results is difficult to implement. Verification of DA results has become more difficult in PDA due to a lack of relatively credible references because actual past climate states could not be accurately captured and measured by instruments. Before the instrumental period (approximately 1850 to present), the accuracy of PDA results (Bhend et al., 2012) maybe verified indirectly only through comparing them with other proxy-based reconstructions or climate model simulations.

(5) Reconstructing time-scales in many studies of PDA are relatively short. In the current PDA studies using either the PF method or the EnSRF method, the reconstruction time-scales in those studies are not too long (no more than the past 1000 years) due to the limited computing power and the basic concept of ensemble prediction behind DA. We should note that, in fact, reconstructing past climates using PDA for longer periods, such as the Holocene and the mid-Holocene, is more beneficial for us to obtain more valuable information on past climate change, and using such information to recognize the modern situation of climate change and predict future scenarios of climate change is more practical.

4. Prospects of PDA

PDA was introduced in 2000, and although its vigorous development is obvious, at present, PDA is still faced with the problems described in Section 3. However, as more researchers set their sights on PDA, we should have sufficient reason to believe that (1) the theory and application of PDA will become increasingly more mature, similar to DA of the atmosphere, oceans, and land surface, and that (2) PDA results used for past climate interpretations will become increasingly more credible and accurate. To achieve the above objectives, the following aspects should be addressed:

(1) Special attention should be given to estimating the observational errors of various proxies. The further study of PDA should focus not only on the discovery and collection of more proxies but also on estimating the observational errors in proxies because the observational errors directly affect the assimilation skill of PDA. Instrumental errors may be accurately estimated through instrument alignment

and correction, as well as error analysis in post-processing analysis; however, how to rationally determine the representative errors of observations is a complex problem, and solving this problem relies on the proxy characteristics and environments.

(2) More efficient PDA methods still require further exploration. PF and EnSRF, two frequently-used PDA methods, are modified from the standard-PF and the standard-EnSRF in atmosphere, ocean, and land surface DA, respectively, to assimilate time-averaged observations. We should note that, in addition, more efficient PDA methods still require exploration because these two PDA methods do not completely consider the characteristics of PDA in the context of modification. The diverse family of DA has a number of branches; hence, there may be one or several DA methods suitable for PDA; for example, a smoothing method, an alternative branch of DA with respect to filter methods, has high potential in PDA as it does not require sequentially updating state variables and initial conditions in time, in contrast to filter methods(Widmann et al., 2010).In addition, although variational methods are not suitable for PDA, ensemble methods (e.g., EnKF) in PDA always show effective performances (Widmann et al., 2010). Therefore, perhaps a new situation for variational methods in PDA can be developed if one can propose a novel DA method that combines ensemble methods with variational methods. Ensemble four-dimensional variational assimilation, a novel DA method proposed by Tian et al. (2008, 2009, 2011), should receive attention in regards to its potential and application in PDA because it inherited the advantages of the ensemble methods and the four-dimensional variational method.

(3) The construction of many more forward models and the improvement of the performances of some existing forward models are two important tasks. These tasks require not only assimilating proxies in the northern hemisphere and over land but also, more importantly, the assimilation of proxies in the southern hemisphere and in the marine realm to obtain more practical estimations of large-scale climate variations. At present, marine proxies mainly include coral and marine sediment. Forward models that relate indices of these proxies to climate variables, such as temperature and precipitation, have not yet been developed; instead, there are only relatively simple empirical models (or statistical models). Therefore, we have to perform two important tasks, including (1) construction of forward models related to coral and marine sediment and (2) validation of these forward models so that these marine proxies can be incorporated into PDA as soon as possible.

(4) To realize the goals proposed in paragraph (3), we should not only successfully construct and validate various forward models of proxies but also propose a theoretical framework on how to assimilate multi-source observations and multi-timescale observations within the same DA process. In general, various proxies show different temporal resolutions. For example, the temporal resolutions of loess sediment and marine sediment are far greater than 1 year, and the highest temporal resolution of these two proxies can reach 10 years. Therefore, assimilating various proxies with different temporal resolutions within the same DA process is still a key issue in PDA.

(5) Simultaneously estimating both model states and model parameters using PDA is a promising approach to be developed in the future. Reconstruction of past climate states is just one of the functions of DA. The other important function of DA is to optimally estimate climate model parameters. Simultaneous estimation of both model states and model parameters is relatively mature in the fields of land surface and hydrological science (Moradkhani et al., 2005; Qin et al., 2009; Nie et al., 2011; Liang et al., 2013; Xie and Zhang, 2013; Bi et al., 2014; Zhang et al., 2015). To optimize model parameters in those fields, DA can improve and perfect the parameterization schemes of models in terms of the physical mechanisms and therefore improve the regional adaptability and simulation skills of those models (Zhang et al., 2015). In the context of PDA with long-term simulation, simultaneous estimation of both model states and model parameters using DA allows us to investigate the temporal heterogeneities of model parameters over a relatively long period of time and thus may help us to optimize those parameters. In addition, models with optimized parameters may show decreased uncertainty and therefore can help researchers improve both the simulation skill of climate models used for studying past climate change and the predictive ability of climate models used for future climate change projections.

Acknowledgements *The authors thank scientific editors of the journal for their helpful instructions, and also thank sincerely the three anonymous reviewers for their valuable suggestions and comments. This work was supported by the National Natural Science Foundation of China (Grant Nos. 91425303, 91225302) and the Chinese Academy of Sciences Interdisciplinary Innovation Team Project.*

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