The Stochastic Calculus Reformulation of Data Assimilation: on Scale

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10 **Abstract.** The understanding of uncertainties in Earth observations and simulations has been hindered by the spatial scale

problem. In addition, errors caused by spatial scale change are an important part of uncertainty in data assimilation (DA).

However, these uncertainties exceed the abilities of current theory. We attempted to address these problems. First, measure

theory was used to propose a mathematical definition such that spatial scale is the function output of a measure given that its

referential element and representative region are confirmed, and then the Jacobian matrix was used to describe the change of

15 scale. Second, the scale-dependent variable was defined to further consider the heterogeneities. Last, under the Bayesian

framework of DA, the scale-dependent uncertainty was studied based on stochastic calculus. The result formulated the scale-

dependent error in DA. If we restrict the scale to a one-dimensional variable, the variation range of this type of error is

proportional to the scale gap. Furthermore, assuming the observation operator is stochastic, we developed an example by

introducing the stochastic radiative transfer equation. The new methodology will extend the recognition of the uncertainty in

20 DA and may be able to address the scale problem.

1 Introduction

Scientists have devoted considerable attentions to understanding uncertainties in Earth observations and simulations.

However, uncertainties caused by spatial scale changes have yet to be fully addressed. Empirical studies have been

conducted only recently (Crow et al., 2012; Gruber et al., 2013; Hakuba et al., 2013; Ran et al., 2016; Huang et al., 2016).

25 Studies found that the absolute bias between point- and footprint-scale measurements of soil moisture is highly significant

(Li and Liu, 2016) and that the uncertainty increases with increases in the difference between spatial scales (Famiglietti et al.,

2008). This uncertainty problem, also known as the "spatial scale problem", may result in significant errors in understanding

geographical parameters.

The uncertainty caused by the scale problem (for brevity, the term "scale" will be used to refer to spatial scale below) is

30 actually derived from the strong spatial heterogeneities (Miralles et al., 2010; Li, 2014) and irregularities (Atkinson et al.,

2000) of geographical parameters across different scales, and both the spatial heterogeneities and irregularities vary nonlinearly with scale. In addition, the scale problem is closely related to dynamic process variations in land surface systems. For example, saturated hydraulic conductivity has different characteristics at the micro- and macro-scales (Gim énez et al., 1999), and some essential soil structures also present complex architectures from the molecular scale to the landscape scale

5   (Lin et al., 2010). Similarly, the parameters of long-term water balance simulations (Merz et al., 2009), the factors controlling the radiative transfer process of vegetation (Jacquemoud et al., 2009), and the environmental conditions that influence the spatial correlations of surface soil moisture (Ryu and Famiglietti, 2006) also vary with scale. Furthermore, the scale problem is also caused by the scale variations of basic physical principles. For example, the validity of Planck's law is dependent on the scale unless surface of blackbody is isothermal (Li, et al. 1999). Focusing on the above researches may

10 substantially improve the understanding of the scale problem. However, these phenomena cannot be explained by ordinary dynamic models because the main factor, scale, is not fully cognitive, and the availability of those researches only works in case studies, which may not be generalizable or appropriate for the theoretical study of scale.

As a generalized methodology for reducing and controlling uncertainties (Li, 2014), data assimilation (DA) remain traps in the scale problem. DA is a dynamic process of information fusion between outputs of numerical model and multi-source

15 direct or indirect observations, and it generally accepted that DA can typically generate creative solutions to the problem of how to use available observational information to improve the predictability of geophysical parameters without any sacrifices to dynamic mechanisms (Talagrand, 1997; Li et al., 2007; Li and Bai, 2010). Recently, scientists have recognized that DA is even a "paradigm" change (Li, 2014) and that a correct characterization of uncertainty will substantially improve the validity of simulations and the accuracy of observations. However, studies of DA uncertainties also encounter the scale

20 problem. The forcing data and parameters of the dynamic models are typically collected by diversified Earth observation techniques or data products; therefore, considerable mismatches problems among the representative spaces may arise. Furthermore, those problems is even more outstanding among the model units and representative spaces of measurements considering that both the dynamic and observation models in DA are likely strongly nonlinear and complex.

Unfortunately, there is still no precise and serious definition of "scale", and its influence on DA uncertainties remains

25 unclear. We believe that the scale problem should begin with an integrated study of all random evolutions of the parameter in its probability distribution space. DA also stresses an integrated understanding of the probability distribution function (PDF) of the state space, which results in an estimation of the first and second moments (data value and error information). By this logic, unlike deterministic processes, a stochastic process-based method can offer advantageous solutions to this problem. However, a conceptual reformation of uncertainty may arise when both the scale problem and stochastic models

30 are introduced in DA.

In this study, we attempt to answer the following questions: what is the mathematical definition of scale, and how does the scale influence the uncertainties of DA? Because these questions cannot be explained using the traditional rules of DA, we look to new theories that have not been considered in DA. We first define an essential concept that will determine the subsequent study. The next section introduces some measure concepts to describe scale, and Sect. 3 presents the Ito process-

formed geographical parameters with respect to the change of their scales. Second, the DA system is reformulated based on the above concepts and stochastic calculus. In Sect. 4, we establish the Bayesian description of DA with time- and scale-dependent stochastic processes and investigate the impact of scale changes on the posterior probability of the system state. An example of this impact is also presented by introducing a stochastic radiative transfer equation (SRTE). Comments and

5   prospects are summarized in the last section.

2 Scale

An accurate conception of scale is extremely beneficial for the study of Earth observations and simulations. However, except for an intuitive conception (Goodchild et al., 1997) and certain qualitative classifications of scale (Vereecken et al., 2007), it is difficult to find a strict definition of scale. This gap partially reflects the complexity of this problem and requires

10   corresponding mathematical tools to illuminate "scale". Because scale is highly dependent on the geometric features of observational region, we first introduce several basic concepts of measure theory.

2.1 Measure and measure space

Let Ω be an arbitrary nonempty space. $\mathcal{F}$ is a $\sigma-field$ of subsets of Ω and satisfies

    (i) $\Omega \in \mathcal{F}$, and the empty set $\Phi \in \mathcal{F}$;

15   (ii) $A \in \mathcal{F}$ implies its complementary set $A^c \in \mathcal{F}$;

    (iii) $A_1, A_2, \cdots \in \mathcal{F}$ implies their union $A_1 \cup A_2 \cup \cdots \in \mathcal{F}$.

If a set function μ on $\mathcal{F}$ satisfies the following conditions:

    (1) $\mu(A) \in [0, \infty)$ and $\mu(\Phi) = 0$; and

    (2) If $A_1, A_2, \cdots \in \mathcal{F}$ is a disjoint sequence, then if $\bigcup_{k=1}^{\infty} A_k \in \mathcal{F}$, the countable additivity of μ is

20

$$\mu\left(\bigcup_{k=1}^{\infty} A_k\right) = \sum_{k=1}^{\infty} \mu(A_k),$$

μ is then called the **measure**. In addition, if $\mu(\Omega) = 1$, μ can be replaced by the probability measure P, and if μ is

finite, P can be calculated as $P(A) = \mu(A) \big/ \mu(\Omega)$. The triple $(\Omega, \mathcal{F}, \mu)$ and $(\Omega, \mathcal{F}, P)$ are the measure space and

probability measure space, respectively. Additional details on measure theory can be found in literatures (Billingsley, 1986).

25   In measure theory, Ω is typically a one-dimensional space, and a multi-dimensional space is formulated by the product spaces. In this study, to avoid an overly complex expression, we define the observational region as a one-dimensional

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measure space with $\Omega \subset R^2$, in which the abstract information about the region of interest is conveyed. In this case, the measure correspondingly turns into $\mu(A) = (a,b)^T, a,b \in [0,\infty)$, which should also obey the countable additivity. This simplification will not negatively affect the definition of scale.

2.2 Definition of scale

5 To connect the measure and scale, the following measures in Earth observation will be considered in advance.

(i) Measure in a line (Lebesgue measure): Let $\left(\Omega, \mathcal{F}, \mu : \Omega = [\alpha,\beta] \subset R\right)$ be a one-dimensional observational region.

$\forall A = [a,b] \in \mathcal{F}$, measure $\mu_i(A) = b - a$, and probability measure $P_i(A) = \dfrac{b-a}{\beta-\alpha}$.

(ii) Measure of a single point measurement: This measure is permanently zero under the condition of the Lebesgue measure. However, in the real world, the representative space of a single point measurement cannot be ignored, and

10 thus, any single point measurement with an absolute zero measure cannot exist.

(iii) Measure of the remote sensing observations: Assuming that a pixel of a remote sensing image is a rectangle,

$\alpha = \left(\alpha_1, \alpha_2\right)^T$, $\beta = \left(\beta_1, \beta_2\right)^T$, $a = \left(a_1, a_2\right)^T$, $b = \left(b_1, b_2\right)^T$, and

$\forall A = [a,b] = [x,y : a_1 \leq x \leq b_1, a_2 \leq y \leq b_2] \in \mathcal{F}$, the measure of an Earth observational region

$\left(\Omega, \mathcal{F}, \mu : \Omega = [\alpha,\beta] = [x,y : \alpha_1 \leq x \leq \alpha_2, \beta_1 \leq y \leq \beta_2] \subset R^2\right)$ is $\mu_{iii}(A) = b - a = \left(b_1 - a_1, \quad b_2 - a_2\right)^T$.

15 Here, the measure is an equivalent expression of the spatial resolution of the remote sensing image.

(iv) Measure of the disc measurement: Due to the conditions (ii) and (iii) of $\mathcal{F}$, it is better to count the circumscribed square of the disc as the subsets of Ω. Using the same notation as in measure (iii), this measure of disc measurement

is $\mu_{iv}(A) = \int_{a_1}^{b_1} dx \int_{-\sqrt{r^2-(x-c_1)^2}+c_2}^{\sqrt{r^2-(x-c_1)^2}+c_2} dy = \dfrac{\sqrt{\pi}}{2}\left(b_1 - a_1, \quad b_2 - a_2\right)^T$, where $b_1 - a_1 = b_2 - a_2$, $r = \dfrac{(b_1 - a_1)}{2}$,

$c_1 = \dfrac{(b_1 + a_1)}{2}$ and $c_2 = \dfrac{(b_2 + a_2)}{2}$. This measure is proportional to the area of the disc.

20 (v) Measure of the footprint measurement: The representative space of this measurement is any bounded closed domain. Just like measure μ_{iv}, we also see the area of the domain as its measure $\mu_v(A) = \iint_A dxdy$. Because this domain is arbitrary and it is difficult to calculate its area directly, we use double integration by substitution to change the variables; define the substitution functions $x = x(u,v)$ and $y = y(u,v)$, which must be injective and continuously first-order differentiable, $\mu_v(A) = \iint_A dxdy = \iint_\Lambda |J(u,v)| dudv$, where the Jacobian determinant

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$$|J(u,v)| = \begin{vmatrix} \partial x / \partial u & \partial x / \partial v \\ \partial y / \partial u & \partial y / \partial v \end{vmatrix} \neq 0$$ and Λ is a bounded closed domain in the $u-v$ coordinate plane, the area of

which can be easily calculated. Thus, the measure μ_v is proportional to the area of Λ. From the definition of the

footprint measure, the measures μ_{iii} and μ_{iv} are special cases of μ_v.

Implicitly, there are spatial coordinates with a given **referential element** in each of the above measures. For example,

5 both μ_i and μ_{ii} are based on the referential element of unit length, and μ_{iii} and μ_{iv} are based on the unit area. Thus, we

may require that the measures of the one- and two-dimensional unit intervals are $\mu([0,1]) = 1$ and

$\mu\left(\left[(0 \quad 0)^T, (1 \quad 1)^T\right]\right) = (1,1)^T$, respectively. The value of the measure depends strongly on the design of the referential

element. Therefore, if the two-dimensional referential element is counted as $\mu\left(\left[(0 \quad 0)^T, \left(\dfrac{\sqrt{\pi}}{2} \quad \dfrac{\sqrt{\pi}}{2}\right)^T\right]\right) = (1,1)^T$,

then $\mu_{iii}(A) = \dfrac{2}{\sqrt{\pi}}(b_1 - a_1, \quad b_2 - a_2)^T$ and $\mu_{iv}(A) = (b_1 - a_1, \quad b_2 - a_2)^T$, respectively. In addition, by introducing

10 the discrete point measure (Billingsley, 1986), which is based on a distinctive referential element, the measure of a single

point measurement will be greater than zero, but other measures are invalid. Additionally, if the spatial coordinates are

replaced by latitude and longitude coordinates, all of the above measures should be adjusted accordingly.

According to the above analysis, we define "**scale**" as the function output of a measure given that its referential element

and representative region are confirmed. That is, let A_0 be a given rectangular referential element, and μ is a measure; for

15 any representative region $A \in \mathcal{F}$, the scale is $s = \mu(A) = \iint_A \mu(A_0) dA_0 = \iint_A \mu(x,y) dx dy$. From a geometric

perspective, the measure refers to the shape of the observation region, and the scale further indicates the size of the region;

therefore, the scale increases with increases in the value of the measure.

We further demonstrate the change of scale. $\forall A_1, A_2 \in \mathcal{F}$, if there are two measures μ_1, μ_2 and two different scales

$s_1 = \mu_1(A_1) = \iint_{A_1} \mu_1(A_0) dA_0 = \iint_{A_1} \mu_1(x,y) dx dy$ and $s_2 = \mu_2(A_2) = \iint_{A_2} \mu_2(A_0) dA_0 = \iint_{A_2} \mu_2(u,v) du dv$.

20 Based on the technique of integration by substitution, we obtain

$s_1 = \iint_{A_1} \mu_1(x,y) dx dy = \iint_{A_2} \mu_1(x(u,v), y(u,v)) |J(u,v)| du dv$, where the substitutions $x = x(u,v)$ and $y = y(u,v)$

and the Jacobian determinant $\left| J(u,v) \right|$ have the same definitions as in measure (v). $J(u,v)$ represents the degree of geometric transformation from A_1 to A_2. In particular, if $J(u,v) = diag(\xi,\xi), \xi \in R^+$ and $\mu_1 = \mu_2$,

$$s_1 = \xi^2 \iint_{A_2} \mu_2 \left(x(u,v), y(u,v) \right) du dv = \xi^2 \mu_2 \left(A_2 \right) = \xi^2 s_2 , \qquad (1)$$

and s_1 and s_2 are then a **one-dimensional law** change.

5   If two scales follow the one-dimensional law, they are geometrically similar. This law simplifies scale as a one-dimensional variable that corresponds to the scale differences between most remote sensing images with various spatial resolutions. For example, for the measure of remote sensing observations, if $J(u,v) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ and $A^* = J \cdot A$,

$\mu_{iii}\left(A^* \right) = 2b - 2a = 2^2 \mu_{iii}\left(A \right)$. Then, these two scales $\mu_{iii}\left(A^* \right)$ and $\mu_{iii}\left(A \right)$ are in a one-dimensional law.

Figure 1 demonstrates the relationships between the referential element, measure and scale. The measure space
10   $\Omega = [\alpha,\beta] = [x,y : 0 \le x \le 4, 0 \le y \le 4]$ is regularly divided by a referential element defined with unit area. Let μ_{C1}, μ_{C2} and μ_{C3} be the measures of the disc measurements $C1$, $C2$ and $C3$, and μ_{D1}, μ_{D2} be the measures of the diamond measurements $D1$ and $D2$. Based on the definition of measure, $\mu_{C1} = \mu_{C2} = \mu_{C3}$ because they can be seen as an area calculation of an inscribed circle in a square region. However, the scale of $C2$ is not equal to the two other scales because of their different areas. However, their scales are in a one-dimensional law because the measures are identical and the Jacobian
15   matrices are diagonal. Similarly, we have $\mu_{D1} = \mu_{D2}$; their scales are also different but are in a one-dimensional law.
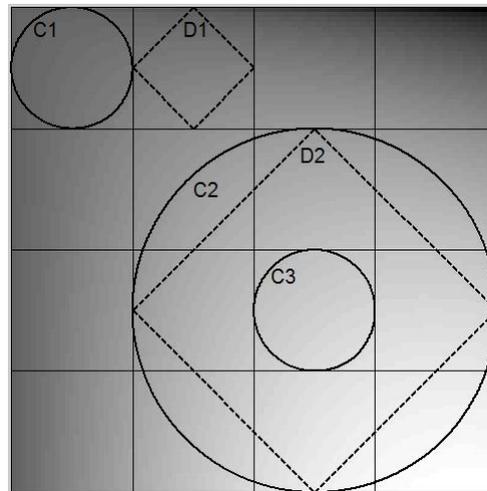

Figure 1. Diagram of the Relationships between the Referential Element, Measure, Scale and Variable.

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We further represent the scale by s, and $s_0 = \mu_0(A_0) = \iint_{A_0} \mu_0(x,y)dxdy = (1,1)^T$ represent the standard scale. In the next section, the system state and observations of DA will be presented as stochastic processes to investigate their evolution with the one-dimensional infinitesimals ds and dt.

3 Stochastic variables in DA

5 Let a real function $V(A)$ be the **variable** if it maps the measure space $(\Omega, \mathcal{F}, \mu)$ onto R. A variable is the measurement of a geographical parameter in a specific region, and $V(s,t) \to R$ denotes that the variable depends on time t and has a scale $s = \mu(A)$.

In Figure 1, if the pixel intensity is the value of a geographical parameter, the entire region is heterogeneous. A variable represents an ensemble average in a specific observational region with a specific scale. Therefore, the variables of $C1$ and
10 $C3$ are not equal considering that their observational regions are different, and the variables of $C2$ and $C3$ are also different because the scale changes. The former introduces the variables that vary with location, and the latter is a scale-dependent variable. Therefore, from the Earth observational perspective, a variable is a nonlinear and heterogeneous mapping function from the observational region to the set of real numbers at a given time.

The dynamic process of the variable clearly depends on time, and we further assume that the variable changes with spatial
15 scale in view of the scale effects. Furthermore, due to the uncertainties in Earth observations and simulations, it is reasonable to assume that the variable is random both in time and on the spatial scale span. Therefore, if the statistical properties of the variable are available, we can construct an explicit stochastic equation of the variable.

We introduce the time-dependent Ito process (See Sect. 4.2) as follows to define the variable process:

$$dV = p(t)dt + q(t)dW(t), \qquad (2)$$

20 where $p(t)$, $q(t)$ and $W(t)$ are the transition probability, volatility and Brownian motion (See Sect. 4.2), respectively. Similarly, the variable is supposed to evolve via a stochastic process for which the dynamic process and uncertainty are allowed to vary with scale:

$$dV = \varphi(s)ds + \sigma(s)dW(s), \qquad (3)$$

where $\varphi(s)$ and $\sigma(s)$ are the scale-based transition probability and volatility, respectively.

25 It should firstly notice that time is one-dimensional unidirectional, but the scale go forward or back on the condition that the scale follows the one-dimensional law. Secondly, the Brownian motion is valid only on the condition that the observation instrument is perfectly calibrated, which indicates that the instrument error of the geophysical parameter is only associated with random error and is free of systematic bias.

The variable of a forecasting model in DA can be expressed as Eq. (2), and if the dynamic model is differentiable,

$dV = \dfrac{\partial M_k}{\partial t_k} dt_k + q(t_k) dW(t_k)$, where the dynamic process is equivalent to the transition probability, and both t_k and the

subscript k denote discrete time. If the future of the system state is based solely on the present state, i.e.,

$x(t_{k+1}) = M_k \big(x(t_k) \big)$, the variable process is Markovian. In the analysis step of DA, the system state does not pertain to

5   time, and we assume that scale has a quantifiable impact on the uncertainties in this step; thus, both the system states and

observations can be defined by Eq. (3). In the following sections we will try to prove this hypothesis.

4 Reformulation of DA

The dynamic and observation operators of a DA system are typically deterministic models. Those models can be effectively

understood in a specific case study but are not applicable in an integrated theoretical study. We offered a solution to this

10   problem by introducing stochastic calculus. Recently, nonlinear dynamic models based on stochastic differential equations

(SDEs), such as the double-well model and stochastic Lorenz model (Miller et al., 1999; Eyink et al., 2004), were studied in

assimilation. In addition, a DA study based on stochastic processes (Miller, 2007) has been proposed. However, the theorems

of calculus based on stochastic processes (or stochastic calculus) are distinct from ordinary calculus; therefore, a theoretical

exploration of DA is essential.

15   In this section, based on the above definition of scale and the variables formed by the stochastic process, we reformulate

the expression of DA by employing basic stochastic calculus laws and further study how the scale influences the

uncertainties of DA.

4.1 Bayesian analysis of DA

We introduce the widely accepted Bayesian theorem of DA (Lorenc, 1995; Miller, 2007; Li and Bai, 2010) to investigate its

20   time- and scale-dependent uncertainties. In the following, we suppose that there is only one system state and one observation

in DA, and the results will be extended to a multi-variable DA at the end of this section.

Consider a nonlinear forecasting system described by

$$X^t \big(t_k \big) = M_{k-1:k} \big(X^t \big(t_{k-1} \big) \big) + \eta(t_k), \qquad (4)$$

where $M_{k-1:k}(\bullet)$, $X^t \big(t_k \big)$ and $\eta(t_k)$ represent a forecasting operator transiting the system state from the discrete time

25   $k-1$ to k, the true system state with prior PDF $p(X)$, and the white noise of the forecasting system at time k,

respectively. In addition, if a new observation is available at time k,

$$Y^o \big(t_k \big) = H_k \big(X^t \big(t_k \big) \big) + \varepsilon(t_k), \qquad (5)$$

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where $H_k(\bullet), Y^o(t_k)$ and $\varepsilon(t_k)$ represent the nonlinear observation operator, true observation with prior PDF $p(Y)$, and observational white noise at time k, respectively.

Comparing Eq. (4) and Eq. (2), it can be deduced that $M_{k-1:k}(\bullet)$ and $\eta(t_k)$ are associated with $p(t)$ and $q(t)$. However, Eq. (5) cannot result in the same conclusion as Eq. (2) because the observation operator is not a time-dependent dynamic model. Based on the reviews in Sect. 1, when the observation operator maps the system state to the observation space, a remarkable change may arise if the observation and state space scales differ. Thus, we assume that the observation operator $H(\bullet)$ is scale dependent in this situation.

Based on Bayes theorem, the posterior PDF of the state conditioned on the addition of a new observation into the system is

$$p(X|Y) = \frac{p(Y|X)p(X)}{p(Y)}, \qquad (6)$$

where $p(X|Y)$ is the posterior PDF and $p(Y|X)$ is a likelihood function. Therefore, the aim of DA is equivalent to finding the posterior PDF $p(X|Y)$.

4.2 Basic knowledge of stochastic calculus

In this section, we have incorporated some necessary concepts and theorems of stochastic calculus. All the classic theorems have been introduced without proofs; their detail derivations can be found in literatures (Itô, 1944; Karatzas et al., 1991; Shreve, 2005).

Compared with the ordinary differential and integral calculus, **stochastic calculus** is defined for integrals of stochastic processes with respect to stochastic processes, such as Brownian motion. **Brownian motion** is one of the simplest stochastic processes, and describes the physical phenomena such as random perturbations and irregular movements of microscopic particles subject to random forces. Brownian motion is named after the Scottish botanist Robert Brown, who observed continuous jittery motions of pollen suspended in water by a microscope. The Brownian motion W defined on a probability measure space $(\Omega, \mathcal{F}, P)$ is characterized as follows:

1) $W(0) = 0$.

2) $\forall t > s \geq 0$, the increments $W(t) - W(s)$ are independent.

3) $\forall t > s \geq 0$, $W(t) - W(s) \sim N(0, t - s)$.

The last two conditions represent that $\forall t_2 > s_2 > t_1 > s_1 \geq 0$, $W(t_2) - W(s_2)$ and $W(t_1) - W(s_1)$ are independent Gaussian random variable. Additionally, because Brownian motion is based on probability measure space, W pertains to probability measure P.

Lemma 1: $\forall s_0 > 0$, let $W^*(0) = W(s_0) - W(s_0), \cdots, W^*(s) = W(s_0 + s) - W(s_0)$; then, $W^*(s), s \geq 0$ is a Brownian motion.

Proof. First, $W^*(0) = W(s_0) - W(s_0) = 0$. $\forall s_{i+1} > s_i \geq 0, i = 1, 2, 3, \cdots$,

$$W^*(s_{i+1}) - W^*(s_i) = \left[W(s_0 + s_{i+1}) - W(s_0)\right] - \left[W(s_0 + s_i) - W(s_0)\right] = W(s_0 + s_{i+1}) - W(s_0 + s_i),$$

which means that the increments $\left[W^*(s_{i+1}) - W^*(s_i)\right]$ are equal to $\left[W(s_0 + s_{i+1}) - W(s_0 + s_i)\right]$. Therefore, $W^*(s), s \geq 0$ is a Brownian motion, with $E\left[W^*(s_{i+1}) - W^*(s_i)\right] = 0$ and $Var\left[W^*(s_{i+1}) - W^*(s_i)\right] = s_{i+1} - s_i$. □

Remark on Lemma 1: This Lemma is practical because scale is certainly greater than zero, which does not fit the definition of Brownian motion whereby the parameter should start at zero. The standard scale s_0 is associated with zero in Lemma 1; thus, it is logical to let $s = 0$ in $W^*(s)$. Lemma 1 further implies that $W(s), s \geq s_0$ is an equivalent expression of $W^*(s), s \geq 0$; therefore, in the following content, we use Brownian motion with a parameter starting at s_0 to define the scale-dependent variables, and some classic expressions should be changed slightly.

The stochastic process Eq. (3) is the differential form of **Ito process**, the integral form of which is

$$V(s) = V(0) + \int_0^s \varphi(u)du + \int_0^s \sigma(u)dW(u).$$

Theorem 1: For any Ito process defined as in Eq. (3), the quadratic variation accumulated up to s is

$$[V,V](s) = \int_0^s \sigma^2(u)du. \tag{7}$$

Remark on Theorem 1:

According to Lemma 1, Eq. (7) is

$$[V,V](s) = \int_{s_0}^s \sigma^2(u)du, \tag{8}$$

and the integral form of the Ito process (3) is

$$V(s) = V_0 + \int_{s_0}^s \varphi(u)du + \int_{s_0}^s \sigma(u)dW(u), \tag{9}$$

where V_0 is the initial value in s_0 and the drift of Eq. (9) is $V_0 + \int_{s_0}^{s} \varphi(u)du$.

As a distinguishing feature of stochastic calculus, the **quadratic variation** and **drift** can be regarded as stochastic versions of the variance and expectation, respectively. That is, variance and expectation are instances of their random variable counterparts with a certain integral path. Therefore, rather than being constants, quadratic variation and drift are more

5   complex.

The quadratic variation is expressed by the second-order variation of a stochastic process. Therefore, the quadratic variation for a continuous differentiable random variable is 0. Equation (7) highly relies on the volatility $\sigma^2(u)$, and thus, the quadratic variation varies with the integration path. Additionally, if the measure obeys the one-dimensional law, the stochastic variable in Eq. (9) is integrated over a one-dimensional continuous interval $[s_0, s]$. However, a more complex

10   situation is that the integral path is random, and thus, the general expression of Eq. (9) is the curvilinear integral

$V(s) = V_0 + \int_{L} \varphi(u)du + \int_{L} \sigma(u)dW(u)$, where L is an arbitrary path from s_0 to s .

Theorem 2 (Ito's Lemma): If the partial derivatives of function $f(u,x)$, viz. $f_u(u,x)$, $f_x(u,x)$ and $f_{xx}(u,x)$ are defined and continuous, and if $s \geq 0$, we have

$$
\begin{aligned}
df(s,V(s)) = {} & f_u(u,V(u))du + f_x(u,V(u))\sigma(u)dW(u) \\
& + f_x(u,V(u))\varphi(u)du + \frac{1}{2}f_{xx}(u,V(u))\sigma^2(u)du
\end{aligned}
, \tag{10}
$$

15   where $V(s)$ is defined in Eq. (9). The integral form of (10) is

$$
\begin{aligned}
f(s,V(s)) = {} & f(0,V(0)) + \int_0^s f_u(u,V(u))du + \int_0^s f_x(u,V(u))\sigma(u)dW(u) \\
& + \int_0^s f_x(u,V(u))\varphi(u)du + \frac{1}{2}\int_0^s f_{xx}(u,V(u))\sigma^2(u)du
\end{aligned}
, \tag{11}
$$

and considering Lemma 1, Eq. (11) becomes

$$
\begin{aligned}
f(s,V(s)) = {} & f(s_0,V(s_0)) + \int_{s_0}^s f_u(u,V(u))du + \int_{s_0}^s f_x(u,V(u))\sigma(u)dW(u) \\
& + \int_{s_0}^s f_x(u,V(u))\varphi(u)du + \frac{1}{2}\int_{s_0}^s f_{xx}(u,V(u))\sigma^2(u)du
\end{aligned}
. \tag{12}
$$

Ito's Lemma is typically used to build the differential of a stochastic model with Ito processes. In this section, Ito's Lemma

20   is applied to study the scale-dependent relationship between the observation operator and system state, and the uncertainties caused by scale in the analysis step.

4.3 Stochastic calculus for DA

Next, we deduce the stochastic calculus results for DA based on the above assumptions and theorems. We first assume that,

Assumption 1: The measures of the system state and observation in DA obey the one-dimensional law defined in Sect. 2.2.

5   In the forecasting step, **Assumption 2**: The simulation units of the model equal the scale of the system state, and both are constant.

In the analysis step, **Assumption 3**: The parameters (including the system state and observation) and observation operator are scale dependent; only one observation is added into the DA system at a time, and the system states and observations at different times are scale independent.

10   Considering assumption 2, the forecasting step is explicitly free of scale, and thus, Eq. (2) is adequate to describe this step.

Based on assumption 3, the analysis step relates to scale; thus, some basic definitions should be presented in advance. According to Eq. (3), the system state and observation in the analysis step are respectively expressed as

$$dX = \varphi_X(s)ds + \sigma_X(s)dW(s), \tag{13}$$

and

15
$$dY = \varphi_Y(s)ds + \sigma_Y(s)dW(s), \tag{14}$$

where $\varphi_X(s)$, $\sigma_X(s)$, $\varphi_Y(s)$ and $\sigma_Y(s)$ represent the scale-dependent transition probability and volatility of system state X and observation Y, respectively. The scale-dependent observation operator is $H(s, X(s))$, which means that the observation operator and its parameters are both susceptible to scale. According to the review in Sect. 1, the parameters can be regarded as Earth observational data, and thus, they may vary with scale. The observation operator also depends on scale because it is

20   a particular physical law. Even if the observation operator is scale invariant in essence, a scale-dependent parameter will again breed its sensitivity to scale.

Assumption 3 implies that when observational information is added in the analysis step, the system state and observation scales are invariant. Regardless of the scale-based transition probability of system state and observation, $\varphi_X(s) = 0$ and $\varphi_Y(s) = 0$. In addition, because the noises are Gaussian, we have $\sigma_X(s) = \sigma_Y(s) = 1$.

25   Based on the above discussion, the differential and integral forms of the system state are

$$dX = dW(s), \text{ and} \tag{15}$$

$$X(s_X) = X_0 + \int_{s_0}^{s_X} dW(s). \tag{16}$$

In addition, for the observation, we have

$$dY = dW(s), \text{ and} \tag{17}$$

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$$Y(s_Y) = Y_0 + \int_{s_0}^{s_Y} dW(s). \tag{18}$$

From the Bayesian equation of DA (Eq. (6)), one can obtain the posterior PDF $p(X \mid Y)$ in association with the likelihood function $p(Y \mid X)$ and the distributions of the system state and observation. Based on Theorem 1 and Eq. (15)-(18), we have $X \sim N\left(X_0, \int_{s_0}^{s_X} ds\right)$ and $Y \sim N\left(Y_0, \int_{s_0}^{s_Y} ds\right)$ under the condition that the variances exist. In addition, because

5 Assumption 1 states that the measures are in the one-dimensional law, the scales vary in one-dimensional space, which results in $X \sim N(X_0, s_X - s_0)$ and $Y \sim N(Y_0, s_Y - s_0)$. Finally, the last point is the calculation of $p(X \mid Y)$.

If the observation operator $H(s, X(s))$ is defined with continuous partial derivatives $H_s(s,x)$, $H_x(s,x)$ and $H_{xx}(s,x)$, in line with Ito's Lemma, we have

$$
\begin{aligned}
H(s_X, X(s_X)) &= H(s_0, X_0) + \int_{s_0}^{s_X} H_s(u, X(u)) du + \int_{s_0}^{s_X} H_x(u, X(u)) dW(u) + \frac{1}{2} \int_{s_0}^{s_X} H_{xx}(u, X(u)) du \\
&= H_0 + \int_{s_0}^{s_X} \left[H_s(u, X(u)) + \frac{1}{2} H_{xx}(u, X(u)) \right] du + \int_{s_0}^{s_X} H_x(u, X(u)) dW(u)
\end{aligned} \tag{19}
$$

10 Assumption 1 suggests that the observation and system state spaces have the same probability measure, and thus, the Brownian motions in these two spaces are equivalent. Let Eq. (18) − (19), we obtain

$$
\begin{aligned}
& Y(s_Y) - H(s_X, X(s_X)) \\
&= Y_0 + \int_{s_0}^{s_Y} dW(u) - \left[H(s_0, X_0) + \int_{s_0}^{s_X} H_s(u, X(u)) du + \int_{s_0}^{s_X} H_x(u, X(u)) dW(u) + \frac{1}{2} \int_{s_0}^{s_X} H_{xx}(u, X(u)) du \right] \\
&= Y_0 - H_0 + \int_{s_0}^{s_Y} dW(u) - \left[H(s_X, X(s_X)) - H(s_0, X(s_0)) \right] - \frac{1}{2} \int_{s_0}^{s_X} H_{xx}(u, X(u)) du - \int_{s_0}^{s_X} H_x(u, X(u)) dW(u) \\
&= Y_0 - \left[H(s_X, X(s_X)) + \frac{1}{2} \int_{s_0}^{s_X} H_{xx}(u, X(u)) du \right] + \left\{ \int_{s_0}^{s_Y} dW(u) - \int_{s_0}^{s_X} H_x(u, X(u)) dW(u) \right\}
\end{aligned} \tag{20}
$$

Equation (20) can be regarded as an Ito process, and its drift is

$$Y_0 - \left[H(s_X, X(s_X)) + \frac{1}{2} \int_{s_0}^{s_X} H_{xx}(u, X(u)) du \right]. \tag{21}$$

15 The integral term in Eq. (21) is the difference of the first-order differential observation operator between the system state scale s_X and the standard scale s_0. This term illustrates that when mapping the system state to the observational space by introducing scale, the mapping should consider not only the function of the observation operator but also the first-order differential term. The former part is typically found in the literature, whereas the latter has been derived in this study for the

first time. This result prompted us to further consider the first-order differential of the observation operator when calculating the observation error.

The quadratic variation of (20) is

$$\left(s_Y - s_0\right) + \int_{s_0}^{s_X} H_x^2(u, X(u))\,du\,, \qquad (22)$$

5 which means that the uncertainty of the observation error includes both the difference between scales S_Y and S_0 and the change of the observation operator from scale S_X to S_0. Therefore, from Eq. (21) and Eq. (22), we obtain

$$P(Y\mid X) = N\left(Y_0 - \left[H(s_X, X(s_X)) + \frac{1}{2}\int_{s_0}^{s_X} H_{xx}(u, X(u))\,du\right], \left(s_Y - s_0\right) + \int_{s_0}^{s_X} H_x^2(u, X(u))\,du\right). \qquad (23)$$

The distributions of $p(Y\mid X)$, X and Y are stochastic functions that depend on scale, and thus, the posterior PDF of the system state is scale dependent as well.

10 In particular, if Y is a direct measurement, viz. $H\left(s, X(s)\right) = X(s)$, the result becomes

$$Y(s_Y) - X(s_X) = \begin{cases} Y_0 - X(s_X) + W(s_Y) - W(s_X), & s_Y > s_X \\ Y_0 - X(s_X) + W(s_X) - W(s_Y), & s_X > s_Y \end{cases}, \text{ and} \qquad (24)$$

$$P(Y\mid X) = N\left\{Y_0 - X(s_X), \left|s_Y - s_X\right|\right\}. \qquad (25)$$

The quadratic variation (22) can be further described by the scale ranging from S_X to S_Y. Under the condition that $s_Y > s_X$, because $W(s_Y) - W(s_X)$ and $W(s_X) - W(s_0)$ are independent, the quadratic variation of (20) becomes

15 $$s_Y - s_X + \int_{s_0}^{s_X} \left[1 - H_x(u, X(u))\right]^2\,du\,. \qquad (26)$$

In the same manner, if $S_X > S_Y$, the quadratic variation of (20) becomes

$$\int_{s_0}^{s_Y} \left(1 - H_x(u, X(u))\right)^2\,du + \int_{s_Y}^{s_X} H_x^2(u, X(u))\,du\,. \qquad (27)$$

The significance of Eq. (20)-(27) is that the effect of scale on the posterior PDF is identified quantitatively. In addition to the model error and instrument error, a new part of the uncertainty of DA has been discovered in the analysis step. The

20 expectation of the posterior PDF may vary with the scale of the system state if Y is an indirect measurement of X, and the uncertainty of the drift depends on the difference between S_Y and S_X (based on Eq. (26) and Eq. (27)) or between S_0, S_Y and S_X (based on Eq. (22)). In addition, if Y is a direct measurement of X (Eq. (24) and Eq. (25)), the expectation of the

posterior PDF is the difference between Y and X, and the uncertainty is equal to the change of scale. Additionally, if the results are not derived from assumption 1, i.e., the measure varies randomly, the posterior PDF should be more complex because its integral path is an arbitrary curve.

4.4 An example: the stochastic radiative transfer equation (SRTE)

5 As a concrete instance of stochastic observation operator $H(s, X(s))$, the SRTE will be employed in the following discussion to further demonstrate how scale influences the uncertainties of the system state.

The SRTE is a stochastic integral-differential equation that describes the radiative transfer phenomena through a stochastically mixed immiscible media and develops an analytical or numerical method for finding the stochastic moments of the solution, such as the ensemble-averaged or variance of the radiation intensity (Pomraning, 1998; Shabanov et al., 2000;
10 Kassianov et al., 2011). Consider the general expression of the SRTE,

$$-\mu \frac{dI(\tau)}{d\tau} = -I(\tau) + J(\tau) + B[T(\tau)], \qquad (28)$$

where $I(\tau)$, $J(\tau)$, $B[\tau]$, μ, τ and T are the radiation intensity, scattering integral term, emission source, coefficient of radiation direction, optical depth and brightness temperature, respectively. To tie into more substantial random optical properties of transfer media, such as absorption and scattering, the optical depth τ is assumed to be stochastic. Because real
15 transfer media is rarely homogeneous, we further suggest that optical depth is a scale-dependent Ito process as

$$d\tau(s) = \varphi_\tau(s)ds + \sigma_\tau(s)dW(s), \qquad (29)$$

which causes the radiation intensity, scattering term and emission source to depend on scale as well.

Regardless of the scattering integral term and emission source, the SRTE simplifies to a homogeneous linear differential equation,

20
$$-\mu \frac{dI(\tau)}{d\tau} = -I(\tau), \qquad (30)$$

and its analytical solution is $I(\tau) = I(0)e^{\tau/\mu}$. Considering that $H(s, x(s)) = I(x) = I(0)e^{x/\mu}$, then $H_s(s, x(s)) = 0$,

$H_x(s, x(s)) = \frac{1}{\mu} I(0)e^{x/\mu}$ and $H_{xx}(s, x(s)) = \frac{1}{\mu^2} I(0)e^{x/\mu}$. Based on Ito's Lemma,

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$$dI(\tau(s)) = dH(s, \tau(s)) = H_s(s, \tau(s))ds + H_x(s, \tau(s))d\tau(s) + \frac{1}{2}H_{xx}(s, \tau(s))d\tau(s)d\tau(s)$$

$$= \frac{1}{\mu}I(0)e^{\tau(s)/\mu}d\tau(s) + \frac{1}{2\mu^2}I(0)e^{\tau(s)/\mu}d\tau(s)d\tau(s)$$

$$= \frac{1}{\mu}I(\tau(s))d\tau(s) + \frac{1}{2\mu^2}I(\tau(s))d\tau(s)d\tau(s)$$

$$= \left(\frac{1}{\mu}I(\tau(s))\right)\sigma_\tau(s)dW(s) + \left(\frac{1}{\mu}I(\tau(s))\right)\varphi_\tau(s)ds + \left(\frac{1}{2\mu^2}I(\tau(s))\right)\sigma_\tau^2(s)ds$$

$$= \left(\frac{\sigma_\tau(s)}{\mu}\right)I(\tau(s))dW(s) + \left(\frac{\sigma_\tau^2(s)}{2\mu^2} + \frac{\varphi_\tau(s)}{\mu}\right)I(\tau(s))ds$$

. (31)

Radiation intensity is a scale-dependent Ito process, for which the rate of the transition probability is $\left(\frac{\sigma_\tau^2(s)}{2\mu^2} + \frac{\varphi_\tau(s)}{\mu}\right)$ and

the rate of volatility is $\frac{\sigma_\tau(s)}{\mu}$. The difference between (31) and the common Ito process is that there is a primitive function

$I(\tau(s))$ in the integral term. Therefore, the other parts of the integral term can be regarded as an evolution rate of the

5   primitive function, and the uncertainty of the radiation intensity is more complex because it is related to not only the change

of scale but also the primitive function.

   Integrating both sides of Eq. (31) yields the general solution of the radiation intensity,

$$I(\tau(s)) = C \cdot \exp\left[\int\left(\frac{\sigma_\tau(s)}{\mu}\right)dW(s) + \int\left(\frac{\sigma_\tau^2(s)}{2\mu^2} + \frac{\varphi_\tau(s)}{\mu}\right)ds\right],$$ (32)

where the constant $C \in R$. Eq. (32) further indicates that $I(\tau(s))$ is a scale-dependent Ito process. Considering that the

10   optical depth τ is the system state, the radiation intensity I is the observation and $I(\tau(s))$ is the observation operator, the

above result in Sect. 4.3 could be easily applied here to study the DA posterior PDF because τ, I and $I(\tau(s))$ are all Ito

processes.

4.5 Extension to multi-variable DA

   In above discussion, we have assumed that there is only one variable in DA. However, there are typically numerous system

15   states. This section will further introduce the **product spaces** to extend the single variable of DA to multiple variables.

Suppose that the independent system states X_k are the variables of the measure spaces $(\Omega, \mathcal{F}_k, \mu_k)$, $k = 1, 2, \cdots, n$, and

$(\Omega^n, \mathcal{F}^n)$ is the product space, where $\Omega^n = \prod_{k=1}^{n} \Omega$ and $\mathcal{F}^n = \prod_{k=1}^{n} \mathcal{F}_k$. According to Fubini's theorem (Billingsley,

1986), there is the only one product measure μ^n in $(\Omega^n, \mathcal{F}^n)$ such that $\mu^n \left(\prod_{k=1}^{n} A_k \right) = \prod_{k=1}^{n} \mu_k (A_k)$, where $A_k \in \mathcal{F}_k$. We

define the vector of the system state $X^n = (X_1, X_2, \cdots, X_n)^T$ as a variable vector of the product measure space

5 $(\Omega^n, \mathcal{F}^n, \mu^n)$. In particular, if all measures μ_k obey the one-dimensional law, we have

$$\mu^n \left(\prod_{k=1}^{n} A_k \right) = \prod_{k=1}^{n} \xi_k^2 \mu_0(A_k) = \left(\prod_{k=1}^{n} \xi_k \right)^2 \mu_0^n \left(\prod_{k=1}^{n} A_k \right),$$

which proves that the product measure is also in a one-dimensional law.

The analysis for the single system state can also be applied to finite multiple states in the product measure space. However, the above results may not hold without the assumption that the system states X_k are independent of each other.

10 **5 Conclusions and outlook**

In this study, we mainly addressed two basic problems: what is scale and how should the impact of scale changes in a DA framework be evaluated? Instead of the empirical and qualitative expression, we employed measure theory and stochastic calculus to define the scale and thus the evolution of uncertainty with respect to scale in DA.

The first problem began with an introduction to measure theory. We revealed that scale is the function of a measure, given

15 that its referential element and representative region are confirmed. Because scale is related to the shape and size of a representative space, this definition regards scale as the measure value, and is according to the spatial transformations between different observation regions. We then defined the variable, which depends on scale, and this step should further consider the heterogeneities of geographical parameters. A variable consequently expresses the ensemble average of a geographical parameter at a specific scale. This study marked a connection between the concepts of measure and scale, and

20 we expected that the problems of scale could be further understood by utilizing the completeness and rigorousness of measure theory. The definition of the change of scale is as important as that of scale because the uncertainties in Earth observations and simulations are partially caused by scale transformations. The change in scale was described using the Jacobian matrix, and it can be further simplified by the one-dimensional law to suit stochastic calculus. This simplification is reasonable for a large portion of Earth observation data, including remote sensing data, because the representative space

25 changes of those data are geometrically similar. However, an in-depth and comprehensive exploration should be conducted in the future to describe other situations in the real world.

For the second problem, we reformulated the expression of DA using a scale-dependent stochastic variable and investigated how the change in scale influences the evolution of uncertainties in DA. The results formulated a new scale-dependent error in DA and further supported previous qualitative knowledge that the analysis error is highly related to changes in scale. It is beneficial to understand the uncertainty under the condition that we separated the scale-dependent error

5   from other errors. Earth observations and simulations can also be improved based on a better description of uncertainty. The results can be derived from the one-dimensional simplification of scale change, and the variables in DA are supposed to evolve regularly based on assumptions 1-3. However, these situations may be more complex in the real world. Therefore, the above results, which are dominated by the structure of the Jacobian matrix and the integral path depending on scale change, will become intricate when adding concrete physical models (such as the SRTE).

10   This work contributes to the understanding of uncertainties in simulations and observations of land surface processes that to define and quantify scale. A scale problem is caused by the scale variations of dynamic processes and basic physical principles, and also from the spatial distributional heterogeneity and irregularity of geographical parameters. Thus, we conducted an integrated study that considered both the geometric transformation of an observation space and the variation in geographical parameters. This integrated study included all possible situations and predictably conforms to each scale-

15   related case study. However, a case study can be seen as a particular solution of the stochastic calculus equation, for which scales change and the scale-dependent Brownian motions evolve in its own integral paths. In addition, the uncertainties of case studies differ because their integral paths differ.

A theoretical exploration was conducted in this work, but the study of the scale problem and nonlinear and stochastic assimilation are far from complete. This reformulation is worthwhile because research on uncertainties in Earth observations

20   and simulations cannot exclude scale-related errors.

6 Notation

	Ω	Observational region
	$\mathcal{F}$	$\sigma - field$
	μ	Measure
25	s	Scale
	S_0	Standard scale
	dV	Variable process
	$W(s)$	Brownian motion
	dX	System state process
30	dY	Observation process

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X_0	Initial value of state in s_0	
Y_0	Initial value of observation in s_0	
s_X	Scale of system state	
s_Y	Scale of observation	
$\tau(s)$	Optical depth	
$I(\tau)$	Radiation intensity	

5

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