A stochastic approach for parameterizing unresolved scales in a system with memory

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ABSTRACT
Complex systems display variability over a broad range of spatial and temporal scales. Some scales are unresolved due to computational limitations. The impact of these unresolved scales on the resolved scales needs to be parameterized or taken into account. One stochastic parameterization scheme is devised to take the effects of unresolved scales into account, in the context of solving a nonlinear partial differential equation with memory (a time-integral term), via large eddy simulations. The obtained large eddy simulation model is a stochastic partial differential equation. Numerical experiments are performed to compare the solutions of the original system and of the stochastic large eddy simulation model.

Key words: Stochastic partial differential equations (SPDEs); stochastic parameterizations; impact of unresolved scales on resolved scales; large eddy simulation (LES); fractional Brownian motion; colored noise.

Mathematics Subject Classifications (2000): 60H30, 60H35, 65C30, 65N35.

Dedicated to Peter E. Kloeden on the occasion of his 60th birthday

1. INTRODUCTION
Stochastic parameterizations have been investigated intensively for quantifying uncertainties in mathematical models of physical, geophysical, environmental, and biological systems. We may roughly classify such uncertainties into two
kinds. The first kind of uncertainties may be called model uncertainty. They involve with physical processes that are less known, not yet well understood, not well-observed or measured, difficult to be described in the mathematical models, or otherwise ignored in the usual deterministic modeling. Parameterizations of model uncertainties have been considered in, for example, [8, 11, 36, 15, 24, 25, 26] and references therein.

The second kind of uncertainties may be called simulation uncertainty. This arises in numerical simulations of multiscale systems that display a wide range of spatial and temporal scales, with no clear scale separation. Due to the limitations of computer power, at present and for the conceivable future, not all scales of variability can be explicitly simulated or resolved. Although these unresolved scales may be very small or very fast, their long time impact on the resolved simulation may be delicate (i.e., may be negligible or may have significant effects, or in other words, uncertain). Thus, to take the effects of unresolved scales on the resolved scales into account, representations or parameterizations of these effects are required [30, 3].

The present paper deals with simulation uncertainty, i.e., stochastically parameterizing the effects of the unresolved scales on the resolved scales. We consider this issue in the context of large eddy simulations (LES) of a nonlinear partial differential equation with memory. Relevant existing works include [10, 1, 13, 12, 16, 31, 2, 5, 37, 38].

In large eddy simulations of fluid or geophysical fluid flows [3, 30], the unresolved scales appear as the so-called subgrid scales (SGS). The SGS term appears to be highly fluctuating ("random"); see the Figure 1 in [22]. Partially motivated by this, stochastic parameterizations of subgrid scales have been investigated in fluid, geophysical and climate simulations, based on physical or intuitive or empirical arguments. Another, perhaps more important, motivation for applying stochastic parameterizations of subgrid scales is to induce the desired backward energy flux ("stochastic backscatter") in fluid simulations [14, 19, 32].

We present one stochastic parameterization scheme of the subgrid scale term in the large eddy simulation of a nonlinear partial differential equation with an extra memory term, which is in fact a nonlinear integro-partial differential equation. The approximation scheme is based on stochastic calculus involving a fractional Brownian Motion, and the "parameter" to be calculated is a spatial function, which is derived using Ito stochastic calculus.

This paper is organized as follows. After introducing large eddy simulations in §2, we discuss fractional Brownian motions and colored noise in §3, and devise a stochastic parameterization scheme of the subgrid scales in details in §3 and §4, respectively. Finally, in §5, we demonstrate this stochastic
parameterization scheme by a few numerical experiments on solving a nonlinear partial differential equation with memory.

2. STOCHASTIC LARGE EDDY SIMULATIONS

As an example, we consider the following nonlinear partial differential equation with a memory term (time-integral term)

\[ u_t = u_{ss} + u - u^3 + \int_0^t \frac{1}{1 + |t - s|^{\beta}} u(x, s) ds, \]  

(1)

under appropriate initial condition \( u(x, 0) = u_0(x) \) and boundary conditions \( u(-1, t) = a, u(1, t) = b \) with \( a, b \) constants, on a bounded domain \( D: -1 \leq x \leq 1 \). Here \( \beta \) is a positive constant. This model arises in mathematical modeling in ecology [39], heat conduction in certain materials [9, 17] and materials science [7, 17]. The time-integral term here represents a memory effect depending on the past history of the system state, and this memory effect decays polynomially fast in time.

The large eddy solution \( \overline{u} \) is the true solution \( u \) looked through a filter: i.e., through convolution with a spatial filter \( G_\delta(x) \), with spatial scale (or filter size or cut-off size) \( \delta > 0 \):

\[ \overline{u}(x, t) := u \times G_\delta = \int_D u(y, t) G_\delta(x - y) dy. \]

In this paper, we use a Gaussian filter as in [3], \( G_\delta(x) = \frac{1}{\pi \delta^2} e^{-\frac{x^2}{\delta^2}} \).

On convolving (1) with \( G_\delta \), the large eddy solution \( \overline{u} \) is to satisfy

\[ \overline{u}_t = \overline{u}_{ss} + \overline{u} - \overline{u}^3 + \int_0^t \frac{1}{1 + |t - s|^{\beta}} \overline{u}(x, s) ds, \]

or

\[ \overline{u}_t = \overline{u}_{ss} + \overline{u} - \overline{u}^3 + \int_0^t \frac{1}{1 + |t - s|^{\beta}} \overline{u}(x, s) ds + R(x, t), \]

(2)

where the remainder term, i.e., the subgrid scale (SGS) term \( R(x, t) \) is defined as

\[ R(x, t) := (\overline{u})^3 - (\overline{u}^3). \]

We can write \( u = \overline{u} + u' \) with \( \overline{u} \) the large eddy term and \( u' \) the fluctuating term. Note that \( \overline{u} = u - u' \). So the SGS term \( R(x, t) \) involves nonlinear
interactions of fluctuations $u'$ and the large eddy flows. Thus $R(x, t)$ may be regarded as a function of $\bar{u}$ and $u'$: $R := R(\bar{u}, u')$.

The leads to a possibility of approximating $R(x, t)$ by a suitable stochastic process defined on a probability space $(\Omega, F, P)$, with $\omega \in \Omega$, the sample space, $\sigma$-field $F$ and probability measure $P$. This means that we treat $R$ data as random data as in [22], which take different realizations, e.g., due to fluctuating observations or due to numerical simulation with initial and boundary conditions with small fluctuations. In fluid or geophysical fluid simulations, the SGS term may be highly fluctuating and time-correlated [22], and this term may be inferred from observational data [27, 28], or from fine mesh simulations.

In fact, in our case study here, the subgrid scale term $R(x, t)$ is clearly time-correlated; see Fig. 1. The (averaged) time correlation function here, over a computational time interval $[0, T]$, is defined as:

$$
Corr(x, s) = \frac{1}{T} \int_0^T \frac{\text{cov}(R(x, t), R(x, t+s))}{\text{STD}(R(x, t)) \cdot \text{STD}(R(x, t+s))} \, dt,
$$

Fig. 1. $\text{Corr}(0, s)$ — Averaged time correlation of the subgrid scale term $R(x, \tau)$, at $x = 0$, for $u_t = u_{xx} + u - u^2 + \int_0^\tau \frac{1}{1 + |t - s|} u(x, s) ds$, $u(x, 0) = 0.53x - 0.47 \sin(1.5\pi x)$, $u(-1, \tau) = -1$, $u(1, \tau) = 1$; $\beta = 2$. 

where cov denotes covariance, and \( \text{STD}(R) = \sqrt{E(R - E(R))^2} \) is the standard deviation.

This further suggests for parameterizing the subgrid scale term \( R(x, t) \) as a time-correlated or colored noisy term.

Before we devise how we parameterize the subgrid scale term \( R(x, t) \) as a colored noise or time-correlated term, we first discuss fractional Brownian motion and colored noise in the next section.

3. STOCHASTIC PARAMETERIZATION VIA A COLORED NOISE

We first discuss a model of colored noise in terms of fractional Brownian motion. The fractional Brownian motion is a generalization of the more well-known process of Brownian motion. It is a centered Gaussian process with stationary increments. However, the increments of the fractional Brownian motion are not independent, except in the standard Brownian case \( (H = 0.5) \). The dependence structure of the increments is modeled by a so called Hurst parameter \( H \in (0, 1) \). For more details, see [21, 23, 6, 18, 35].

Definition of fractional Brownian motion: For \( H \in (0, 1) \), a Gaussian process \( B^H(t) \), or \( \text{fBM}(t) \), is a fractional Brownian motion if it starts at zero \( B^H(0) = 0 \), a.s., has mean zero \( E[B^H(t)] = 0 \), and has covariance \( E[B^H(t)B^H(s)] = 0.5 \left(|t|^{2H} + |s|^{2H} - |t - s|^{2H}\right) \) for all \( t \) and \( s \). The standard Brownian motion is a fractional Brownian motion with Hurst parameter \( H = 0.5 \).

Some properties of fractional Brownian motion: A fractional Brownian motion \( B^H(t) \) has the following properties:

(i) It has stationary increments;
(ii) When \( H = 1/2 \), it has independent increments;
(iii) When \( H \neq 1/2 \), it is neither Markovian, nor a semimartingale.

The exact simulation of \( B^H(t_1), ..., B^H(t_n) \) is in general computationally very expensive. The Cholesky decomposition method, which is to our knowledge a known exact method for the non-equidistant simulation of fractional Brownian motion, requires \( O(n^3) \) operations. Moreover the covariance matrix, which has to be decomposed, is ill-conditioned. If the discretization is equidistant, i.e., \( t_i = i/n, i = 1, ..., n \), the computational cost can be lowered considerably. For example, the Davis-Harte algorithm for the equidistant simulation of fractional Brownian motion has computational cost \( O(n \log(n)) \); see, e.g., Craigmile [4].

Here we use the Weierstrass-Mandelbrot function to approximate the fractional Brownian motion. The basic idea is to simulate fractional Brownian
motion by randomizing a representation due to Weierstrass. Given the Hurst parameter $H$ with $0 < H < 1$, we define the function $w(t)$ to approximate the fractional Brownian motion:

$$w(t_i) = \sum_{j=0}^{\infty} C_j r^{jH} \sin(2\pi r^{-j}t_i + d_j)$$

where $r = 0.9$ is a constant, $C_j$’s are normally distributed random variables with mean 0 and standard deviation 1, and the $d_j$’s are uniformly distributed random variables in the interval $0 \leq d_j < 2\pi$. The underlying theoretical foundation for this approximation can be found in [29, 20]. Figure 2 shows a sample path of the fractional Brownian motion, when Hurst parameter $H = 0.75$.

The increments of fractional Brownian motion are correlated in time. This motivates us to parameterize the subgrid scale term $R(x, t)$, which is time-correlated, by using colored noise $\frac{dB^H_t}{dt}$.

We thus parameterize the subgrid scale term $R(x, t)$ term (3) above as a mean component plus a colored noise. To be more specific, we model $R(x, t)$ as follows:

$$R(x, t) = f(\bar{u}) + \sigma(x) \frac{dB^H_t}{dt},$$

(4)

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Fig. 2. A sample path of fractional Brownian motion $B^H(t)$, with $H = 0.75$. 

where \( \frac{dB^H_t}{dt} \) is a colored noise, and

\[
\sigma(x) = a_0 + a_1 u + a_2 u^2 + a_3 u^3,
\]

is the mean component of the subgrid scale term \( R(x, t) \). Moreover, the noise intensity \( \sigma(x) \) is a non-negative deterministic function to be determined from fluctuating SGS data \( R \). The subgrid scale term \( R(x, t) \) may be inferred from observational data [27, 28], or from fine mesh simulations as we do here. We represent the mean component \( f(\bar{u}) \) in terms of the large eddy solution \( \bar{u} \). The specific form for \( f \) depends on the nature of the mean of \( R \). Here we take \( f(u) = a_0 + a_1 u + a_2 u^2 + a_3 u^3 \), where coefficients \( a_i \)'s are determined via data fitting by minimizing \( \int_0^T \int_0^T [a_0 + a_1 u + a_2 u^2 + a_3 u^3 - \mathbb{E}(R(x,t))]^2 \, dx \, dt \). Moreover, we take \( B_t^H \) as a scalar fractional Brownian motion.

Note that \( \sigma \) is to be calculated or estimated from the fluctuating SGS data \( R \), either from observation or (in this paper) from fine mesh simulations; see detailed discussions in [22, 5]. So this is an inverse problem. As in usual inverse problems [33], the stochastic parameterizations for the SGS term \( R \) is not unique. This offers an opportunity for trying various stochastic parameterization schemes, much as one uses various smoother functions (e.g., polynomials or Fourier series) to approximate less regular functions or data in deterministic approximation theory.

To estimate the unknown parameter (function) \( \sigma(x) \), we start with (4)–(5) to get the following relation:

\[
R(x, t) - \mathbb{E}(R(x, t)) = \sigma(x) \frac{dB^H_t}{dt}.
\]

Taking time integral over a computational interval \([0, T]\) on both sides, we obtain

\[
\int_0^T \left[ R(x, t) - \mathbb{E}(R(x, t)) \right] dt = \int_0^T \sigma(x) dB^H_t = \sigma(x) B^H_T.
\]

Therefore, taking mean-square on both sides,

\[
\mathbb{E} \left( \int_0^T \left[ R(x, t) - \mathbb{E}(R(x, t)) \right] dt \right)^2 = \sigma^2(x) T^{2H}.
\]

Thus an estimator for \( \sigma(x) \) is
which can be computed numerically.

By the stochastic parameterization (4) on the SGS term $R$, with $f$ determined from (5) and $\sigma$ from (7), the LES model (2) becomes a stochastic partial differential equation (SPDE) for the large eddy solution $U \approx \bar{u}$:

$$
U_t = U_{xx} + U - U^3 + \int_0^t \frac{1}{1+|t-s|^\beta} U(x,s)ds + f(U) + \sigma(x) \frac{dB^x_t}{dt},
$$

with boundary conditions $U(-1, t) = a, U(1, t) = b$ and filtered initial condition

$$
U(x, 0) = \bar{u}_0(x).
$$

4. NUMERICAL EXPERIMENTS

We use a spectral method to solve nonlinear system (1) and (8) numerically. For more details, please see [34]. We take the following initial and boundary conditions:

$$
u(x, 0) = u_0 = 0.53x - 0.47 \sin(1.5\pi x), u(-1, t) = -1, u(1, t) = 1
$$

![Solution to the original system on a fine mesh, $\beta = 2$, mesh size $\Delta x = 0.001.$](image)
Fine mesh simulations of the original system with memory (1) are conducted to generate benchmark solutions or solution realizations, with initial conditions slightly perturbed; see Fig. 3. These fine mesh solutions $u$ are used to generate the SGS term $R$ defined in (3) at each time and space step. The filter size used in calculating $R$ is taken as $\delta = 0.01$. The mean $f$ is calculated from (5) via cubic polynomial data fitting (as discussed in the last section), and

$$u_t = u_{xx} + u - u^3 + \int_0^t \frac{1}{1 + |t - s|^\beta} u(x, s) ds, \beta = 2.$$  

Fig. 4. Solution to the original system with NO stochastic parametrization on the mesh four times coarser than the mesh used in Fig. 3,

$$u_t = u_{xx} + u - u^3 + \int_0^t \frac{1}{1 + |t - s|^\beta} u(x, s) ds, \beta = 2.$$  

Fig. 5. Solution to LES model with stochastic parametrization on the mesh four times coarser than the mesh used in Fig. 3,

$$U_t = U_{xx} + U - U^3 + \int_0^t \frac{1}{1 + |t - s|^\beta} U(x, s) ds + f(U) + a(x) \dot{B}_t^H, \beta = 2, H = 0.75.$$  

Fine mesh simulations of the original system with memory (1) are conducted to generate benchmark solutions or solution realizations, with initial conditions slightly perturbed; see Fig. 3. These fine mesh solutions $u$ are used to generate the SGS term $R$ defined in (3) at each time and space step. The filter size used in calculating $R$ is taken as $\delta = 0.01$. The mean $f$ is calculated from (5) via cubic polynomial data fitting (as discussed in the last section), and
The parameter function $\sigma(x)$ is calculated as in (7). The stochastic LES model (8) is solved by the same numerical code but on a coarser mesh. Note that a four times coarser mesh simulation with no stochastic parameterization for the original system (1) does not generate satisfactory results; see Fig. 4. The stochastic LES model (8) is then solved in the mesh four times coarser than the fine mesh used to solve the original equation (1). The stochastic parameterization leads to better resolution of the solution as shown in Fig. 5. The root-mean-square error, $\text{error}(x,t) := \sqrt{\mathbb{E}|u(x,t) - U(x,t)|^2}$, between the fine mesh solution $u$ (Fig.3) and this stochastic LES solution $U$ (Fig. 5) is plotted in Fig. 6.

5. DISCUSSIONS

We have discussed the issue of modeling the impact of unresolved scales on the resolved ones, in the context of large eddy simulation of a nonlinear partial differential equation with memory. The resulting model is a stochastic partial differential equation, which describes large scale evolution with some effects of unresolved scales taken into account.

It would be very interesting to investigate whether this stochastic approach works for simulation of other complex systems, such as climate systems, fluid flows, biological systems and materials.
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