Mesoscale Organized Convection in Climate Models: A Stochastic Scheme and Uncertainty Quantification

Gino Chen

University of Miami, gchen0119@gmail.com

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MESOSCALE ORGANIZED CONVECTION IN CLIMATE MODELS: A STOCHASTIC SCHEME AND UNCERTAINTY QUANTIFICATION

By

Gino Chen

A DISSERTATION

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MESSOSCALE ORGANIZED CONVECTION IN CLIMATE MODELS: A STOCHASTIC SCHEME AND UNCERTAINTY QUANTIFICATION

Gino Chen

Approved:

__________________________________  _______________________________________
Ben Kirtman, Ph.D.                    Mohamed Iskandarani, Ph.D.
Professor of Atmospheric Sciences     Professor of Ocean Sciences

__________________________________  _______________________________________
Sharanya Majumdar, Ph.D.             Guillermo Prado, Ph.D.
Professor of Atmospheric Sciences     Dean of the Graduate School

__________________________________  _______________________________________
Omar Knio, Ph.D.
Professor of Applied Mathematics and Computational Science
King Abdullah University of Science and Technology
Mesoscale organized convection is generally misrepresented in the large-scale convective parameterizations used in contemporary climate models. This impacts extreme weather events (e.g., Madden-Jullian Oscillation (MJO)) and the general circulation driven by the significant amount of latent heat released from mesoscale organized convection. Studies show that the missing processes could be partially recovered by embedding a 2D cloud-resolving model in each GCM columns, i.e., super-parameterization. Despite successfully resolving the MJO, the study of mesoscale organization mechanism across the CRM and GCM cells remains sparse in this multiscale modeling framework. We apply rigorous detection and hierarchical clustering algorithms on the 3-hourly 2D resolved Mesoscale Convective Systems (MCSs) embedded in the cloud-permitting Super-Parameterized Community Atmosphere Model 5.2 (SPCAM). We then examine the fields of a long-lived and large MCS cluster at the central Pacific. The MCS cluster shows a squall line-like circulation throughout the lifecycle in SPCAM. The growth of deep shear surrounding the MCS cluster is presumably caused by the upgradient momentum transport of squall line organization. We simultaneously obtain the 3-hourly CAM cumulus parameterization outputs based on the timestep-wise perfect initial conditions given by SPCAM. This allows pure model physics comparison without introducing initial condition errors. The re-
results show that CAM has a systematically biased stratiform cooling and moistening response below 3km to the given SPCAM deep convection favoring conditions. We show that this bias is mainly due to the CAM’s stratiform microphysics scheme. The mesoscale organization in SPCAM thus provides a baseline for improvements of convective parameterization of CAM. The details of the systematic differences are revealed by a composite analysis. Results show SPCAM has a realistic growth to decay deep convection mode dominant in the large-scale heating and moisture sink in the composite. On the other hand, CAM strongly favors a steady stratiform dipole mode. CAM also shows little to no deep convection variation in the MCS organized environment given by SPCAM. The lack of variation commonly seen in deterministically parameterized large-scale models is often remedied by stochastic parameterization to represent the missing subgrid processes. By decomposing CAM’s cumulus parameterization schemes, we proposed a stochastic scheme to represent the mesoscale organization processes in CAM using the results from SPCAM.

We perform a simple model proof-of-concept study to reach the goal of applying the stochastic scheme to a complex climate model. The time-independent perturbed parameter scheme shows comparable forecast skill when compared to the standard stochastic schemes. This time-independent perturbation scheme allows us to treat the forecast model as a black box with minimal intrusion to the model codes. The major standout of the new scheme is its ability to significantly reduce the simulation cost by building a stochastic spectral “surrogate model”, i.e., Polynomial Chaos Expansion (PCE). The surrogate model thus performs ensemble forecasts without the need to integrate the actual forecast model. The results show more reliable prediction and extended predictability compared to a deterministic scheme. The new scheme also
shows comparable forecast skill when compared to the well known additive stochastic parametrization scheme. We incorporate the necessary components (i.e., Bayesian posterior sampling algorithm and global sensitivity analysis) on top of the stochastic scheme to form a more comprehensive forecast system for uncertainty quantification of the model parameters and tendencies. This study is the building block to the future application of the new forecast system to the climate model in the hope of representing convective organization.
Acknowledgements

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Gino Chen

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CHAPTER 1

Introduction

One of the challenges in climate prediction is to accurately parameterize some of the fundamental processes that are well represented in weather models but missing in climate models. A long-standing uncertainty lies in the moist convective parameterization, which represents the primary vertical transport of heat, moisture, and dynamical quantities into the atmosphere. The convective organization with an upscale-cascade of energy ([Del Genio, 2012; Moncrieff and Liu, 2006]) is often misrepresented in traditionally mass-flux-based convective parameterization ([Ooyama, 1971; Arakawa and Schubert, 1974]) in most climate models. A higher resolution, but computationally intensive, global cloud resolving model (CRM) is often applied for the purpose of explicitly resolving the convective organization processes. We propose a cost-effective parameterization (i.e., stochastic scheme) by quantifying the detailed structure of MCSs in a cloud-permitting general circulation model (GCM) to represent organized convection in a conventional GCM.

Conventional parameterization unrealistically assumes scale separation between cumulus processes and the environment ([Yano et al., 2014]; [Plant and Yano, 2015]). The misrepresented parameterization has major impacts on the Mesoscale Convective Systems (MCSs) which organize in and above the unresolved scale $O(10-100\text{km})$ of
large-scale models. The small-scale cumulus convection in active MCSs requires low-level environmental shear to interact with the cold outflow from convective downdraft [Bryan et al., 2007]. The cold pool dynamics further lifts the conditionally unstable air to rejuvenate convection ([Moncrieff and Green, 1972; Moncrieff, 1992]) (Figure 1.1).

In the sheared environment, a propagating deep convective system provides upscale growth by up-gradient momentum transport [LeMone, 1983; Moncrieff and Klinker, 1997], as opposed to the down-gradient mixing effects in mass-flux-based schemes. The “downgradient” comes from the Prandtl mixing-length theory which parameterizes the turbulent mixing as a linear function of the background gradient

$$
\overline{w's'} = -K \frac{\partial \bar{s}}{\partial z},
$$

(1.1)
where the eddy viscosity $K$ is strictly positive. The turbulent mixing thus tends to destroy the background gradient. Whereas “upgradient” violates the mixing length parameterization, and $K$ results in a negative value. Therefore the background gradient is enhanced by the turbulent transport term (e.g., pressure gradient force altering the eddy momentum transport). In terms of upgradient momentum transport, an MCS shows upper-level outflow strengthening as it evolves (Figure 1.2). The upscale energy growth led by the mechanism is crucial for an MCS to form large-scale stratiform clouds with overturning circulation that extends the system lifetime.

![Figure 1.2: Figure from Houze Jr [2014] reprinted from Houze [1989].](image)

MCSs contribute nearly half of the total rainfall in the observed tropics ([Schumacher and Houze Jr, 2003; Yuan and Houze Jr, 2010]) and in regions where climate models have difficulty in representing the rainfall frequency and distribution [Moncrieff et al., 2012]. Given a favorable large-scale environment [Laing and Fritsch, 2000], an MCS can evolve into long-lasting flooding events. An MCS contains individual cells of cumulonimbus, a precipitating stratiform raining region, and an extended
non-precipitating ice water detraining anvil region (see lifecycle of an observed MCS in Figure 1.3). The three cloud features may occur separately or entangled in the same cloud complex [Houze Jr, 2014].

Figure 1.3: Figure from Houze Jr [2014] reprinted from Leary and Houze Jr [1979].

There are distinct differences between the stratiform and convective cloud momentum transport [Zipser, 1977] and net heating profiles [Houze, 1989]. LeMone
[1983] pointed out the momentum flux in a tropical squall line is contributed mostly by the leading convective region and little from the stratiform region. The heating in the convective region focuses on lower-levels, and the stratiform region exhibits a lower-level cooling and upper-level heating dipole mode [Lin et al., 2004]. The latent heating of the upper troposphere in the tropics is maximized by both convective and stratiform components [Houze, 1989] (Figure 1.4).

![Figure 1.4: Figure from Houze Jr [2014] reprinted from Schumacher et al. [2004].](image)

The latent heating is further reinforced by the radiative effects of the upper-level anvil clouds [Machado and Rossow, 1993]. The anvil clouds significantly affect the radiative heating profile in the tropics [Ackerman et al., 1998].

To incorporate the missing organization processes in GCMs, Grabowski and Smolarkiewicz [1999] embedded a 2D CRM in each column of the GCM to allow cloud-scale physics to interact with the large-scale environments. Preliminary research by LeMone and Moncrieff [1994] found that the bulk effects of the mesoscale organized convection were surprisingly well captured in a 2D CRM, which holds true even with periodic lateral boundary conditions [Grabowski et al., 1996]. Randall et al. [2003] coined “superparameterization” for this cloud-permitting parameterization. Khairoutdinov et al. [2005]; Khairoutdinov and Randall [2001] replaced the con-
ventional parameterization with superparameterization in Community Atmosphere Model (CAM) and formed super-parameterized CAM (SPCAM).

Studies of mesoscale organization processes [Pritchard et al., 2011; Kooperman et al., 2013] show that SPCAM captures nocturnal eastward propagating MCSs, which accounts for up to 60% of summer rainfall to the central United States. Most climate models have difficulty in simulating the period and amplitude of the Madden Julian Oscillation (MJO) [Slingo et al., 1996; Lin et al., 2006]; thus, improvements in MJO representation can be partially attributed to the MCS organization process. Grabowski [2003] discovered a realistic intraseasonal MJO with an eastward-moving convective envelope in SPCAM. The detailed structure of the MJO in SPCAM was verified with observations by Benedict and Randall [2009]. Kim et al. [2009] and Klingaman et al. [2015] found that SPCAM produced the most realistic MJO out of 8 and 15 state-of-the-art atmospheric GCMs respectively. Hannah et al. [2015] compared the most up-to-date CAM and SPCAM and found a better fluctuation of precipitation and zonal wind associated with the MJO.

Operational GCMs have been slow to incorporate convective processes in their traditionally mass-flux based parameterization [Yano, 2014]. For instance, the upgradient momentum transport is missing [Yano and Moncrieff, 2016], and the only deep convection scheme in GCMs that incorporates mesoscale downdraft and convective-scale vertical velocity is the Donner scheme [Donner, 1993; Donner et al., 2001]. These missing processes are novel properties of mesoscale organization processes [Moncrieff and Klinker, 1997; Houze Jr, 2014], and lead to common biases in rainfall frequency and intensity. For example, conventional GCMs have the tendency to rain too often and too weakly in conventional GCM [O’Gorman and Schneider, 2009]. The
quasi-equilibrium assumptions further break down at higher resolutions for mass-flux schemes [Jones and Randall, 2011].

Despite these limiting factors, there remain possibilities to incorporate the missing mesoscale processes into the conventional schemes. Yano and Moncrieff [2016] tested the organized convection parameterization with upgradient momentum transport in an intermediate large-scale model [Yano et al., 2010]. Both deterministic [Khouider et al., 2011] and stochastic multi-cloud parameterization [Deng et al., 2015; Goswami et al., 2017, 2016] show improvements in representing organized convection. A stochastic deep convective parameterization of the standard Zhang-McFarlane scheme in CAM5 also improved the simulation of tropical precipitation variability [Wang et al., 2016].

Stochastic parameterization simulates the subgrid-scale processes in a cost-effective way, which is generally 5 to 6 times cheaper than global CRMs. This motivates us to study the detailed structure of MCSs in SPCAM to find the possibility for representing organized convection as a stochastic process in CAM. A large and long-lasting squall-like MCS shows that the up-gradient momentum transport mechanism is presumably better represented in SPCAM. We compare the GCM output fields of the SPCAM and CAM in the deep convection favoring environment and found that CAM has a systematically biased response as a stratiform dipole heating profile. We seek to generalize this systematic difference to the entire population of MCSs by composite analysis to further quantify and parameterize the upscale organization processes from both models. The current composite study shows that CAM responds as a near steady stratiform mode in a deep convection favored environment. We conduct a
thorough composite analysis to conclude the systematic differences of the two model in representing organized convection.

The systematic difference between the large-scale heating and moisture profile has statistical relationships that enables us to propose a stochastic spectral scheme, which acts as a cost effective sampling “surrogate model” of the forecast model. Finally we show in an idealized simple model system that the proposed scheme has comparable forecast skill when compared to a stochastic parametrization scheme. In addition, the proposed scheme shows the ease to be applied to forecast improvement methods (e.g., Bayesian inference, sensitivity analysis, etc).
CHAPTER 2

Organized convective systems in climate models

In this study, we provide further evidence that the large-scale GCM environment reacts as an organized cloud cluster to the embedded small-scale 2D CRM convection organization. In section 2.1, we develop a 2D-CRM MCS detection and clustering algorithm and the global geographical distribution of the clusters are shown. We examine a single long-lived MCS cluster with squall line-like circulation in the tropics in section 2.2. We compare large-scale GCM cell outputs of SPCAM and CAM using the exact same initial condition at every timestep. Hence simplifying the problem to a pure model physics comparison.

2.1 Materials and methods

2.1.1 Forecast model

The 2D cloud-resolving model, System for Atmospheric Modeling (SAM Version 6.8.2), is zonally embedded in each of the GCM columns of SPCAM to replace the CAM convective parameterization. The Morrison et al. [2005] two-moment microphysics scheme [Wang et al., 2011a,b] is used for SAM. The zonal domain of the 2D
CRM is periodic, so the CRM cells do not communicate through lateral boundaries of the GCM cells. One can view the zonally aligned CRM as a “ring” embedded in each GCM cells. The CRM tendency fields, except the momentum, are zonally averaged and used to update the GCM states. Detail formulation of SPCAM can be seen in Khairoutdinov et al. [2005].

A two months spin-up period is performed and discarded prior to a one-year “free running” simulation of SPCAM, where data are saved 3-hourly. The zonal grid of the 2D CRM is set to a 4km resolution and uses the same bottom 28 vertical levels of CAM5.2. We set the zonal domain to 128km to reduce the systematic mean state issues [Pritchard et al., 2014]. The horizontal grid for CAM5.2 is set to 1.25° (longitude) × 0.9424° (latitude) resolution with 30 vertical levels. The present-day monthly climatology (1981-2011) of SST and sea ice are prescribed. We outputted the “offline” CAM5.2 data from the free running SPCAM’s one year simulation. Therefore, the model outputs of SPCAM and CAM are obtained based on the same initial conditions at every given timestep. This eliminates initial condition errors to compare pure model physics differences.
Table 2.1: MCS detection criteria

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cloud top height ($h_{\text{top}}$)</td>
<td>Maximum height where ice mixing ratio $&gt; 10^{-3}$ g/kg</td>
</tr>
<tr>
<td>Cloud top temperature ($T_{\text{top}}$)</td>
<td>Temperature at $h_{\text{top}}$</td>
</tr>
<tr>
<td>High cloud complex (HCC)</td>
<td>Continuous region with $T_{\text{top}}$ contained within 260K isotherm</td>
</tr>
<tr>
<td>High cloud system (HCS)</td>
<td>Portion of HCC associated with a local minima $T_{\text{top}}$ a</td>
</tr>
<tr>
<td>Precipitation Feature (PF)</td>
<td>A region contoured by rain rate 0.1 mm hr$^{-1}$</td>
</tr>
<tr>
<td>Raining core (RC)</td>
<td>Portion of any PF overlapping and/or located within an HCS</td>
</tr>
<tr>
<td>Heavy rain area (HRA)</td>
<td>Portion of PF $&gt; 6$mm hr$^{-1}$</td>
</tr>
<tr>
<td>Mesoscale convective system</td>
<td>Any HCS with its largest RC satisfying:</td>
</tr>
<tr>
<td></td>
<td>1) Exceeds 48 km $\approx$ diameter of a 2,000 km² circle</td>
</tr>
<tr>
<td></td>
<td>2) Occupies more than 70% of the total HCS area</td>
</tr>
<tr>
<td></td>
<td>3) $T_{\text{top}} &lt; 220$K exists</td>
</tr>
<tr>
<td></td>
<td>4) More than 10% occupied by HRA</td>
</tr>
</tbody>
</table>

*aIf multiple $T_{\text{top}}$ local minimas exist in an HCC, we define them as different HCSs only if the $T_{\text{top}}$ local maximas between these minimas are at least 10°C higher. These maximas become the boundaries of the new set of HCSs. When changing the threshold to 20°C, the change in total number of MCSs detected are insensitive (< 0.5%).*

### 2.1.2 MCS detection

The general definition of MCS according to Houze Jr [2014], “a cumulonimbus cloud system that produces a contiguous raining region of approximately 100 km or more in at least one direction”. We adopted the MCS detection criteria developed by Yuan and Houze Jr [2010] as shown in Table 2.1 and applied to the 2D CRM domain separately over all GCM columns in SPCAM. The periodicity of the 2D CRM is accounted to eliminate the boundaries for the detection algorithm. Once an MCS is detected (covering at least 78% of the 2-D domain), the entire GCM cell is considered as a single MCS. This allows clustering of neighboring large-scale cells otherwise not possible.
Figure 2.1: Hierarchical clustering with minimum-linkage criteria resulting in (a) a single cluster and (b) two distinct clusters.
2.1.3 MCS clustering (Hierarchical Cluster Analysis)

Each MCS detected in the CRM domain of a GCM column of SPCAM represents a separate convective entity. The CRM domain is zonally periodic, hence the CRM’s state variables are only updated through GCM’s tendency terms with the neighboring columns. Therefore the only way to treat two MCS cells as the same convective cluster is to do this in the steps, 1) detect the MCSs separately by previous algorithm; 2) determine if they are neighboring cells in space and time; 3) cluster the neighboring cells into an “MCS cluster”. Therefore we need an algorithm to unify or separate the individually detected MCSs in space and time to study a complete cloud cluster lifecycle. Previous studies ([Williams and Houze Jr, 1987; Mapes and Houze Jr, 1993]) are able to spatially connect cold cloud pixels in satellite image frames into cloud clusters. Once spatially clustered, any two cloud clusters adjacent in time frames will become a time cluster when meeting the time-tracking criteria, “cluster elements of areas overlapping at least 50% or $10^4$ km$^2$ from a 3-h satellite snapshot”.

We developed an algorithm based on the same idea of clustering cells adjacent in space and time, but doing them simultaneously with Hierarchical Clustering Analysis (HCA) ([Kaufman and Rousseeuw, 2009]), and we call this algorithm a space-time HCA.

In the space-time HCA, we modified the time-tracking criteria to “at least two spatial points between two timeframes of cluster elements are neighbors”, since a GCM cell ($\sim 10^4$ km$^2$) is the highest resolution available. The HCA measures the distance of the GCM cells with MCSs located both in space and time. We used the Euclidean distance $d(g, p) = \sqrt{\sum_{i=1}^{3} (g_i - p_i)^2}$, which sums the squared difference over all three dimensions (x,y,t). The g and p are triplet integer index coordinate values
in space and time. For example, \( g = [1, 1, 2] \) and \( p = [2, 2, 3] \) represents two spatially neighboring index values \([1, 1]\) and \([2, 2]\) between two adjacent time indices at 2 and 3. The farthest Euclidean distance qualified as neighboring points is decided by the cutoff distance \( D = d(g, p) = \sqrt{1^2 + 1^2 + 1^2 + \epsilon} \approx 1.75 \), where \( \epsilon = 0.02 \) is just a small offset value. By measuring all the points between cluster pairs (i.e., more than one point can form a cluster), the minimum-linkage criteria [Johnson, 1967] finds the closest two points between two clusters and uses \( D \) to decides whether they are the same cluster. The triplet allows simultaneous clustering in space and time, which gives the name space-time HCA.

For illustration purposes, at a fixed time, both Figure 2.1 (a) and (b) shows two spatially located red and blue clusters ready to be determined as being the same or distinct clusters. Each grid box is centered on an index coordinate value, hence the Euclidean distance is measured using these values. Minimum-linkage criterion selects the closest grid boxes (thickly outlined boxes) between the two clusters, and determine if the two boxes are neighbors. Figure 2.1 (a) shows the two clusters with minimum-linkage distance \( d = \sqrt{1^2 + 1^2} = \sqrt{2} \) (dashed line) less than the cutoff distance \( D = 1.75 \), thus the two clusters qualify as the same cluster. Whereas Figure 2.1 (b) shows the minimum-linkage distance \( d = \sqrt{2^2 + 1^2} = \sqrt{5} > 1.75 \), thus qualify as two different clusters with linkage being trimmed in the HCA algorithm.

The total number of MCS clusters detected in each seasons is 4,464 in DJF, 4,542 in MAM, 4,737 in JJA, and 4,123 in SON. Approximately 60% (40%) belongs to the tropics between 23.5S to 23.5N (subtropics between 23.5 and 66.5) in DJF, 50% (49%) in MAM, 52% (47%) in JJA, 58% (41%) in SON. The maximum number of GCM cells of an MCS cluster and the duration of an MCS cluster has a significant
positive correlation of 0.77 in DJF, 0.80 in MAM, 0.80 in JJA, 0.70 in SON. The positive correlation is expected as long-lived MCS clusters create more dissipating stratiform clouds covering larger areas.

Approximately 10% of the global clusters are long-lived and large clusters, and more than half of these are over the tropical ocean. A cluster is long-lived and large when it lasts at least 12 hours and covers at least 5 GCM cells (≈ 50,000 km²). In the tropics, approximately 73% (DJF), 76% (MAM), 80% (JJA), and 84% (SON) of these clusters are over the ocean. The average maximum cluster size is approximately 3 (2) GCM cells over the ocean (land) in all seasons. The frequency of large clusters over the ocean (land) is approximately 11% (3%). The above statistics show that SPCAM produces more long-lived and large clusters over the ocean. Larger areal coverage over the ocean compared to land is consistent with the idea that MCS sizes are set by the convective sustainability of the environment [Yuter and Houze, 1998]. Where the ocean generally provides warmer air at the boundary layer for new convections with less nocturnal cooling to inhibit convection compared to the land. However, a stronger low-level jets can advect moist maritime air during the night time to counteract diurnal cooling, e.g., larger MCSs east of Andes and east of Rocky Mountains.
Figure 2.2: MCS population. The total number of MCSs passing over each GCM cell is added over the entire season and shown in shading.
Figure 2.3: Accumulated precipitation in each season by the MCSs shown in shading.
Figure 2.2 shows the MCS population in the boreal summer and winter for SP-CAM. In general, the higher population zones are collocated with long-lived and large MCS clusters. Figure 2.3 shows the accumulated precipitation over each GCM cells in each seasons by the detected MCSs. The tropical patterns of MCS population and precipitation closely follow the satellite observation in the boreal summer [Fiolleau and Roca, 2013a; Chambon et al., 2013] in Figure 2.4. Notice the accumulated precipitation in Figure 2.3 is only contributed by the MCSs. The monsoonal rain belt
(e.g., Bay of Bengal) and intertropical convergence zone (ITCZ) features are both well seen.

2.2 A long-lived MCS cluster lifecycle

The persistent rainfall caused by long-lived and large MCSs are often associated with significant and damaging flood events. We examined one of the long-lived and large MCS clusters to assess how realistic the convective organization behaves in SPCAM.

The selected MCS cluster propagated westward from 0.47N 176.25E at local time 11:45 on June-11 to 0.47S 166.25E at local time 14:05 on June-12, remaining over the ocean for the entire lifetime. It grew to a maximum size of 10 GCM cells (≈ 100,000km$^2$) and sustained above 5 GCM cells for at least 6 hours. The MCS cluster propagates westward at an average speed of 8ms$^{-1}$. The propagation speed of the MCS cluster is coarsely estimated from the lower 6km averaged wind over a $7^\circ \times 7^\circ$ centered at the centroid of the MCS cluster. All the horizontal velocity fields shown in the figures are computed relative to the propagation speed.

We define the common parameters used for studying the organization of MCSs here. Observations show that strong thunderstorms are maintained in a sheared environment by producing rotating updrafts at the flanks [Rotunno and Klemp, 1982]. Organized MCSs such as squall lines rejuvenate themselves by older convective cells producing rain-chilled outflows, which interacts with the sheared environment at its gust front [Rotunno et al., 1988]. The rain-chilled gust front is highly rotational due to its sharp horizontal buoyancy gradient with the environment. When this rotational gust front is in a conditionally unstable environment with low-level shear, further lift-
ing can lead to instability with new convective cells ([Rotunno et al., 1988; Mapes, 2000]). The new updraft cells further act to maintain the jump updraft of MCS as a gravity wave response [Raymond, 1984] and enable MCS to propagate to a more buoyant and convection-favoring region. This jump updraft transitions older convective cells to stratiform structures. With sufficient large-scale potential vorticity, the system can evolve into a long-lived MCS with a potential vorticity anomaly supporting stratiform updraft. Thus for long-lived clusters, the key parameters we focused on are the low-level shear, surface buoyancy, and potential vorticity anomaly.

The 0 to 3km low-level environmental shear and Lifted Index (LI) are both included in the potential MCS genesis index ([Jirak and Cotton, 2007]). We defined 0-3km shear as the absolute difference of the SPCAM’s GCM column zonal velocity (i.e., environmental wind for the embedded CRM) at 3km and the lowest model level (approximately 100m). Our results show that the cluster-averaged 0-3km low-level shear have high values of 8.7m s$^{-1}$ and 7.3m s$^{-1}$ over land (7.5m s$^{-1}$ and 8.4m s$^{-1}$ over the ocean) in JJA and DJF, respectively. Both land and ocean show strong shear in the mean sense for the detected MCSs.

The LI is a measure of surface parcel buoyancy, with more negative (positive) values relating to more positive (negative) buoyancy. Hereafter, LI means the zonally averaged LI in the CRM domain since we are concerned about large-scale boundary layer buoyancy. Our results show that the cluster-averaged LI is $-3.66K$ and $-3.43K$ over the ocean ($-2.08K$ and $-1.77K$ over land) in JJA and DJF, respectively. Since values of less than $-1K$ are favored for thunderstorm development, the negative averaged values show the overall importance of LI in MCS organization in SPCAM.
The higher LI over ocean also reflects why most of the long-lived large clusters are over ocean in Figure 2.2.

Potential vorticity (PV) anomaly is a signature for long-lived MCS owing to the large-scale stratiform heating created updraft [Hertenstein and Schubert, 1991]. With slight modification according to Raymond and Jiang [1990], when vertical velocity is weak, the total potential vorticity can be approximated as

\[ q = \frac{1}{\rho} \left[ -\frac{\partial v}{\partial z} \frac{\partial \theta}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial \theta}{\partial y} + (f + \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}) \frac{\partial \theta}{\partial z} \right] \]  \hspace{1cm} (2.1)

and the mean potential vorticity

\[ q_0 = \frac{f}{\rho_0} \frac{d\theta_0}{dz}, \]  \hspace{1cm} (2.2)

where \( \theta_0 \) and \( \rho_0 \) are the zonally averaged ambient vertical profiles in the CRM domain. Thus the potential vorticity anomaly

\[ q' = q - q_0. \]  \hspace{1cm} (2.3)

Notice we used the Potential Vorticity Unit (PVU) where 1 PVU = \( 10^{-6} \) m\(^{-2}\) s\(^{-1}\) K kg\(^{-1}\). Despite the fact that PV anomaly may not be a sufficient condition for identifying MCS genesis potential [Jirak and Cotton, 2007], it can still be used for identifying the dynamical response of convection development in the detected MCS.

We will further examine the systematic differences in CAM’s convective parameterized response in the MCS environment given the SPCAM fields. Three major GCM column fields we examined are the cumulus heating source \( Q_{1c} \) (i.e., the apparent heat source \( Q_1 \) without the GCM column radiative heating), apparent moisture sink \( Q_2 \), and eddy moist static energy flux \( Q_{1c}-Q_2 \). The three variables are the bulk response of the large-scale environment given the embedded cumulus cloud ensembles
and are originated from the groundbreaking work by Yanai et al. [Yanai et al., 1973].

Where

\[ Q_1 = \frac{\partial \bar{s}}{\partial t} + \nabla \cdot sV + \frac{\partial s\bar{\omega}}{\partial p} = Q_R + L(c - e) - \frac{\partial s'\omega'}{\partial p} \]  

(2.4)

thus

\[ Q_{1c} = Q_1 - Q_R. \]  

(2.5)

Where the radiative heating \( Q_R \), dry static energy \( s = c_pT + gz \), latent heat of condensation \( L \), condensation rate \( c \), re-evaporation rate \( e \), vertical velocity \( \omega \), and horizontal velocity \( V \). Similarly

\[ Q_2 = -L\left(\frac{\partial \bar{q}}{\partial t} + \nabla \cdot qV + \frac{\partial \bar{q}\bar{\omega}}{\partial p}\right) = L(c - e) + L\frac{\partial q'\omega'}{\partial p}. \]  

(2.6)

Finally, the total heating from vertical eddy transport becomes

\[ Q_{1c} - Q_2 = -\frac{\partial}{\partial p}(s' + Lq')\omega', \]  

(2.7)

where \( s' + Lq' \) is the eddy moist static energy. The \( \bar{\ } \) represents the large-scale horizontal average, and \( (\ )' \) represents the deviation from the average. Dividing both \( Q_{1c} \) and \( Q_2 \) by a constant heat capacity of air \( c_p \) changes the units from J day\(^{-1}\) to K day\(^{-1}\), we will hereafter use \( Q_{1c} \) and \( Q_2 \) as a convenient shorthand for \( Q_{1c}/c_p \) and \( Q_2/c_p \). An “offline” evaluation of CAM’s \( Q_{1c} \) and \( Q_2 \) are computed as:

\[ Q_{1c} \text{ or } Q_2 = P_{\text{deep}} + P_{\text{evap/snow}} + P_{\text{shallow}} + P_{\text{micro}} + P_{\text{macro}} = \sum_{i=1}^{5} P_i, \]  

(2.8)

where \( P_i \)'s are just the parameterized heating or moisture sink processes from CAM. The two models’ outputs are compared at the same timesteps using identical instantaneous state inputs, thus does not induce initial condition errors to the integration. The only difference between the two models will be caused by their individual parameterized moist convection physics.
Figure 2.5: Horizontal 3-hourly snapshots of the field evolution surrounding an MCS cluster (black boxes). The figure is centered at the MCS cluster centroid latitude and longitude with a dashed line overlapping the 850-200hPa deep shear unit vector (black arrow). Fields include the 0-3km low level shear (shading) and total precipitation rate of 1 mm hr$^{-1}$ and 3 mm hr$^{-1}$ (red contours).
Figure 2.6: Similar to Figure 2.5, but with the fields LI (shading) and surface $\theta_e = -3$K anomaly (pink dashed contour). The velocity field is computed relative to the MCS cluster westward propagation velocity.
2.2.1 Plan view

Figure 2.5 and 2.6 show the 3-hourly snapshots of the long-lived MCS. The active MCS cluster started out with one GCM cell in (a) and gradually evolve into a multi-cell meridionally elongated cluster in (e). The meridional elongation is also shown in the total precipitation rate contour. The cluster is embedded in a negative low-level 0-3km sheared environment in Figure 2.5 throughout its lifetime. The cluster propagates westward to a more buoyant environment with stronger LI in Figure 2.6 (f). This westward propagation is a result of cold pool dynamics, where rain-chilled outflow in a sheared and buoyant environment creates lifting and leads to downshear (i.e., westward) development of new convective cells. As the cluster propagates westward, we see from Figure 2.6 (f) that the inflow with stronger LI is forced into the system and the cluster extends its life cycle.

A negative equivalent potential temperature anomaly contour is shown throughout Figure 2.5. This is the return flow of the stratiform rain-induced downdraft cold anomalous air of an organized MCS system. Notice the negative contour is always located down the deep shear vector. This shows that there is some tilting of the updraft flow creating dissipating stratiform clouds towards the east of the system. The tilting will be shown later when taking a vertical cross-section over the dashed-line outlined by the deep shear vector.
2.2.2 Vertical view

2.2.2.1 SPCAM

Figure 2.7: The surrounding fields of the MCS cluster on the vertical plane drawn from the dashed line in Figure 2.5 (a). The 0km on the horizontal axis indicates the MCS cluster centroid latitude and longitude. Notice the three transparent black arrows are hand-drawn to emphasize the squall line-like branch flows. The fields include the Q1c (shadings), $\theta_e$ anomaly (pink contour), and PV anomaly (dark blue contour). The relative velocity vector field of horizontal and vertical wind is scaled by 0.1, and 10, respectively.
Figure 2.7 shows the vertical cross section of the Q1c surrounding the MCS cluster. As previously mentioned, the vertical cross section is sampled along the MCS propagation direction (i.e., dashed black line in Figure 2.5 (a)). The MCS cluster horizontal relative wind vectors $\vec{u} = (u, v)$ are projected onto the unit deep shear vector $\vec{u}_s$, by simply taking the dot product $\vec{u} \cdot \vec{u}_s$, where a unit vector is the original vector divided by its length. This projected value (i.e., dot product) is the new horizontal wind speed used in Figure 2.7. This allows one to see the amplitude of the full horizontal velocity in the direction of the deep shear vector, as opposed to using zonal or meridional velocity alone.

The MCS cluster propagates westward according to the low-level shear vector (i.e., downshear). The three hand-drawn black arrows, a jump updraft and two overturning flows, indicate the existence of squall line-like mean flow pattern [Moncrieff, 1992, 2010] (Figure 2.8) in the background field. This squall line-like flow persisted and strengthens (i.e., deep shear magnitude increases approximately 1ms$^{-1}$ from start to end of life cycle) through the life cycle. The flow mechanics are fundamentally distinct from classical mass-flux-based parameterization as used in CAM’s deep convection. According to up-gradient momentum transport [LeMone, 1983; Moncrieff and Klinker, 1997], the horizontal pressure gradient force from the
inflow jet and positive buoyancy from the deep convective plume accelerate the mean flow. Pritchard et al. [2011] show that CAM’s deep convection scheme produces a down-gradient mixing of horizontal momentum, which slows down the mean flow and counteracts the organization process. The correct representation of the up-gradient momentum transport shows the SPCAM resolving organized convective system, and is the major finding in our study.

The positive convective heating shading shows a gradual deepening from $-400\text{km}$ to $400\text{km}$, which indicates the rejuvenation of convective cloud downshear of the system with high $\theta_e$ inflow air located at $-400\text{km}$. The stratiform layer trails the convective line and is a consequence of dissipating convective cells. The trailing edge at $500\text{km}$ shows stratiform cooling and the subsiding low $\theta_e$ dry air entrained by the overturning downdraft. Notice the stratiform cloud may be trailing or leading the convective line throughout the life cycle depending on the propagation speed [Parker and Johnson, 2000, 2004].

A significant positive PV contribution of $0.5$ PVU contour collocates with the stratiform cloud deck. Raymond and Jiang [1990] shows that PV anomaly is largely due to convection redistributing mass, where removing (adding) mass between two isentropic surfaces causes positive (negative) PV anomaly. The positive PV anomaly from stratiform updraft may be the precursor for long-lived MCS.
Figure 2.9: The Q1c, Q2, and Q1c-Q2 (shadings) comparison between SPCAM (left) and CAM (right) sampled at 0-hour lifetime over the black dashed line of Figure 2.5 (a) as Figure 2.7.
Figure 2.10: Similar to Figure 2.9, but sampled at 12-hour lifetime over the black dashed line of Figure 2.5 (e).
Figure 2.11: Similar to Figure 2.9, but sampled at 27-hour lifetime over the black dashed line of Figure 2.5 (j).
2.2.2.2 SPCAM v.s. CAM

Figure 2.9 - 2.11 are the vertical cross sections of the Q1c, Q2, and Q1c-Q2 sampled at the associated lifetime.

In Figure 2.9 (b), CAM shows a low to mid-level “cooling response” with a moisture source peak in (d) above $z = 2$km ($\sim 800$hPa) near 400km. This cooling with moisture source above $z = 2$km is collocated with deep convection heating with moisture sink in SPCAM (c). At the same location, SPCAM shows strong convective updraft, high rain rate, and low cloud base (not shown but approximately follows the zero Q1c shading). According to the idealized large-scale heating profile [Schumacher et al., 2004], this low to mid-level cooling response is due to high stratiform fractional rain rate (i.e., greater than 70%). In observations, the stratiform cooling coexists with mesoscale downdraft, weak stratiform rain, and mid-level cloud base. These conditions favoring the cooling are closer to 600km, as oppose to 0km to 500km. This cooling response is the major caveat of CAM when deep convection condition from SPCAM are fed to the offline computation, and persists throughout the active MCS life cycle.

There are two moisture sink peaks in SPCAM at approximately 3km and 7km in Figure 2.9 - 2.11 (c), which is also observed in nature [Zermeño-Díaz et al., 2015] during active phases of large MCSs. Whereas in CAM, there is no moisture sink but a moisture source at 3km throughout the MCS life cycle. Moreover, the maximum Q1c, Q2, and Q1c-Q2 above 4km from SPCAM are on the order of 10 K day$^{-1}$ larger than that of CAM over the life cycle. These results indicate that the deep convection is either weak or absent in the GCM cells over the MCS lifecycle of CAM.
In conclusion, a squall-like circulation is detected in SPCAM with conditions favoring long-lived MCS. SPCAM shows a deep convective heating profile with CAM responding as a stratiform-like dipole heating profile over the deep convection core and the rejuvenated convective cells.

![Graph](image)

Figure 2.12: Decomposition of CAM’s parameterized scheme at the centroid GCM cell at 0h lifetime of the selected cluster case. The Q1\textsubscript{CAM} is the offline evaluation of the CAM’s total parameterized cumulus heating. The total heating is just the sum of all decomposed heating according to equation 3.1.

### 2.2.2.3 CAM parameterization

CAM has major discrepancies in the convective parameterization, which creates a stratiform-like cooling profile in a deep convection favoring environment as previously shown. CAM uses five sequential parameterizations to update the heat tendency, namely the deep convection [Zhang and McFarlane, 1995], convective evaporation...
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[Sundqvist, 1988], shallow convection [Park and Bretherton, 2009], stratiform microphysics [Morrison and Gettelman, 2008], and stratiform macrophysics [Park et al., 2014]. Figure 2.12 shows that the stratiform microphysics is the major contributor to the stratiform cooling below 3km. The stratiform microphysics cooling overwhelms the weaker deep convective heating below 3km.

2.3 Summary

We developed an algorithm to detect and cluster the MCSs in SPCAM. As expected, most of the long-lived large clusters are over the warm ocean in the tropics. The strong low-level shear and high surface buoyancy provide a favorable environment for the downshear development of organized MCS.

We studied a long-lived large MCS cluster and found some results distinguishing the convective organization processes of SPCAM from CAM:

1. For SPCAM, the long-lived MCS cluster shows realistic squall line-like circulations over the GCM cells throughout the lifecycle. Studies have identified similar circulation in the cloud-scale 2D CRM cells in SPCAM [Pritchard et al., 2011]. The circulation in the 2D CRM and the GCM cells thus show self-similarity across scales [Mapes et al., 2006; Moncrieff et al., 2017]. The growth of deep shear indicates that the upgradient momentum transport is presumably the main mechanism of the enhanced squall line-like circulation. This differentiates SPCAM from traditional mass-flux-based climate models with downgradient mixing effects.
2. Regions of deep convection profiles in SPCAM are replaced by strong stratiform rain-evaporative cooling in CAM. The experiment is set up so that SPCAM and CAM respond to the exact same states, so the regions with hydrometeors and strong updraft supporting deep convection should not have stratiform cooling existing. Hence SPCAM is presumably better in capturing the response of deep convection. This is solely an argument based on the response of CAM given the deep convection favoring states from SPCAM. A future comparison of SPCAM and CAM’s response to a given observational state favoring deep convection could provide further validation.

3. CAM’s stratiform microphysics is presumably the major scheme producing the strong low-level cooling at regions of deep convection for SPCAM.

We identified the self-similarity of squall line-like morphology on the scale of GCM cells for SPCAM, and a systematically biased stratiform mode response for CAM. A further composite study will generalize the findings to MCS clusters in the tropics and sub-tropics. The MCSs are the major contributor to rainfall variability in both regions, with latent heat release greatly affecting the general circulation. The detection and clustering algorithm can be applied to climate change experiments in SPCAM (e.g., [Hannah and Aiyyer, 2017]) to examine atmospheric circulation (e.g., [Wu et al., 2013]) impacted by MCSs. This will allow an unprecedented view on how MCSs contribute to climate change and the impacts from CAM’s weaker deep convection mode. In addition, we propose to utilize the two model timestep-wise difference of the GCM column profiles (similar to [Shutts and Palmer, 2007; Chen et al., 2015]) to develop a stochastic scheme for the deterministically parameterized CAM. We suggest enhancing (weakening) the deep convection (stratiform) response in CAM by
the stochastic scheme to improve upscale organization process missing in mass-flux based parameterization.
CHAPTER 3

Composite analysis of MCS clusters

To further show that the organized processes apply to the entire cluster samples, we applied the MCS lifecycle composite analysis of the GCM output convection-related fields in 3.2 and 3.3. Realistic diversified deep convection and stratiform modes with a growth to decay lifecycle in SPCAM are shown in this section. A strong stratiform mode response of CAM is shown for both heating and moisture profiles. The lack of diverse modes is a result of missing subgrid-scale physics caused by CAM’s deterministic parametrization. Therefore we propose a stochastic scheme in section 3.4 to induce the subgrid effects in the deterministic parametrization by stochastic perturbation from SPCAM’s outputs.

3.1 Materials and methods

The detection and clustering method to obtain MCS cluster samples are shown in our previous study [Chen and Kirtman, 2018]. We have appended an extra sample to both the starting and ending time of the detected clusters. For instance, if a detected cluster is only a single timestep (i.e., 3 hours), then the appending makes it a three-timestep cluster. The extra two timesteps represent the growth- and decay-phase samples of this active MCS cluster. Therefore all detected clusters will have at least
three timesteps to represent the three phases of MCS lifecycle from growth, mature to decay (i.e., 0%, 50% to 100% lifetime).

The total detected clusters in the two selected seasons are 8,931 in JJA and 8477 in DJF. Approximately 52% (47%) belongs to the tropics (subtropics) in JJA, 60% (40%) in DJF and less than 1% travel between or beyond the two zones. Tropics is 23.5S to 23.5N, and subtropics is 66.5S to 23.5S and 23.5N to 66.5N. We defined an MCS cluster to belong to one zone if it stays 90% of its life cycle there. In the tropics, approximately 73% (27%) are ocean (land) clusters in JJA and 64% (36%) in DJF. In the subtropics, approximately 60% (40%) are ocean (land) clusters in JJA and 82% (18%) in DJF. A land cluster stays over the land for its entire lifetime, otherwise defined as an ocean cluster.

Three different composite analyses are performed on the detected cluster samples:

1. Percentage lifetime composite analysis following Fiolleau and Roca [2013b] to interpolate the MCSs onto the same time frame allows understanding of the mean features of MCS lifecycle. A cluster is horizontally averaged over the GCM cells at each timestep and interpolated onto the same time frame. Thus with vertical and time dimensions remaining.

2. Contoured Frequency by Altitude Diagrams (CFAD) [Yuter and Houze Jr, 1995] are performed at the three MCS phases: 0%, 50%, and 100% lifetime. This allows more samples of the vertical profiles to be used without the previously applied horizontal averaging.

3. Principal Component Analysis (PCA) is separately applied on vertical profiles of all three aforementioned MCS phases. The PCA will filter out the highest
variance vertical modes of Empirical Orthogonal Functions (EOFs), and relate the two models from Principal Component (PC) correlations.

A matured MCS shows convective and stratiform clouds providing different feedback mechanisms to maintain the organized system and generate diverse precipitation. Thus in order to study the vertical structure of the detected MCS in SPCAM, we applied a slightly modified algorithm from Sui et al. [2007] to handle separation of convective and stratiform rain in the 2D CRM:

1. Precipitation greater than 20 mm h$^{-1}$ is classified as convective.

2. When a cell with rain rate twice as large as the average of both neighboring cells, this cell and its neighboring cells are classified as convective.

3. All other cells will be classified as stratiform, unless the following convective criteria are met:

   (a) When precipitating (rain rate greater than 0.1 mm h$^{-1}$), (1) cloud water exceeds 0.05 g kg$^{-1}$ below the melting level, or (2) updraft above 600 mb exceeds 5 m s$^{-1}$.

   (b) When non-precipitating (rain rate less than 0.1 mm h$^{-1}$), (1) cloud water exceeds 0.025 g kg$^{-1}$, or (2) updraft below melting level exceeds 5 m s$^{-1}$.

This algorithm extracts and zonally large-scale averages the cloud-scale fields only on the MCS with the largest raining core in the 2D CRM columns. The large sample mean field life cycle in the following section using the convective-stratiform separation algorithm does not have a sensitive dependence on small changes to the threshold values (e.g., rain rate, and cloud water mixing ratio thresholds).
We applied percentage lifetime analysis on the fractional rain rate and vertical velocity fields conditioned on the convective and stratiform clouds obtained from the embedded CRMs in SPCAM. This is to show the response of MCS in the 2D CRM cells limited to SPCAM. For the two model comparison, we used all three composite analyses on the Q1c and Q2 from the GCM cells.

**Figure 3.1:** Composite fractional rain rate of convective and stratiform clouds over ocean and land. Fractional rain rate is calculated by summing the conditioned rain rate and divide by the total rain rate in each MCS cluster. The median composite is done over all MCS clusters in each season.
3.2 MCS composite lifecycle: SPCAM

Figure 3.1 shows the monotonic increasing stratiform fractional rain rate, indicating the clusters grew with more stratiform cloud coverage with relatively less convective rain rate with time. The only exception is over the ocean in the subtropics in both seasons, where the stratiform fractional rain rate increases before 50% lifetime and decreases afterward. The weakening stratiform fractional rain rate indicates the clusters are decaying after 50% lifetime.

The decaying of stratiform fractional rain rate after 50% lifetime and the low convective fractional rain rate from the beginning both indicate that the ocean in subtropics is unfavorable for MCS growth. To explain what causes the unfavorable condition, and why subtropics still supports active MCS, we look at two of the most important MCS genesis potential indices: Lifted Index (LI) and 0-to-3km low-level shear. The composite LI is highly positive (i.e., negatively buoyant) throughout the composite lifecycle over the ocean (LI ≈ 4) and land (LI ≈ 1) in the subtropics, which indicates an unfavorable condition for MCS upscale growth. Whereas in the tropics, the composite LI stays highly negative over the ocean (LI ≈ −3) and land (LI ≈ −2) throughout the composite lifecycle to support MCS upscale growth. The reason why the subtropics still supports MCSs, despite unfavorable LI, can be explained by the higher 0-3km low-level zonal shear. Low-level shear is a required condition for MCS upscale growth. In the subtropics, the ocean (land) has mean absolute low-level shear of approximately 14m s$^{-1}$ (11m s$^{-1}$) throughout the composite lifecycle. The values are higher compared to the tropics with ocean (land) of approximately 7m s$^{-1}$ (9m s$^{-1}$). Therefore MCS cluster composite is still supported by low-level shear-generated lifting in the subtropics.
Due to the similarities of the composite profiles between JJA and DJF, we will hereafter focus on just the summer season JJA.

**TROPICS**

**OCEAN**

(a) convective

**LAND**

(b) convective

(c) stratiform

(d) stratiform

Figure 3.2: Composite of vertical velocity (shaded) of the convective and stratiform region over the ocean and land. Ice mixing ratio of convective clouds (dark red contour, higher values are thicker) and non-precipitating liquid water mixing ratio of stratiform clouds (dark blue contour) spaced at 0.02 g kg$^{-1}$ starting from 0.02 g kg$^{-1}$. 
Figure 3.2 shows the composite lifecycle of vertical velocity conditioned on convective and stratiform rain in the tropics. Convective cloud shows the composite updraft reaches 400hPa and peaks at 600hPa over both ocean and land. The updraft reaches a maximum at 50% lifetime and gradually weakens. The peak updraft gives a maximum ice mixing ratio at 200hPa near 50% lifetime. Over the land, the weaker convective updraft at 700hPa, and weaker ice water peak at 200hPa in Figure 3.2 (b) is associated to the less fractional convective rain over land in Figure 3.1 (a) and (c). Which indicates that land is generally dryer with weaker convective cells and rain.

Stratiform cloud shows low- to mid-level downdraft peaking at 700 to 800hPa, with relatively weak updraft above 500hPa. The upper-level updraft in MCS is caused by the convective jump updraft flow which is crucial for ice particles to grow by vapor deposition and falls out as stratiform rain. The peak of the liquid water mixing ratio at 600hPa is related to the 0C radar bright band created by ice melt, which is a character of MCS stratiform cloud. The stronger stratiform downdraft at 700hPa and liquid water peak at 600hPa are associated with higher fractional stratiform rain over land in Figure 3.1 (a) and (c).

Figure 3.3 in the subtropics, the convective updraft peaks much lower over the ocean at 800hPa compared to the tropics in Figure 3.2. As mentioned earlier, the weak buoyancy (i.e., positive LI) is the main reason for the weak convection, which also leads to significantly weaker stratiform downdraft.
Figure 3.3: Composite of vertical velocity (shaded) of the convective and stratiform region over the ocean and land. Ice mixing ratio of convective clouds (red contour) and non-precipitating liquid water mixing ratio of stratiform clouds (blue contour) spaced at 0.01 g kg$^{-1}$ starting from 0.05 g kg$^{-1}$. 
3.3 MCS composite lifecycle: SPCAM vs. CAM

The previous section showed SPCAM capturing the fundamental cloud-scale structures of MCS with regional variability in the composite sense. This composite result and the previous case study of a realistic upscale organization [Chen and Kirtman, 2018] provides a qualitative basis to further compare the composite responses of the two climate models. The question is whether SPCAM remains superior in resolving a growth to decay transition of MCS cluster composite and if CAM is still systematically biased. As previous case study [Chen and Kirtman, 2018] pointed out, CAM shows systematic low-level stratiform cooling and moistening response to a deep convection-favoring environment given by SPCAM. We are motivated to show that the conclusions can be applied to the composite studies on the two major GCM output fields: apparent cloud heating (Q1c) and apparent moisture sink (Q2).

When deep convection mode or stratiform mode are mentioned, we are referring to the GCM’s large-scale averaged Q1c or Q2 profile being deep convection-like or stratiform-like.

3.3.1 Mean Q1c lifecycle

According to the idealized heating profile [Schumacher et al., 2004], the deep convection mode (greater than 50% convective fractional rain rate) has a peak heating between 700hPa and 400hPa. There is also a surface cooling depending on the fraction of stratiform rain rate. Whereas stratiform mode (greater than 50% stratiform rain rate) has a peak heating above 400hPa and a strong cooling below 700hPa.
Figure 3.4: Composite lifecycle of Q1c in JJA. All clusters’ lifetime are linearly interpolated onto an evenly spaced percentage lifetime. The median composite is performed.
Figure 3.5: Composite lifecycle of Q1c in JJA. All clusters’ lifetime are linearly interpolated onto an evenly spaced percentage lifetime. The median composite is performed.
Figure 3.4 shows tropics Q1c for SPCAM (top), CAM (middle), and the difference of the two (bottom). SPCAM’s Q1c in (a) and (b) is dominated by a deep convection mode throughout the lifecycle. The stratiform cooling gradually cancels out the low-level heating near 700hPa at later lifecycle.

As a stark contrast in (c) and (e), CAM shows a strong Q1c stratiform dipole heating mode (greater than 70% of stratiform rain fraction [Schumacher et al., 2004]) throughout the entire period. As pointed out in the case study [Chen and Kirtman, 2018], the strong stratiform cooling profile shows up at the cumulonimbus core of an active MCS. Therefore the stratiform dipole heating mode is a systemic bias caused by CAM’s convective parametrization. The composite Q1c difference of SPCAM and CAM in (e) shows a peak near 700 (≈ 3km) exceeding 30 K day$^{-1}$ over both ocean and land.

Figure 3.5, subtropics ocean Q1c in (a) shows a deep convection mode that has relatively lower fractional stratiform rain rate compared to tropics ocean Q1c (a) in Figure 3.4. Given less stratiform rain rate, CAM’s Q1c in (c) also responds with much less stratiform cooling bias.

3.3.2 Mean Q2 lifecycle

Figure 3.6 (a) and (b) show SPCAM with two strong moisture sinks on the order of 25 K day$^{-1}$ at 700hPa and 400hPa. These two moisture sinks are related to deep convection condensation peaks at 700hPa and 400hPa as seen in Yanai et al. [1973].
Figure 3.6: Composite lifecycle of Q2 in JJA. Computed as Figure 3.4.
Figure 3.7: Composite lifecycle of Q2 in JJA. Computed as Figure 3.5.
A single Q2 peaking at 400hPa in the late lifecycle indicates decaying MCSs with increasing stratiform downdraft moisture source at the low levels canceling out the moisture sink at 700hPa. This moisture sink evolution is also seen in large organized convective systems [Zermeno-Diaz et al., 2015]. Therefore SPCAM’s Q2 composite also satisfies the expected growth to decay lifecycle.

As a stark contrast in the ocean (c) and land (d), CAM shows a stratiform moisture source dominating below 600hPa throughout the entire lifecycle. The moisture source becomes strongest at 50%, collocated with the strongest cooling in Figure 3.4 (c) and (d), which is supposed to be at the strongest deep convection phase of MCS in SPCAM. The composite difference in (e) and (f) shows the peak value at 700hPa, which is associated with the strongest moisture source of CAM and the strongest moisture sink of SPCAM.

### 3.3.3 Probabilistic distribution of Q1c and Q2 with height

So far the case study [Chen and Kirtman, 2018] and composite study show consistency, with SPCAM showing upscale growth to decay MCS cluster lifecycle, and CAM showing stratiform biased Q1c and Q2 modes. For a probabilistic comparison of the vertical profiles at a fixed lifetime, we performed the Contoured Frequency by Altitude Diagrams (CFAD from [Yuter and Houze Jr, 1995]) on Q1c and Q2 profiles at the mature phase (i.e., 50% lifetime).
Figure 3.8: Contoured Frequency by Altitude Diagram (CFAD) of Q1c at 50% lifetime for tropics. The probability distribution of Q1c at each level is individually obtained. The bin size of Q1c is equally spaced at 0.5 K day\(^{-1}\) to get the probability mass.
Figure 3.9: Figure 3.8 continued for subtropics.
Figure 3.10: CFAD of Q2 at 50% lifetime for tropics.
SUBTROPICS Q2

Figure 3.11: Figure 3.10 continued for subtropics.
Figure 3.8 shows a significant contrast of Q1c profile between SPCAM and CAM in the tropics. The shape between 10- and 90-percentile of both models follow approximately the mean vertical profile, i.e., deep convection (stratiform) mode for SPCAM (CAM). The difference (bottom) shows the highest variance at 700hPa, which is where stratiform cooling shows up in CAM when SPCAM has deep convection heating.

Figure 3.9 over the ocean (a) and (c) shows less dramatic difference at the lower levels. As pointed out in the case study [Chen and Kirtman, 2018], when MCS clusters weaken with negatively buoyant boundary layer air (LIA<0) in SPCAM, the stratiform biased mode also weakens in CAM. In (e), we can see that the two model difference at below 600hPa is much smaller than in Figure 3.8 (e). Therefore in the composite study, we see that a stronger deep convection with strengthened stratiform clouds also leads to more Q1c difference between the two models.

Figure 3.10 (a), Q2 shows the double-peaked moisture sink at 400hPa and 700hPa associated to deep convection. The second peak at 400hPa is absent over the ocean in the subtropics (Figure 3.11 (a)). Similar to the Q1c conclusion, the stronger (weaker) deep convection and stratiform clouds leads to more (less) Q2 difference at below 600hPa in (e) (in Figure 3.11 (e)).

3.3.4 Vertical variance mode decomposition

We have shown that SPCAM follows a strengthening to weakening deep convection Q1c and Q2 “mean” mode. Whereas CAM reacts as a strengthening to weakening stratiform mode. The CFAD analysis also shows that 10%- and 90%-tile are following the shape of the mean. But are the variations actually contributed by the mean mode, or are there modes that contribute to the variance that are hidden in the
data? Principal Component Analysis (PCA) [Zhang and Hagos, 2009; Siqueira and Kirtman, 2016] will provide the highest variance modes (i.e., Empirical Orthogonal Function (EOF)). The correlations of the two models can then be done on the Principal Component (PC) samples associated to the highest variance EOF modes. This allows us to analyze whether CAM’s Q1c or Q2 coherently respond to SPCAM. In our study, the EOF is a function of height and PC is a function of the MCS vertical profile samples.

We only use the top two highest variance modes (i.e. EOF1 and EOF2), and their associated PC correlation between the two models. The EOF1 and EOF2 are associated with PC1 and PC2 variances ordered by their magnitude. The percent variance (%Var) is the individual PC variance of a mode divided by the total sum of the variance of all modes and multiplied by 100. The magnitude of the %Var shows the relative contribution of each mode to the total variation of the cluster population. Also, we will focus on the mode evolution (0%, 50%, and 100%) in the tropics since the results are very similar in the subtropics. The sign of the EOF mode is objectively determined by the associated mean PC value multiplied by the EOF mode. Despite being objective, the mean PC value may sometimes be near zero, which makes the sign less meaningful.

### 3.3.4.1 Variance modes of Q1c

Figure 3.12 (a) at 0% lifetime over the ocean, the deep convection mode of EOF1 has %Var dominating over stratiform mode EOF2 in SPCAM. This EOF1 is similar to the shape of the mean Q1c mode in Figure 3.8 (a).
**TROPICS Q1c 0% lifetime**

**OCEAN**

(a) SPCAM

(b) SPCAM

**LAND**

(c) CAM

(d) CAM

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Figure 3.12: EOF modes and PC correlation table for Q1c in the tropics at 0% lifetime.
Figure 3.13: Figure 3.12 continued.
Figure 3.14: Figure 3.13 continued.

Whereas over the land in (b), EOF1 is a stratiform mode which does not match the mean deep convection Q1c mode in Figure 3.8 (b). We suspect the higher variance
in stratiform mode is related to the larger stratiform fractional rain rate observed in Figure 3.1.

Figure 3.12 (c) shows EOF1 as stratiform mode and EOF2 as a weaker stratiform mode or shallow cumulus-like mode (i.e, fair weather cumulus and cumulus congestus shown in Schumacher et al. [2004]) when sign flips. The PC correlation of 0.59 is highest between the stratiform modes of both models. The second highest correlation (0.32) is between both modes of SPCAM and stratiform mode of CAM. This indicates that CAM’s stratiform mode is highly responsive to both modes of SPCAM. Over the land in (b) and (d), the two models show the highest correlation in the stratiform mode.

Figure 3.13 in the mature phase (50% lifetime) over the ocean, (a) and (c) shows the highest correlation becomes shared between the two modes of SPCAM with the stratiform mode of CAM. This indicates that CAM responds strongly as a stratiform Q1c mode irrespective of the given conditions. Whereas over the land in (b) and (d), the highest correlation (-0.69) is still between the stratiform EOF1 modes of the two models.

Figure 3.14 in the decay phase (100% lifetime) over the ocean, (a) and (c) shows the highest correlation (0.72) between the stratiform modes of the two models. A second highest correlation of 0.44 is seen between the deep convection EOF1 mode of SPCAM and weak stratiform EOF2 mode of CAM. The two correlations indicate that CAM is still responding mostly as a stratiform-like mode to SPCAM’s deep and stratiform conditions. Whereas over the land in (b) and (d), there is a comparable correlation of 0.55 and -0.54 of between both SPCAM’s modes and CAM’s (shallow- and stratiform-like) EOF1 mode.
TROPICS Q2 0% lifetime

OCEAN

(a) SPCAM

(b) SPCAM

LAND

(c) CAM

(d) CAM

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Figure 3.15: EOF modes and PC correlation table for Q2 at 0% lifetime.
TROPICS Q2 50% lifetime

OCEAN

(a) SPCAM

(b) SPCAM

(c) CAM

(d) CAM

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Figure 3.16: Figure 3.15 continued.
TROPICS Q2 100% lifetime

OCEAN

(a) SPCAM

(b) SPCAM

(c) CAM

(d) CAM

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Figure 3.17: Figure 3.16 continued.
3.3.4.2 Variance modes of Q2

Figure 3.15 (a) at 0% lifetime over the ocean, SPCAM has highest %Var in a double sink deep convective EOF1 mode and a dipole stratiform EOF2 mode. In (c), CAM shows two low- to mid-level moisture source EOF1 and EOF2 modes. The highest correlation (0.51) is between CAM’s stratiform-like EOF1 and SPCAM’s stratiform EOF2 mode. Over the land, SPCAM’s EOF1 in (b) shows a weaker deep convection profile having the highest correlation (0.53) to CAM’s weaker deep convection EOF1 mode in (d).

Figure 3.16 at 50% lifetime over the ocean, the same conclusion can be drawn as 0% lifetime, i.e., the two models have the highest correlation (0.56) in the stratiform modes. Over the land, SPCAM’s shallow convection EOF1 mode in (b) shows the highest correlation (-0.47) to CAM’s stratiform dipole EOF1 mode. The second highest correlation (0.44) is between the weaker stratiform EOF2 modes of the two models.

Figure 3.17 at 100% lifetime over the ocean, the two models have the highest correlation (0.51) between SPCAM’s stratiform EOF1 mode and CAM’s stratiform-like EOF1 mode. Over the land, SPCAM’s stratiform-like EOF2 mode has the highest correlation (0.60) to CAM’s stratiform-like EOF1 mode. Whereas SPCAM’s shallow convection EOF1 mode has the second highest correlation (0.55) to CAM’s shallow convection EOF2 mode.
Figure 3.18: Normalized mean profiles of CAM’s Q1c and Q2 parametrizations at 0% lifetime in JJA over the ocean. The means are normalized by its vertical standard deviation to compare the shape of each parametrization.

3.4 Relating to the stochastic parametrization

In previous sections, we have shown the SPCAM’s ability to represent MCS multiscale organization. We have also obtained the statistical relationships of Q1c and Q2 modes between the two models. This section will show how to use these relationships to model the missing MCS organization effects by stochastically parameterizing the deterministic scheme of CAM.

There are five main parametrization schemes to determine the Q1c and Q2 in CAM, namely the deep convection [Zhang and McFarlane, 1995], convective evaporation [Sundqvist, 1988], shallow convection [Park and Bretherton, 2009], stratiform
microphysics [Morrison and Gettelman, 2008], and stratiform macrophysics [Park et al., 2014]. In a generalized form

\[ Q_{1c}^{\text{CAM}} = P_{\text{deep}} + P_{\text{evap/snow}} + P_{\text{shallow}} + P_{\text{micro}} + P_{\text{macro}} = \sum_{i=1}^{5} P_i, \quad (3.1) \]

where the parametrizations are written in the order, \( i \), of state updates. i.e., the state updated by \( P_{\text{deep}} = P_1 \) is given to \( P_{\text{evap/snow}} = P_2 \), and so on. This is how CAM ensures a balance between parametrizations.

Figure 3.18 shows the composite means over all MCS clusters of the parametrizations in CAM. The \( P_{\text{deep}} \) is showing up as the deep convective EOF1 of SPCAM. The \( P_{\text{evap}}, P_{\text{micro}}, \) and \( P_{\text{macro}} \) all show a stratiform-related profile. This indicates that \( P_{\text{deep}} \) is overwhelmed by the three schemes that give CAM a strong stratiform mode. Multiplying the \( P_{\text{deep}} \) with a larger number and the other stratiform related \( P_i \) by smaller numbers brings the profile closer to SPCAM. Therefore assume the relationship of \( Q_{1c} \) at a given time and height can be approximated by

\[ Q_{1c}^{\text{SPCAM}} \approx Q_{1c}^{\text{CAM}} + \sum_{i=1}^{5} r_i P_i = \sum_{i=1}^{5} (1 + r_i) P_i. \quad (3.2) \]

This is the multiplicative noise formulation [Arnold et al., 2013] related to stochastic parametrization when \( r_i \) is substituted by a random variable. Essentially adding some stochasticity to the parameterized CAM fields to imitate the MCS organization in SPCAM. We proposed an approach to determine the stochastic \( r_i \). Suppose \( y = Q_{1c}^{\text{SPCAM}} - Q_{1c}^{\text{CAM}} \), equation 3.2 becomes

\[ y = \sum_{i=1}^{5} r_i P_i. \quad (3.3) \]

The known values from the model outputs are \( y \) and \( P_i \), and vector \( r = [r_1, \ldots, r_5] \) is the only unknown. \( r \) is determined by the least squares approximation at each of
the N time samples. PCA applied to this N × 5 matrix of r determines the highest variance EOF1 mode of r and its PC1. A normal random variable, e, with the mean and variance of the PC1 time series substitutes r and Eq. 3.3 becomes

\[ y \approx e \sum_{i=1}^{5} \text{EOF1}_i P_i. \]  

(3.4)

Substituting back the Q1c gives

\[ Q1c_{\text{SPCAM}} \approx \sum_{i=1}^{5} (1 + e\text{EOF1}_i) P_i. \]  

(3.5)

Our goal is to induce stochastic perturbation of e on EOF1 to act as the MCS organization for CAM. Since e is a scalar variable, we can apply either time-dependent perturbation [Arnold et al., 2013] or time-independent perturbation [Chen et al., 2015] as the stochastic parametrization.
CHAPTER 4

Informed stochastic spectral scheme

Our goal from the previous chapter is to induce stochastic perturbation to represent the missing subgrid-scale organized convection processes in large-scale climate models. The complex parametrizations in climate models requires a testbed before fully implemented. In the present proof of concept investigation a new reliable and efficient perturbed parameter scheme is shown to be comparable to an additive stochastic parametrization scheme in resolving systematic model error. The experiments are conducted using two Lorenz 63 (L63) models coupled to mimic the ocean-atmosphere system, and the atmospheric L63 is further coupled to a spatially-resolved convective-scale Lorenz 96 (L96). The entire system of equations is treated as the “truth” model, and is simulated using a parameterized “forecast model”. The L96 is treated as a subgrid-scale process and parameterized using one of three schemes: (i) deterministic, (ii) additive stochastic parametrization, and (iii) perturbed parameter. Perfect initial conditions are applied to investigate uncertainties caused by model errors. The systematic biases are significantly reduced in the perturbed parameter scheme when “informative” perturbations are applied. An informative perturbation is the difference between the true tendency and the deterministically parameterized tendency. Moreover, the proposed scheme uses a stochastic spectral method, Polyno-
mial Chaos Expansion (PCE), to build a low cost surrogate model of the perturbed forecast model. The PCE surrogate is an analytic function of the perturbation which effectively produces an unbiased forecast statistics at large ensemble size, without the need to integrate the actual perturbed forecast model.

Operational weather and climate prediction centers rely on probabilistic ensemble forecasts to account for model and measurement errors. This study will focus on two ensemble forecast schemes, perturbed parameter scheme and additive stochastic parametrization, both introduce perturbations to the model parameter to represent model errors. For the perturbed parameter scheme, a perturbation is randomly sampled prior to each model integration and held fixed throughout the simulation. Whereas the stochastic parametrization applies time-varying perturbations to the model parameter throughout the model integration. In Arnold et al. [2013], the stochastic parametrizations (e.g., additive, multiplicative, etc) were shown to produce significantly more reliable forecasts than the steady perturbed parameter counterpart. A time-varying perturbation is argued to be important as it represents the missing subgrid-scale processes [Palmer, 2001]. However, our study shows that the perturbed parameter scheme could be improved to be equally reliable when informative perturbations are applied. An informative perturbation is the difference between the true tendency and the parameterized tendency. The schemes are tested on a truncated L63 model mimicking the ocean-atmosphere system with unresolved cloud-scale processes, and produces reliable forecasts comparable to an additive stochastic parametrization. Furthermore, a surrogate model, Polynomial Chaos Expansion (PCE), of the perturbed forecast model (i.e., the forecast model with a perturbed parameter scheme)
is built to enable one to effectively obtain unbiased forecast statistics with a large ensemble size.

There are generally two sources of uncertainties: model error and initial condition error. Model errors are caused by bulk parametrization of subgrid-scale processes, discrete integration, inexact representation of physics, etc; whereas the initial condition errors are caused by imperfect instruments, lack of continuous measurements to accurately serve a discretized model, etc. The two types of errors are not mutually exclusive, may interact non-linearly during the model simulation, and may lead to large uncertainties in the forecast states. By using perfect initial conditions in this study, we focus on quantifying only the model errors. The ensemble forecast schemes to represent model errors include the perturbed parameter scheme [Bowler et al., 2008], stochastic parametrizations [Buizza et al., 1999; Majda and Khouider, 2002; Lin and Neelin, 2003; Palmer et al., 2009; Bowler et al., 2008; Plant and Craig, 2008; Arnold et al., 2013], multi-model [Kirtman et al., 2014] and multi-parametrization [Stensrud et al., 2000] schemes. An appropriate representation of the errors will ensure good forecasts.

The main issue for an ensemble generated by a best single model is the unresolved subgrid-scale process which causes highly correlated underdispersed ensembles leading to systematic bias [Palmer, 2001; Stensrud et al., 2000] (i.e, the ensemble spread does not cover the observation [Buizza et al., 2005]). Despite multi-model ensemble approach captures the true state better by resolving structural uncertainty [Tebaldi and Knutti, 2007], the underdispersed states in individual models remain an issue. A recent study of 24 models in CMIP [Pennell and Reichler, 2011] concluded that the effective number of independent models is between 7.5 and 9. This indicates that
the models are not as independent as expected. In addition, quantifying the errors for multiple models remains ad hoc when different sources of model errors interplay [Palmer et al., 2009]. Multi-parametrization [Houtekamer et al., 1996] using the same dynamical core also suffers from these issues.

The single model strategies such as the stochastic parametrizations and the proposed perturbed parameter scheme overcame the systematic bias and enabled quantification of the model errors. The unreliable forecasts with perturbed parameter scheme [Doblas-Reyes et al., 2009; Weisheimer et al., 2011; Arnold et al., 2013] may be attributed to: 1) The use of arbitrary distributions for each perturbed parameter. 2) Small sample size for each parameter does not allow sample statistics to converge probabilistically to the expected values (i.e., central limit theorem). The first issue is analogous to applying a white noise process, instead of an autoregressive process, to the stochastic parametrization. Therefore, the proposed scheme applies informatively distributed perturbations to the perturbed parameter to generate the ensemble. The second issue is generally resolved by repetitively integrating the model whenever a perturbation is generated to create a large ensemble, but at a high computational cost. The expense increases significantly as the number of perturbed parameter increases, such as four parameters used by Arnold et al. [2013]. Therefore, we propose to build a PCE-accelerated surrogate model with the ability of fast convergence to the state outputs of the perturbed forecast model [Lucor et al., 2001]. Once built, we need only to evaluate the analytic PCE function to generate ensemble forecasts nearly free of cost. The PCE received considerable attention in a wide range of engineering applications, such as computational fluid mechanics [Hosder et al., 2006], and was recently applied to an ocean GCM [Alexanderian et al., 2012].
The two innovations of the proposed perturbed parameter scheme summarizes as 1) using informative perturbations with a 2) PCE-accelerated surrogate model to generate reliable ensemble forecasts.

The experimental setup in Section 4.1 includes a coupled L63-L96 system as the “truth model”. The truth model states are simulated using a “forecast model” where L96 is treated as a subgrid-scale process and parameterized by different schemes. A deterministic parametrization in Section 4.2 and an additive stochastic parametrization in Section 4.3 are formulated to compare with the PCE-accelerated informative perturbed parameter scheme in Section 4.7. Forecast consistency of the two ensemble forecast schemes is discussed in Section 4.5. Finally, to conclude the proposed scheme being effective, all forecast schemes are compared using a variety of forecast skill scores in Section 4.6.

Table 4.1: Lorenz Model Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma$</td>
<td>10</td>
<td>standard parameters ($\sigma$, $r$ and $b$) of L63</td>
</tr>
<tr>
<td>$r$</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>$8/3$</td>
<td></td>
</tr>
<tr>
<td>$a$</td>
<td>0.08</td>
<td>coupling parameter for the ocean-atmosphere L63 system</td>
</tr>
<tr>
<td>$k$</td>
<td>-10</td>
<td>offset parameter</td>
</tr>
<tr>
<td>$\tau$</td>
<td>0.1</td>
<td>time-scale ratio for the oceanic L63</td>
</tr>
<tr>
<td>$a_z$</td>
<td>1</td>
<td>coupling parameter for the atmospheric L63 and L96</td>
</tr>
<tr>
<td>$s_z$</td>
<td>10</td>
<td>spatial-scale ratio for the L96</td>
</tr>
<tr>
<td>$\tau_z$</td>
<td>2 or 10</td>
<td>time-scale ratio for the L96</td>
</tr>
</tbody>
</table>
4.1 Experimental setup

4.1.1 Coupled Lorenz system

We use a two time-scale, coupled L63 model [Lorenz, 1963; Arnold et al., 2013] where the fast component is analogous to the atmosphere and the slow component is analogous to the ocean. The atmospheric component is further coupled to a spatially-resolved convective-scale L96 [Lorenz, 1996] composed of four identical dynamical equations each representing a spatial grid point with nonlinear interaction with the neighbors. The first and last grid point share the boundary. A deterministic parametrization of the spatially resolved process is analogous to the bulk parametrization of the cloud processes in the weather and climate models.

The atmospheric component:

\[
\frac{dX_1}{dt} = \sigma(X_2 - X_1) - a(Y_1 + k) - U^* \\
\frac{dX_2}{dt} = rX_1 - X_2 - X_1X_3 + a(Y_2 + k) \tag{4.1} \\
\frac{dX_3}{dt} = X_1X_2 - bX_3 + aY_3
\]

The oceanic component:

\[
\frac{dY_1}{dt} = \tau \left( \sigma(Y_2 - Y_1) \right) - a(X_1 + k) \\
\frac{dY_2}{dt} = \tau(rY_1 - Y_2 - Y_1Y_3) + a(X_2 + k) \tag{4.2} \\
\frac{dY_3}{dt} = \tau(Y_1Y_2 - bY_3) + aX_3
\]

where \( U^* = \frac{a\tau_s}{s_z} \sum_{i=1}^{4} Z_i \) (the term to be parameterized) is associated to the spatially resolved system:

\[
\frac{dZ_i}{dt} = \tau_s \left( -s_zZ_{i+1} + Z_{i-1} - Z_i + \frac{a_z}{s_z} X_1 \right); \quad i = 1, \ldots, 4 \tag{4.3}
\]
where $Z_0 = Z_4$, and $Z_5 = Z_1$. The spatially resolved system represents the subgrid-scale processes after $U^*$ is parameterized. (See Table 4.1 for the parameter descriptions).

### 4.1.2 Truth model

The entire set of equations (4.1), (4.2) and (4.3) is defined as the truth model. The equations are integrated by an adaptive fourth-order Runge-Kutta (RK4) time-stepping scheme. A true time series of 1600 Model Time Units (MTU) is generated (transient phase is removed) for the forecast models to compare with. This study conducts a total of 300 forecast events (each of 25 MTU) with initial conditions selected from the 1600 MTU truth time series at intervals of 5 MTU where the atmospheric states generally lose correlation.

Following Arnold et al. [2013], we designed two experiments by varying the time-scale ($\tau_z = 2$ and $\tau_z = 10$) for the spatially resolved system. The results by using L96 in Wilks [2005] shows that the slow evolving case ($\tau_z = 2$ in our case) better represents a real atmospheric convective-scale process. Whereas the L96 in $\tau_z = 10$ behaves like a white-noise process with less correlation between the time samples. The contrasting subgrid-scale dynamics gives us the opportunity to test the limits of our methodology.

### 4.1.3 Forecast model

The forecast model uses the atmosphere (4.1) and ocean (4.2), and parameterizes $U^*$ with $U_p$, thus removing the spatially resolved system (4.3) and treat it as the
subgrid-scale process. The following sections will go through the three schemes of $U_p$ for the forecast model: (i) deterministic, (ii) additive stochastic parametrization and (iii) the proposed perturbed parameter scheme.

In order to set a maximum forecast lead time for the atmospheric states to remain predictable by the model, we calculated the *error-doubling time*, which is approximately two atmospheric days in a GCM [Lorenz, 1996]. The error-doubling time calculated by the deterministic forecast model approximately gives 1 MTU = 1.5 (= 2) atmospheric days for $\tau_z = 2$ ($\tau_z = 10$). Therefore the maximum forecast lead time for the atmospheric states in both experiments is set to 5 MTU, which is in the range of 7 to 10 atmospheric days.

### 4.2 Deterministic parametrization

![Figure 4.1](image)

Figure 4.1: The density contours of the ($U^{*k}, X^k_1$) time samples in (a) $\tau_z = 2$ and (b) $\tau_z = 10$. The deterministic curve $\bar{U}$ (solid) and the perturbed curve (dashed) $U_p$. 
Figure 4.1 shows the density contours of the cloud of time samples of \((X_1^k, U^*(X_1^k))\), where \(k\) is the discrete time index. A cubic linear regression fit (solid black line) through the cloud gives the deterministic parametrization

\[
\bar{U} = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3.
\] (4.4)

The difference between a time sample of true \(U^*\) and \(\bar{U}(X_1^k)\) is the true residual

\[
r^k = U^*(X_1^k) - \bar{U}(X_1^k).
\] (4.5)

Therefore, the density contours in Figure 4.1 can also be seen as formed by the \(r^k\) with zero values centered at the deterministic curve, and larger values away from the curve. A total of 320,000 \(r^k\) samples are drawn from the 1600 MTU time series every 0.005 MTU. The true residuals are the subgrid-scale uncertainties caused by the deterministic parametrization, and will be modeled by the two schemes in the following sections.

Figure 4.2: Lag-n autocorrelation coefficient \(\gamma(n)\) of the \(r^k\) time samples in (a) \(\tau_z = 2\) and (b) \(\tau_z = 10\).
4.3 Stochastic parametrization

We have chosen to model $r^k$ as an additive stochastic parameter $e^k$ based on the reliable forecast skill shown in *Arnold et al.* [2013]. Therefore, the additive stochastic parametrization for $U^*$ is

$$U_p = \bar{U} + e^k. \quad (4.6)$$

Figure 4.2 shows the time-lag autocorrelation coefficient of the true $r^k$ samples, with slow (fast) decay in the $\tau_z = 2$ ($\tau_z = 10$) experiment. The high autocorrelation in $\tau_z = 2$ (Figure 4.2 (a)) shows that it is reasonable to model $r^k$ as a lag-1 autoregressive process (AR1) [Wilks, 2011]. The AR1 represents the discrete time samples of $e^k$ as a simple linear regression

$$e^{k+1} = \gamma e^k + \epsilon$$

$$= \gamma e^k + (1 - \gamma^2)^{1/2} \sigma_r z,$$  \quad (4.7)

where the predictand $e^{k+1}$ is updated by the predictor $e^k$ at the previous time sample, $\gamma$ is the lag-1 autocorrelation coefficient from the true residual, and $\epsilon$ is the error of the simple regression. Figure 4.1 (c) and (d) show higher densities near the deterministic curve. Therefore $\epsilon$ is modeled as a centered Gaussian process, with a standard normal random variable $z$, and the standard deviation $\sigma_r$ of the true residuals. The ensemble forecast of the additive stochastic parametrization contains a total of 40 ensemble members for any event.

It is intuitive to represent the subgrid-scale uncertainties with a time-varying $e^k$ since $r^k$ is constantly changing. But, there is no theoretical proof that a time-fixed $e$ is invalid. This leads to the perturbed parameter scheme where $e$ is fixed in time, which is no longer a stochastic process.
4.4 Proposed efficient perturbed parameter scheme

The proposed perturbed parameter scheme treats $r^k$ as a time-invariant perturbation, $e_s$, on the $\beta_0$ coefficient,

$$U_p = \bar{U} + e_s = (\beta_0 + e_s) + \beta_1 X + \beta_2 X^2 + \beta_3 X^3,$$

where the $k^{th}$ time index is dropped and replaced with the subscript $s$ representing “stationarity”. This single perturbed parameter $\beta_0$ is used in the proposed scheme (in contrast to using all four parameters/regression coefficients in Arnold et al. [2013]). As shown in Figure 4.1, the perturbed $\beta_0$ shifts the deterministic curve by $e_s$. The perturbed forecast model is thus integrated along this perturbed curve (dashed black line) once a fixed value of $e_s$ is sampled prior to the model integration. As mentioned in Section 4.2, the true perturbation $r^k$ has higher densities near the deterministic curve ($r^k$ is zero on the curve). Therefore, it is reasonable to sample $e_s$ according to the density of $r^k$ (e.g., sample more $e_s$ near the deterministic curve). A proper distribution of $e_s$ will capture the probabilistic behaviour of the subgrid-scale $r^k$ fluctuation. We assigned informative distributions to the $e_s$ (Subsection 4.4.2) to test the impact of proper distributions on the reliability of the ensemble forecast. Furthermore, in order to obtain an unbiased statistics with a large number of perturbed model simulations, we built a surrogate model of the perturbed forecast model. The PCE-based surrogate is built by integrating the perturbed forecast model on a selected set of perturbations, and spectrally expanded as an analytic function of $e_s$ (Subsection 4.4.1). The analytic function allows one to easily generate large ensemble forecasts (e.g., $> 10^4$ ensemble members) by sampling different distributions of $e_s$ without the need to integrate the actual perturbed forecast model after its built. The PCE was initially developed
by Wiener [1938] to address problems in statistical mechanics; it was applied in engineering mechanics to quantify uncertainties in stochastic Gaussian processes by Ghanem and Spanos [1990], and generalized to a wider range of stochastic processes by Xiu and Karniadakis [2002].

4.4.1 PCE of a perturbed state variable

PCEs express the dependence of the model output variables on the input perturbation $e_s$ as a spectral series of the form [Le Maître and Knio, 2010]:

$$ f(t,e_s) = \sum_{i=0}^{N} \hat{f}_i(t) P_i(\xi). \tag{4.9} $$

where $f(t,e_s)$ is a perturbed model output variable (e.g., $X_1(t,e_s)$; separate independent PCEs can be constructed for any output quantity of interest), $\hat{f}_i(t)$ are the series coefficients, $P_i(\xi)$ are polynomial basis functions, $N$ is the maximum degree of the polynomial $^1$, $\xi$ is a standardized variable that maps the standard domain $-1 \leq \xi \leq 1$ to the perturbation domain $r_{\text{min}} \leq e_s \leq r_{\text{max}}$ $^2$. PCEs can be viewed as Fourier-like expansions in the perturbed parameter and thus inherit their approximation properties; in particular PCEs converge spectrally fast when $f(t,e_s)$ varies smoothly with $e_s$. We suppress the time dependence of $f$ and $\hat{f}_i$ from now on to simplify notation.

The basis functions are polynomials that are orthogonal with respect to an inner product defined by

$$ \left\langle P_i, P_j \right\rangle = \int P_i(\xi) P_j(\xi) p(\xi) d\xi = \delta_{ij} \left\langle P_i^2 \right\rangle \tag{4.10} $$

$^1N$ is selected to allow the relative error between the PCE approximation and the exact perturbed model output to be sufficiently small.

$^2$A linear mapping of the form $e_s = (r_{\text{max}} - r_{\text{min}}) \frac{\xi + 1}{2} + r_{\text{min}}$ is sufficient. Here $r_{\text{min}} = \min_k r^k$ and $r_{\text{max}} = \max_k r^k$ are the extrema of the true residual (equation 4.5).
where \( \delta_{ij} = 1 \) if \( j = i \) and zero otherwise, and where \( p(\xi) \) is a weight function\(^3\). This study uses Legendre polynomials for \( P_i \), which are orthogonal with respect to the uniformly distributed \( \xi \) in the standardized domain \([-1 1]\), hence \( p(\xi) = 1/2 \) is just constant over the domain. The assumption of a uniformly distributed \( \xi \) is not restrictive since, once the series coefficients are known, one could simply sample it with any probability distribution desired. A carefully selected distribution of \( e_s \) will guarantee reliable forecasts since the sampling of \( e_s \) affects directly the ensemble forecast state distributions. This will be discussed in Subsection 4.4.2.

*Spectral projection* can be used to obtain the coefficients \( \hat{f}_i \), i.e., one takes the inner product of equation (A.3) with each of the basis functions \( P_i \) and invokes orthogonality to obtain:

\[
\langle f, P_i \rangle = \left\langle \sum_{j=0}^{N} \hat{f}_j P_j, P_i \right\rangle = \hat{f}_i \langle P_i^2 \rangle, \text{ or } \hat{f}_i = \frac{\langle f, P_i \rangle}{\langle P_i^2 \rangle}.
\]

(4.11)

Since \( f \) is not an analytic function, we use quadrature (i.e., numerical integration) to approximate the numerator in (4.11):

\[
\langle f, P_i \rangle = \int_{-1}^{1} f P_i p(\xi) d\xi \approx \sum_{q=1}^{n} w_q f(\xi_q) P_i(\xi_q)
\]

(4.12)

\( \xi_q \) are the quadrature points, \( n \) is the number of quadrature points and \( w_q \) are the associated quadrature weights. \(^4\) The evaluation of the series coefficients requires thus an ensemble of model runs to obtain \( f(\xi_q) \) (the ensemble members correspond to setting the perturbed parameter to its value at the quadrature point and running

\(^3\)When the weight function coincides with the probability distribution of \( e_s \) the inner product can be interpreted as an expectation estimate of \( P_i P_j \); it is easy to show that the mean of \( f \) w.r.t. \( \xi \) is then simply the zeroth coefficient \( \hat{f}_0 \).

\(^4\)We have employed the Clenshaw-Curtis nested quadrature rule [Clenshaw and Curtis, 1960] in which accuracy can be improved by increasing \( n \); \( l \)-level Clenshaw-Curtis quadrature rule gives \( n = 2^{l-1} + 1 \) quadrature points to exactly integrate \( \langle fP_i \rangle \), with maximum polynomial of degree \((n-1)\). Therefore, \( P_i \) has highest degree polynomial of \( N = (n-1)/2 \) rounded to the lowest integer.
the model); no code modification is needed. Equation (4.11) becomes

\[ \hat{f}_i = \frac{\sum_{q=1}^{n} w_q f(\xi_q) P_i(\xi_q)}{\langle P_i^2 \rangle}. \]  

(4.13)

The combination of equations (4.13) and (A.3) completes the PCE-accelerated surrogate model for the perturbed forecast state variable.

As mentioned earlier, \( \tau_z = 2 \) may be closer to a real atmosphere-ocean coupled system, and the atmospheric variables exhibit a relatively smooth variations with \( e_s \). A relatively short spectral series is then expected to represent accurately this dependency. The \( \tau = 10 \) experiment, on the other hand, exhibits large jump discontinuities (and ensuing Gibbs oscillations) whose number increases with longer lead time (\( \geq 10 \text{MTU} \)). The discontinuities hinder the convergence rate of the PCE and a longer series is then needed to represent the functional relationship between the state variables and the perturbation. The \( \tau = 10 \) experiment required a 64\textsuperscript{th} degree polynomial, hence an ensemble size of 129 is needed for the quadrature. We used 129 for the \( \tau = 2 \) experiment even though a 16\textsuperscript{th} degree polynomial (and 33 ensemble members) would have been sufficient for the smoother perturbed state. The observed jump phenomena will be discussed in Subsection 4.4.4.

Once built, PCE of a perturbed forecast state variable allows one to test any distribution of \( e_s \) without actually integrating the model. The perturbed parameter scheme is thus performed by sampling the \( e_s \) from the PCE with a proper distribution to give an ensemble state distribution that generates reliable forecast.
4.4.2 Distributions of “true error” samples

In this study, $e_s$ is defined to be “informative” when the samples contain the true residuals $r^k$, and “uninformative” when they are sampled from an arbitrarily assigned distribution.

We assigned three distributions to $e_s$: $e_{\text{unif}}$, $e_{\text{clim}}$ and $e_{\text{AR1}}$. The $e_{\text{unif}}$ distribution is uninformative and its samples are randomly generated from a uniform distribution with domain $r_{\text{min}} \leq e_{\text{unif}} \leq r_{\text{max}}$, whereas $e_{\text{clim}}$ and $e_{\text{AR1}}$ contain informative samples of $r^k$. The $e_{\text{clim}}$ distribution is designed to verify the existence of a single climatological distribution of $e_s$ for all forecast events; $e_{\text{clim}}$ is expected to be the most informative since it is based on the entire time series (1,600 MTU) of true $r^k$ samples. Figure 4.3 shows the distribution of the $e_{\text{clim}}$ using all 320,000 $r^k$ time samples. The $e_{\text{AR1}}$ distribution is based on the collection of all $e^k$ samples generated by the 40 ensemble members (25 MTU each) of the AR1-process for any forecast event. The $e_{\text{AR1}}$ remains
informative since the AR1 process begins with a single true $r^k$ sample. A total of 300 distributions (corresponding to 300 forecast events) are constructed for $e_{AR1}$ to check whether using the samples from the stochastic parametrization and modifying them into a stationary distribution could achieve equivalent forecast skill.

4.4.3 Summary of the proposed scheme

- Obtain the spectral coefficients (4.13) following the quadrature rule.

- Construct the analytic PCE (A.3) of the perturbed forecast state variables $X$’s and $Y$’s by using the spectral coefficients.

- Sample the analytic PCE with different input distributions of $e_s$ to generate output distributions for the state variables at the given lead times.
Figure 4.4: Time series of the RMSD between the exact perturbed state outputs and the PCE approximations at \( \tau_z = 2 \) (top) and \( \tau_z = 10 \) (bottom).

Figure 4.5: The evolution of the exact (grey) versus PCE approximated (black) perturbed forecast states (\( X_1 \) (top) and \( Y_1 \) (bottom)) as a function of the uniformly distributed \( \xi \) in the standard domain \([-1 1]\) at \( \tau_z = 2 \).
4.4.4 Numerical consistency of PCEs

In order to measure whether the PCE approximations have converged sufficiently to the exact perturbed forecast states (i.e., a good surrogate for the perturbed forecast model), we calculated the Root Mean Squared Difference (RMSD) between the two outputs. The exact perturbed forecast outputs are generated by directly integrating the perturbed forecast model from a uniformly sampled \( e_s \). The same collection of \( e_s \) is then evaluated by the PCE. The RMSD is then calculated between the exact outputs and the PCE approximations.

Figure 4.4 is the time series of RMSD averaged over 300 events. It shows how well the PCE captures and how fast it diverges from the exact outputs given different subgrid time-scale \( \tau_z \). In an ideal smooth perturbed state we expect the RMSD to stay as low as possible, which is the case for the ocean (black) earlier in time (<

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5Keep in mind, RMSD is unrelated to the PCE forecast skill. RMSD measures only the numerical accuracy of PCE as a surrogate of the perturbed forecast model.
The earlier bifurcations in the atmospheric states (grey) with larger jump discontinuities deteriorate the PCE approximation and cause RMSD to grow faster.

The qualitative differences in PCE approximations and exact outputs are shown in Figure 4.5 ($\tau_z = 2$) and Figure 4.6 ($\tau_z = 10$). The two figures show the forecast state as a function of the input perturbation $e_{\text{unit}}$ at different forecast lead times (shown above each panel) from the view of a single event. They show how different time-scale of the subgrid-scale system impacts PCE approximations. The $\tau_z = 10$ case exhibits fast evolving states and multiple big jump discontinuities, which is harder for the PCE to converge. Although the ocean component bifurcates multiple times in both experiments, the overall state spread remained in a relatively narrow range (with small amplitude jumps), and the errors in the PCE-accelerated ocean ensemble remained small.

Figure 4.7 and Figure 4.8 show the evolution of the perturbed state p.d.f.\(^6\) of the exact versus PCE outputs with respect to Figure 4.5 and Figure 4.6. The two figures are needed to further confirm that as the PCE converges to the exact perturbed states the distributions also converged. The features of the p.d.f. shown in this event are ubiquitous in other forecast events. The distributions of the atmospheric states in $\tau_z = 10$ (top panels in Figure 4.8) spread along a wider range with larger variances in all lead times and constantly changing shapes (non-Gaussian). The perturbed ensemble with large spread indicates the necessity of applying informative input distributions of $e_s$ to better represent the correct shapes of the perturbed output distributions. Notice the largely bifurcated nature in $\tau_z = 10$ hinders the accuracy of PCE on

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\(^6\)Apply kernel density estimation following Botev et al. [2010]
approximating the exact states at longer lead time (e.g., the bottom rightmost panel in Figure 4.8).

Figure 4.7: The evolution of the exact (grey) versus PCE approximated (black) perturbed forecast state p.d.f. ($X_1$ (top) and $Y_1$ (bottom)) at $\tau_z = 2$.

Figure 4.8: As Figure 4.7, the exact (grey) versus PCE approximated (black) perturbed forecast state p.d.f. at $\tau_z = 10$. 
4.5 Forecast consistency

According to Leutbecher and Palmer [2008], a consistent forecast requires

$$\frac{1}{M} \sum_{m=1}^{M} \epsilon_m^2 \to \frac{1}{M} \sum_{m=1}^{M} \frac{N+1}{N-1} s_m^2 \quad \text{as} \quad M \to \infty,$$

(4.14)

where $M$ is the total number of forecast events, $N$ is the ensemble size for any event, $\epsilon_m^2$ is the squared error between the ensemble mean and the true state at the $m^{th}$ event, $s_m^2$ is the ensemble variance at the $m^{th}$ event, $\frac{N+1}{N-1}$ is a correction factor.

Condition (4.14) for forecast consistency requires the Mean Square Error (MSE) to converge to the Mean Ensemble Variance (MEV) at large $M$ (e.g., 300 for our study) with a correction factor. Hence, Figure 4.9 shows the convergence relationship, MSE : MEV = 1 : 1 (black line), with 6 pairs of (MSE, MEV) generated by the two schemes: additive stochastic parametrization $Stoch$ (triangle), and perturbed parameter scheme with $e_{\text{unif}}$ (circle). The 6 pairs are calculated by sorting 300 pairs of $(\epsilon_m^2, s_m^2)$ by $s_m^2$ and incrementally divide and average in 6 quantiles (i.e., each with
$M = 50$ pairs). As expected, the two schemes have points scattering near the black line, which implies forecast consistency.

### 4.6 Forecast skill

The forecast skill of the ensemble schemes is evaluated by three scores, Reliability (REL), Ignorance Skill Score (IGNSS) and Ranked Probability Skill Score (RPSS).

REL (a component of Brier Score for dichotomous events) measures whether the model is well-calibrated. IGNSS is a measure of the ensemble dispersion with penalty on underdispersed ensembles that cause systematic errors. RPSS evaluates a multi-category event with penalty on the ensemble members further away from the category of occurrence (i.e., penalizes with a distance measure). For RPSS and IGNSS, the forecast states are divided into 10 categories, which are the deciles of the climatological distribution.

Figure 4.11 ($\tau_z = 2$) and Figure 4.10 ($\tau_z = 10$) show the time evolution of the three scores, RPSS (top), IGNSS (middle) and REL (bottom) generated by the schemes: (I) Uninformative perturbed parameter ($e_{\text{unif}}$), (II) Informative perturbed parameter ($e_{\text{clim}}, e_{\text{AR1}}$), (III) Additive stochastic parametrization ($Stoch$), (IIII) Deterministic parametrization ($Det$). The PCE for the perturbed parameter scheme in the two figures is approximated by 64$^{th}$ degree polynomial. As expected, without a probabilistic feature, $Det$ performed poorly over all scores. Therefore, we only compare the $Stoch$, and the perturbed parameter scheme using $e_{\text{clim}}, e_{\text{AR1}}$ and $e_{\text{unif}}$ in the following.
Figure 4.10: As Figure 4.11, forecast scores RPSS, IGNSS and REL at $\tau_z = 10$.

Results in Figure 4.11 and Figure 4.10 show consistent and nearly identical scores by $e_{\text{clim}}$ and $e_{\text{AR1}}$. This supports the hypothesis of applying informative distributions to the perturbed parameter scheme, regardless of the highly bifurcated states in $\tau_z = 10$.

In $\tau_z = 10$, the uninformative $e_{\text{unif}}$ performs poorly in Figure 4.10 (a) and (c). The failure is attributed to the wide ensemble spread (caused by strong bifurcations) in $\tau_z = 10$. Suppose the wide-spread case ($\tau_z = 10$) and the small-spread case ($\tau_z = 2$) both forecast low density at the category of occurrence by using $e_{\text{unif}}$. The small-spread case will remain reliable with the entire ensemble contained in (or in close proximity to) the category of occurrence. Whereas the wide-spread case using the uninformative input may have its highest density erroneously far from the category.
of occurrence, resulting in a penalty in RPSS. This explains why it is necessary to apply informative $e_s$, especially when forecasting the wide-spread cases.

Figure 4.11: Forecast scores RPSS (top), IGNSS (middle) and REL (bottom) at $\tau_z = 2$ generated by $e_{\text{unif}}$ (black circle), $e_{\text{clim}}$ (black upper triangle), $e_{\text{AR1}}$ (black lower triangle), $\text{Stoch}$ (grey square), and $\text{Det}$ (grey dashed-line), with PCE approximated by 64th degree polynomial.

In contrast to $\tau_z = 10$, the $\text{Stoch}$ in $\tau_z = 2$ underperformed in Figure 4.11 (c), (d) and (e) with the possible reasons: 1) In $\tau_z = 2$ ($\tau_z = 10$), the slow (fast) varying, less (more) white noise like, subgrid-scale dynamics is harder (easier) to be modeled by a stochastic process, and 2) the Gaussian stochastic term $\epsilon$ in equation (4.7) may not (may) represent a non-Gaussian (Gaussian-like) true residual in Figure 4.3 (a) (in Figure 4.3 (b)).
Figure 4.12: As Figure 4.11, forecast scores RPSS, IGNSS and REL at $\tau_z = 2$, with PCE approximated by 16th degree polynomial.

In order to demonstrate the overall cost reduction by the PCE, a low order PCE (16th degree polynomial, built by 33 ensemble members) forecast is shown in Figure 4.12 with other schemes identical to Figure 4.11. There are nearly no changes in the atmospheric scores between Figure 4.11 and 4.12. This indicates a low cost PCE built with less simulations is applicable when the perturbed state is relatively smooth. The weaker oceanic scores (Figure 4.12 (d), (f)) at longer lead times ($\geq 10$ MTU) for $e_{\text{clim}}$ and $e_{\text{AR1}}$ is caused by low order PCE converging slower when the jump discontinuities begin to increase. Despite the weakness, PCE with $e_{\text{clim}}$ and $e_{\text{AR1}}$ remains comparable at predictable weather lead times ($\leq 5$ MTU).
4.7 Uncertainty quantification and forecast problem

Previously, we have proposed to implement a surrogate model on the stochastic scheme. The next natural approach is whether we can combine tools to form an efficient probabilistic forecast system to quantify the uncertainty carried out by the perturbations. A probabilistic forecast system is consisted by three main components: a numerical model, observations and random errors. A deterministic model is presented as

\[ f(x, t, \theta) = F(f), \quad (4.15) \]

with a nonlinear differential operator \( F \) and the model state \( f \in \mathbb{R}^{N_f} \). The model state relates to the true observations \( y \) with a function \( g : \mathbb{R}^{N_f} \rightarrow \mathbb{R}^{N_y} \),

\[ y = g(f) + \epsilon_{mod} \quad (4.16) \]

by some model error \( \epsilon_{mod} \) (e.g., discrete integration of the numerical model with truncation error, bulk effect parametrization of subgrid processes fails when unresolved scale dominates over grid scale motions, chaotic dynamics from high nonlinearity, etc.), where \( y \in \mathbb{R}^{N_y} \). From satellites or other measurements, we collect observations \( d \in \mathbb{R}^{N_y} \), which are deviated from the truth \( y \) by some measurement errors \( \epsilon_{meas} \). The relationship is denoted by

\[ d = y + \epsilon_{meas}. \quad (4.17) \]

Thus combining (4.17) and (4.16)

\[ d = g(f) + \epsilon_{mod} + \epsilon_{meas}. \quad (4.18) \]
In order to capture the observations statistically, it is necessary to perturb the two main input error sources, model parameters (representing model errors) and initial conditions (representing measurement errors), for model to generate a cloud of output states. The inputs and outputs are both random variables, where the outputs are functions of inputs. Therefore, a correct input statistics indicates a correct output statistics, vice versa, leading to a reliable forecast. A correct input generates output that include or overlap the spread of other error sources which are intrinsic to a model or measurements but often hard to present as random variables. A good probabilistic forecast thus rely on selecting an effective input source and correct input distribution.

The input is a real-valued random variable. A single perturbed model run is a probability event, where the perturbation is brought out by the input to generate a sequence of output random variables indexed by time and space (i.e., random process and random field). The real-valued random variables are manageable and we will proceed on by using the notation \( X(\omega) \) to represent random variables (either input or output) for any function \( X \) on a perturbed model event \( \omega \). Therefore, the relationship in (4.18) including the two input random variables, model parameters \( \theta(\omega) \) and initial conditions \( \theta_0(\omega) \), becomes

\[
d = g(f(x, t, \theta(\omega), \theta_0(\omega))) + \epsilon_{\text{mod}}(\omega) + \epsilon_{\text{meas}}(\omega).
\]

We define a “forward model” \( G : \mathbb{R}^{N_\theta} \to \mathbb{R}^{N_y} \) between the random inputs and observations, and let \( \epsilon(\omega) = \epsilon_{\text{mod}}(\omega) + \epsilon_{\text{meas}}(\omega) \). The model thus follows a general relationship

\[
d = G(\theta, \theta_0) + \epsilon
\]
to capture the observations statistically (we dropped $\omega$ for simplicity of notation), where $\epsilon$ becomes an additive error in pragmatic Bayesian framework.

Our priority from this relationship is to reduce the cost for model simulations by developing a PCE surrogate $\tilde{G}$ for the model and apply sensitivity analysis to reduce the dimensions of inputs to $N$-dim without $\theta_0(\omega)$ (i.e., assuming $\theta(\omega)$ will deliver the output distribution overlapping $\theta_0(\omega)$). The relationship thus becomes,

$$d = \tilde{G}(\theta_N) + \epsilon. \quad (4.21)$$

Apply Bayesian inference following this new relationship to generate a corrected input distribution $p(\theta_N|d)$. This is the general relationship of the low cost probabilistic forecast system we proposed.

As a comparison, the initial condition input method in numerical weather prediction (NWP) generates the corrected input distribution by 1) singular vectors (SV): applied by European Centre for Medium-Range Weather Forecasts (ECMWF), 2) bred-vector (BV): applied by National Centers for Environmental Prediction (NCEP) and 3) ensemble data assimilation, (e.g., ensemble Kalman filtre (EnKF)), making corrections directly on the output as the subsequent initial condition input. EnKF is a sequential Bayesian filter algorithm which perturbs the initial condition by the input $\theta_0(\omega)$ and corrects the output distribution $p(f(\theta_0)|d)$ by providing observations at given analysis time stages $t$. EnKF achieves the correction assuming no parameters $\theta$ perturbation.
The $\theta_0(\omega)$ input method is a flow-dependent \cite{Leutbecher and Palmer, 2008} uncertainty correction, where the correction changes day to day. The $\theta(\omega)$ input method is also flow-dependent, but the physical parameter correction allows physical explanation on what the flow depends on \cite{Alexanderian et al., 2012} (e.g., stronger wind flow might depend more on viscosity than other parameters, which produce more sensitivity and better distribution correction on the viscosity coefficient).

In addition to the single parameter PCE “surrogate” model in section, our surrogate model can handle multi-dimensional parameter space. This multi-dimensional non-intrusive PCE and cost reduction numerical integration scheme (e.g., sparse quadrature) will be more adaptable to climate models with higher dimensional parameters. Furthermore, the multi-dimensional PCE and other application of uncertainty quantification tools (i.e., sensitivity analysis, Bayesian inference and sampling methods) are integrated in our forecast system (see Appendix A). These tools allows us to effectively explore the probabilistic behaviour of model parameters and tendencies. The generalized discussion to multi-dimensional PCE are seen in Appendix A.1, where previous case only focused on a single parameter. When the parameter dimension becomes huge, this requires adaptive methods to reduce the cost of climate model ensemble simulation. Therefore, we incorporated Dimension Adaptive Sparse Quadrature (DASQ) algorithm (Appendix A.1.5.6) to deal with the cost reduction as applied in Winokur et al. \cite{2013}; Huan \cite{2010}. We can easily apply sensitivity analysis (Appendix A.2) on the surrogate model on each selected parameter, and examine which parameter contributes most to the total variance. Thus leads to model parameter selection in the future ensemble forecast. The application of the surrogate
model to Bayesian inference is further explored (Appendix A.3). Bayesian inference, commonly used in data assimilation [Wu et al., 2015; Majumdar et al., 2011], allows us to estimate the posterior probability distribution of the selected parameters and leads to discussion of physical parameters [Sraj et al., 2014]. We developed a dimension adaptive sampling algorithm (Appendix A.4.2), i.e., Delayed Rejection Adaptive Metropolis (DRAM) sampler, to sample effectively over the highest probability domain. Above are all the tools that are included in the current ensemble forecast system to quantify the uncertainties of model parameters and tendencies.

4.8 Summary

We have implement an idealized coupled ocean-atmosphere model with cloud-scale process in the atmospheric component. By using this testbed, the perturbed parameter scheme generates reliable forecasts through the employment of informative perturbations. The PCE surrogate model further reduces the cost of generating large ensemble for unbiased statistics. The numerical integration (i.e., quadrature) to build the PCE function requires no change to the model codes, which is advantageous when applied to complex GCMs.

Due to the highly bifurcated states at longer lead times in a fast varying system ($\tau_z = 10$), the exact perturbed state is approximated by a higher order PCE. These multiple large jump discontinuities may not be observed in a realistic dynamical system; the proposition of PCE being efficient is not violated when the system is relatively smooth and realistic ($\tau_z = 2$) or at weather predictable lead times ($< 5$ MTU).
As shown in Shutts and Palmer [2007], by treating the cloud resolving model outputs as the truth, the true perturbations were coarse-grained to the resolution of an operational model. This approach allows the PCE-accelerated informative perturbed parameter scheme and stochastic parametrizations to be applied to complex GCMs properly. Furthermore, the PCE is developed to build a surrogate with multiple perturbed parameters (e.g., multiple tendency terms) efficiently. A further comparison with a multiplicative noise is needed, where Arnold et al. (2013) shows it to be the most reliable stochastic parametrization.

Further application of multi-dimensional uncertainty quantification tools on the stochastic scheme is required to fully explore a complex climate model with high dimensional parameter space.
CHAPTER 5

Conclusion

Our research focuses on quantifying the mesoscale convective organization processes in two climate models, SPCAM and CAM, sharing the same large-scale GCM dynamical core. The two models are compared based on the same initial conditions (i.e., CAM “offline” evaluation) at every timestep, without inducing initial condition errors. This allows us to see the response of pure model physics reacting to the same given convective organization environments. Based on previous studies showing SPCAM’s ability to resolve realistic mesoscale organized systems, we develop a rigorous algorithm to detect and cluster the MCSs in SPCAM and evaluate the response of CAM. The case study of a long-lived MCS cluster shows that the SPCAM produces a squall line-like MCS circulation. The case also shows realistic growth to decay of SPCAM’s column-wise heating and moisture fields in the deep convection and stratiform clouds. However, CAM responds with an unrealistic stratiform dipole heating mode when given the deep convection-favoring environment. CAM also shows a decaying stratiform mode when given rejuvenated convection conditions, which suggests a lack of upscale convective organization. CAM’s discrepency lies in the stratiform microphysics scheme that dominates the strong cooling at below $z = 3km$. Composite analysis for SPCAM shows diversity, especially over land, in the dominant modes (i.e.,
deep convection and stratiform), whereas CAM shows a uniform stratiform dominant mode plaguing the entire lifecycle. This lack of diversity and variation are often seen in deterministic parameterization, therefore we proposed a stochastic scheme to perturb CAM’s convective parameterization scheme. As a testbed for proof-of-concept, we develop a stochastic scheme which effectively produces a reliable ensemble forecast in the Lorenz coupled model. Unlike conventional stochastic schemes, which require perturbations in time, our scheme relies on time-fixed perturbations. This allows us to develop a “surrogate model” that includes stochasticity in the parameter space, which permits cost-effective ensemble sampling. Results show promising forecast skill compared to a conventional stochastic scheme. The surrogate model is developed with imbedded ability for global sensitivity analysis. The Bayesian inference can be applied to the surrogate model to effectively sample the posterior distribution of these high dimensional parameters. The multi-dimensional uncertainty quantification tools (i.e., DASQ and DRAM algorithms) are included in our forecast system, and are ready to deploy in a complex climate model. The promising forecast skill in the simplified model indicate future application of the time-independent stochastic scheme to a fully coupled GCM is a strong possibility. We expect the new parameterization to enhance the moist convective organization processes missing from CAM. This may result in better representation of upscale organization phenomena such as the MJO and better climatological precipitation in the tropics.
APPENDIX A

Uncertainty Quantification Tools

A.1 Polynomial Chaos Expansion (PCE)

The Polynomial Chaos Expansion (PCE) [Wiener, 1938] is a stochastic spectral expansion method for any random variable or random processes (e.g., model parameters, model state variables, etc.). Our purpose is to use PCE to generates a surrogate of the stochastic model for (1) sensitivity analysis of model parameters and (2) efficient sampling for inverse parameter probability estimation [Marzouk et al., 2007], as oppose to relatively expensive Monte Carlo sampling which requires large numbers of model simulations.

If given any probability outcome event $\omega$, we get a value $f$, this defines a random variable $f(\omega)$. Whereas, if given any $\omega$, we get a function of time (or space) $x$, $f(x)$, this defines a random process (or random field), $f(x, \omega)$. At any fixed $x$, the random process will define a random variable $f(\omega)$. (Notice random process (or random field) could be defined as a sequence of random variables if the time or space are a discrete index set.)
A.1.1 PCE of random variables

For any second-order finite variance random variable \( f: \Omega \to \mathbb{R}, f \in L^2(\Omega, \mathcal{P}) \).

For any random event \( \omega \), \( f(\omega) \) admits a PCE representation [Wiener, 1938]

\[
f(\omega) = \hat{f}_0 \Gamma_0 + \sum_{i_1=1}^{\infty} \hat{f}_{i_1} \Gamma_1(\xi_{i_1}(\omega)) + \\
\sum_{i_1=1}^{\infty} \sum_{i_2=1}^{\infty} \hat{f}_{i_1,i_2} \Gamma_2(\xi_{i_1}(\omega), \xi_{i_2}(\omega)) + \\
\sum_{i_1=1}^{\infty} \sum_{i_2=1}^{\infty} \sum_{i_3=1}^{\infty} \hat{f}_{i_1,i_2,i_3} \Gamma_3(\xi_{i_1}(\omega), \xi_{i_2}(\omega), \xi_{i_3}(\omega)) + \ldots ,
\]

where \( \{\xi_i\}_{i=1}^{\infty} \) is a sequence of i.i.d. random variables. The Polynomial Chaos (PC) \( \{\Gamma_p\}_{p=1}^{\infty} \) in \( \{\xi_i\}_{i=1}^{\infty} \) are mutually orthogonal polynomials w.r.t. the joint PDF \( p(\xi) \), e.g., for Gaussian random variables, the corresponding polynomials are the Hermite polynomials. Any order \((> 0)\) of a PC involves all the combinations of the random variables \( \{\xi_i\}_{i=1}^{\infty} \), which is why PC are called random functionals (function of random function). The deterministic coefficients (i.e., non-random) \( \hat{f}_i \) are called PC coefficients.

Example A.1.1 A function on two random variables

\[
f(\xi_1, \xi_2) = \hat{f}_0 \Gamma_0 + \hat{f}_1 \Gamma_1(\xi_1) + \hat{f}_2 \Gamma_1(\xi_2) + \\
\hat{f}_{1,1} \Gamma_2(\xi_1, \xi_1) + \hat{f}_{2,1} \Gamma_2(\xi_2, \xi_1) + \hat{f}_{2,2} \Gamma_2(\xi_2, \xi_2) + \\
\hat{f}_{1,1,1} \Gamma_3(\xi_1, \xi_1, \xi_1) + \hat{f}_{2,1,1} \Gamma_3(\xi_2, \xi_1, \xi_1) + \hat{f}_{2,2,1} \Gamma_3(\xi_2, \xi_2, \xi_1) + \hat{f}_{2,2,2} \Gamma_3(\xi_2, \xi_2, \xi_2) + \ldots
\]

represented in terms of the PCE.
This form of spectral expansion converges to the true solution in the mean-square sense:

$$\lim_{p \to \infty} E \left[ \left( \hat{f}_0 \Gamma_0 + \ldots + \sum_{i_1=1}^{i_{p-1}} \sum_{i_p=1}^{\infty} \hat{f}_{i_1, \ldots, i_p} \Gamma_p(\xi_{i_1}, \ldots, \xi_{i_p}) - f \right)^2 \right] = 0$$  \hspace{1cm} (A.2)

A compact form of random variable PCE:

$$f(\omega) = \sum_{|i|=0}^{\infty} \hat{f}_i \Psi_i(\xi_1, \xi_2, \ldots)$$  \hspace{1cm} (A.3)

$$|i| = \sum_{k=1}^{\infty} i_k$$  \hspace{1cm} (A.4)

where \( i = (i_1, i_2, \ldots) \) is an infinite dimensional order index, and

$$\Psi_i(\xi_1, \xi_2, \ldots) = \prod_{k=1}^{\infty} \psi_i(\xi_k)$$  \hspace{1cm} (A.5)

The orthogonality of the basis w.r.t. to the joint PDF shown as

$$\langle \Psi_i, \Psi_j \rangle = \int_{\Theta} \Psi_i(\xi) \Psi_j(\xi) p(\xi) d\xi = \delta_{ij} E[\Psi_i^2]$$  \hspace{1cm} (A.6)

where \( \delta_{ij} = 1 \) if \( i = j \), zero otherwise. For computational purpose, the infinite-dimensional polynomial basis will be truncated at some finite order \( n_p \) and stochastic dimension at \( d \)

$$\mathcal{P}_{n_p} f = \sum_{|i|=0}^{n_p} \hat{f}_i \Psi_i(\xi_1, \ldots, \xi_d)$$  \hspace{1cm} (A.7)

$$\Psi_i(\xi_1, \ldots, \xi_d) = \prod_{k=1}^{d} \psi_i(\xi_k)$$

where \( \mathcal{P}_{n_p} \) is the truncated PCE operator. Notice since \( i \) is a vector of multidimensional index, there will be \( n_{pc}(> n_p) \) expansion terms, where \( n_{pc} \) depends on the specific truncation of the PC basis.
Due to orthogonality of the basis,
\[
\langle f, \Psi_j \rangle = \left\langle \left( \sum_{|i|=0}^{n_p} \hat{f}_i \Psi_i \right), \Psi_j \right\rangle = \hat{f}_i \langle \Psi_i^2 \rangle,
\]
the \(i\)-th coefficient is
\[
\hat{f}_i = \frac{\langle f, \Psi_i \rangle}{\langle \Psi_i^2 \rangle},
\]
which minimizes the error norm \(E[(f - P_n f)^2]\). This is only ONE way to define the coefficients, other error norms (metrics) are sometimes more appropriate to minimize.

**Example A.1.2** To demonstrate the finite order, finite dimensional form of spectral expansion, suppose \(n_p = 2\) and \(d = 2\) yields
\[
P_2 f = \sum_{|i| \leq 2} \hat{f}_i \psi_i(\xi_1, \xi_2)
\]
\[
= \hat{f}_{00} + \hat{f}_{10} \psi_1(\xi_1) + \hat{f}_{01} \psi_1(\xi_2) + \hat{f}_{20} \psi_2(\xi_1) + \hat{f}_{02} \psi_2(\xi_2) + \hat{f}_{11} \psi_1(\xi_1) \psi_1(\xi_2)
\]
This also illustrates the total order expansion, that is \(|i| \leq 2\) as opposed to \(\max(i) \leq 2\) which would have included an \(f_{22}\) term.

We see that the expectation of \(f\) is given by
\[
E[f] = \langle f \rangle = \langle \Psi_0, f \rangle = \sum_{i=0}^{n_p} \hat{f}_i \langle \Psi_0, \Psi_i \rangle = \hat{f}_0,
\]
after assuming that \(\|\Psi_0\|^2 = 1\). Therefore, \(\hat{f}_0\) is in fact the mean of the random variable \(f\). Further, the variance
\[
\sigma^2(f) = E[(f - E[f])^2] = E[(f - \hat{f}_0)]
\]
\[
= E\left[ \left( \sum_{i=1}^{n_p} \hat{f}_i \Psi_i \right)^2 \right]
\]
\[
= \sum_{i=1}^{n_p} \hat{f}_i^2 \langle \Psi_i^2 \rangle
\]
which is a weighted sum of its squared PC coefficients.
A.1.2 Pseudospectral stochastic projection method

A spectral projection, as (A.9), recovers the PCE coefficients

$$\hat{f}_i = \frac{\langle f, \Psi_i \rangle}{\langle \Psi_i^2 \rangle},$$

where the denominator could be analytically integrated and satisfies the orthogonality of generalized polynomial chaos (gPC) [Xiu and Karniadakis, 2002] w.r.t. the distribution of the input random parameter. In contrast, the numerator is not possible to integrate analytically for an unknow function, thus requires numerical integration, hence the name pseudo-spectral. This is generally approximated by the MC sampling or quadrature (i.e., cubature) rule. The MC sampling of the input parameters requires numerous model evaluations for the solution to converge. Whereas, quadrature rules require model runs on fixed parameter values with rather fewer model runs and fast convergence. Here we focus on certain quadrature rules to perform the pseudo-spectral stochastic method of gPC [Xiu, 2007] with model runs restricted to the associated quadrature points. This method is also known as non-intrusive polynomial chaos [Hosder et al., 2006], where an uncoupled method is applied without re-designing the deterministic model as apposed to the “intrusive” Galerkin method which requires spectral projection. A simple example of Galerkin method,

**Example A.1.3** Suppose a model $G(X,Y) = 0$, where $G$ is a model operator on the random variables $X$ and $Y$. $X$ and $Y$ could be written in PC expansion such that

$$G(\sum_{i=1}^{n_p} \hat{x}_i \Psi_i, \sum_{i=1}^{n_p} \hat{y}_i \Psi_i) = 0.$$ 

The equation is thus solved by taking spectral projection

$$\left\langle G(\sum_{i=1}^{n_p} \hat{x}_i \Psi_i, \sum_{i=1}^{n_p} \hat{y}_i \Psi_i), \Psi_j \right\rangle = 0, \quad j = 1, \ldots, n_p$$
This shows that the Galerkin method requires solving a set of $n_p$ equations for all $n_p$ coefficients by redesigning the entire system of equations.

In contrast, the non-intrusive method treats the forward model as a black-box and evaluated on the quadrature input points to generate realizations. The pseudospectral coefficient becomes

$$\tilde{f}_i = \frac{Q_l(f \Psi_i p(\xi))}{\langle \Psi_i^2 \rangle}$$  \hspace{1cm} (A.13)

where $Q_l$ is quadrature rule, $l$ is the quadrature level with the associated total numbers of quadrature points $n_l$, $p(\xi)$ is the probability associated with the basis (in the remaining content, assume Legendre polynomial with $p(\xi) = 1$ for the sake of simplicity),

$$\lim_{n_l \to \infty} \tilde{f}_i = \hat{f}_i$$  \hspace{1cm} (A.14)

The result is a pseudo-spectral type approach for the random variable of interest,

$$S_{n_p} f = \sum_{|i|=0}^{n_p} \tilde{f}_i \Psi_i(\xi)$$  \hspace{1cm} (A.15)

where $S_{n_p}$ is the pseudospectral operator. The solution converges in the limit to the truncated PCE

$$\lim_{n_l \to \infty} S_{n_p} f = P_{n_p} f$$  \hspace{1cm} (A.16)

Following classical approximation theory, the pseudospectral approximation converges in the mean square sense w.r.t. the associated probability function $p(\xi)$

$$\|f - S_{n_p} f\|_{L^2_{p(\xi)}}^2 = \int_{\Xi} (f - S_{n_p} f)^2 p(\xi) d\xi \to 0, \quad n_p \to \infty, \quad n_l \to \infty$$  \hspace{1cm} (A.17)
A.1.3 Pseudospectral approximation aliasing

The quadrature approximation incurs an additional error which can be expressed as follows in the $L_2$-norm:

$$
(||P_{np} f - S_{np} f||_2)^2 = \sum_{j=0}^{np} (\hat{f}_j - \tilde{f}_j)^2,
$$

where we have used orthonormality for PCE basis. Substituting $\tilde{f}_j$ with its quadrature approximation gives

$$
\sum_{j=0}^{np} (\hat{f}_j - \tilde{f}_j)^2 = \\
\sum_{j=0}^{np} \left( \hat{f}_j - Q(f\psi_j) \right)^2 = \\
\sum_{j=0}^{np} \left( \hat{f}_j - Q(\sum_{k=0}^{\infty} f_k \psi_k \psi_j) \right)^2 = \\
\sum_{j=0}^{np} \left( \hat{f}_j - Q(\sum_{k=0}^{np} f_k \psi_k \psi_j + \sum_{k=np}^{\infty} f_k \psi_k \psi_j) \right)^2 = \\
\sum_{j=0}^{np} \left( \hat{f}_j - \sum_{k=0}^{np} f_k Q(\psi_k \psi_j) - \sum_{k=np}^{\infty} f_k Q(\psi_k \psi_j) \right)^2.
$$

The term $Q(\psi_k \psi_j)$ can give rise to internal aliasing: if the quadrature is not accurate enough to preserve the orthogonality of the low degree polynomials retained in the series expansion. If it is accurate the first two terms cancel out. The third term is the external aliasing when $k+j$ exceeds the exactness order (see below) of the quadrature.

Internal aliasing occurs when both $\psi_k$ and $\psi_j$ are included in the truncated expansion. External aliasing occurs when only $\psi_j$ is involved in the expansion. We want to select the smallest quadrature level that brings the internal aliasing (first two terms) to zero, since those are the actual polynomials included in the truncated expansion. Finally,
for any function $f$, the error for the pseudo-spectral approximation becomes

$$
(||f - S_{n_p}f||_2)^2 = \sum_{j=0}^{n_p} \left( \hat{f}_j - \sum_{k=0}^{n_p} f_k Q(\psi_k \psi_j) - \sum_{k=n_p}^{\infty} f_k Q(\psi_k \psi_j) \right)^2 + \sum_{j=n_p+1}^{\infty} \hat{f}_j^2, \quad \text{(A.20)}
$$

where the last term is the truncation error.

### A.1.3.1 Quadrature Exactness condition

The polynomials of order up to $n_p$ obtains exact numerical integration by a ($n_l$)-point quadrature rule.

**Example A.1.4** Suppose $\psi(\xi)$ is of order $n_p$, the 1D quadrature exactness could be written as:

$$
\int_{\Xi} \psi(\xi)d\xi = Q_l \psi(\xi) = \sum_{q=1}^{n_l} w_q \psi(\xi_q) \quad \text{(A.21)}
$$

### A.1.3.2 Accurate set

In order to keep track of multi-dimensional quadrature levels, one rewrites the quadrature operator with the level index $l$. Hence

$$
\alpha(Q_l) = \{ \psi_i : Q_l(\psi_i) = Q(\psi_i), \forall i \leq n_p \}. \quad \text{(A.22)}
$$

One can always find a quadrature of sufficient order to integrate a polynomial of degree up to $n_p$ exactly.

### A.1.3.3 Half Accurate set

$$
\alpha_{1/2}(Q_l) = \{ \psi_i : Q_l(\psi_i^2) = Q(\psi_i^2), \forall i \leq \text{floor}(n_p/2) \}. \quad \text{(A.23)}
$$
This is the set that avoids internal aliasing where \(< \psi_i, \psi_j > = Q_l(\psi_j \psi_j) = \delta_{ij} \| \psi_i \|^2\).

This condition suggests a definition of the multidimension PCE when quadrature rules are anisotropic between dimensions (e.g., sparse quadrature).

A.1.4 1D quadrature rule

Suppose the support of a parameter is \([-1, 1]\), the quadrature is exact if

\[
\int_{-1}^{1} f(\xi) d\xi = Q_l^{(1)} f = \sum_{q=1}^{n_l} w_q f(\xi_q^l),
\]

where it depends on function values at a finite set of points

\[
\{ \xi_1^l, \ldots, \xi_{n_l}^l \} \subset [-1, 1].
\]

For now, we focus on a specific type of nested quadrature rule for the practicality of adaptive construction of the PC series. By taking advantage of the nested property, the numbers of function evaluations could be greatly reduced by reusing previous results during adaptation. The nested points of univariate quadrature rule are the maxima of polynomials, such as the Chebyshev roots. According to Trefethen [2008], the order of convergence is the same between the Clenshaw-Curtis (CC, nested) and the Gauss-Legendre (GL, non-nested) quadrature rule, but with a factor of 2 between the exactness of the formulae. In fact, both N-point Gaussian and Clenshaw-Curtis quadrature have error bounded by \(O((2N)^{-k}/k)\) for a \(k\)-times differentiable integrand.

According to Conrad and Marzouk [2013], Gauss-Paterson (GP, nested) has the best exactness property with the nested property. We use only the nested rules as our sparse quadrature construction for practical purpose. The relationship of levels and
numbers of quadrature points for GP,

\[ n_1 = 1 \]
\[ n_l = 2^l - 1, \ l \geq 2 \] \hspace{1cm} (A.26)

and for CC,

\[ n_1 = 1 \]
\[ n_l = 2^{l-1} + 1, \ l \geq 2 \] \hspace{1cm} (A.27)

The results in Table A.1 summarize the quadrature exactness condition given the quadrature rules.

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<td>5</td>
<td>17</td>
<td>17</td>
<td>8</td>
<td>31</td>
<td>46</td>
<td>23</td>
</tr>
</tbody>
</table>

Table A.1: The two nested quadrature rules with the numbers of quadrature points \( n_l \), the maximum order of accurate polynomial set \( n_a \) and the maximum order of half accurate set \( n_{ha} \) associated to the given levels \( l \).

The quadrature points for CC are the roots of the Chebyshev Polynomial. Simply,

\[ x_q = \cos\left(\frac{q\pi}{n_l}\right), \ q = 0, 1, 2, \ldots, n_l \] \hspace{1cm} (A.28)

The CC weights \( w_q \) could be obtain in \( O(n \log n) \) by Fast Fourier Transform (FFT) [Waldvogel, 2006].
A.1.5 Multidimension quadrature rule

A.1.5.1 Full tensor product quadrature

The naive approach to the multidimension quadrature is to form a linear combination of the maximum level 1D quadrature over all dimension,

\[
Q^{(D)}_l f = \sum_{q_1=1}^{n_{l_1}} \ldots \sum_{q_d=1}^{n_{l_d}} w_{q_1}^{l_1} \ldots w_{q_d}^{l_d} f(\xi_{q_1}^{l_1}, \ldots, \xi_{q_d}^{l_d})
\]

where \( l = (l_1, \ldots, l_d) \) is the quadrature level vector and \( D = (1, \ldots, d) \) is the dimension vector. We can see the first equality is summed over all the 1D quadrature points (A.25) in all dimensions by full tensorized grid.

\[
\mathcal{H}^{(D)}_l = \xi^{l_1} \times \ldots \times \xi^{l_d} \subset [-1,1]^d.
\]

A.1.5.2 Full tensor pseudospectral approximation

Given an arbitrary function \( f(\boldsymbol{\xi}) \),

\[
Q^{(D)}_l f = (Q^{(1)}_{l_1} \otimes \ldots \otimes Q^{(d)}_{l_d}) f(\boldsymbol{\xi})
\]

where \( l = (l_1, \ldots, l_d) \) is the quadrature level vector and \( D = (1, \ldots, d) \) is the dimension vector. We can see the first equality is summed over all the 1D quadrature points (A.25) in all dimensions by full tensorized grid.

\[
\mathcal{H}^{(D)}_l = \xi^{l_1} \times \ldots \times \xi^{l_d} \subset [-1,1]^d.
\]

Apply the pseudospectral approximation to each dimension individually requires a tensor product pseudospectral operator,

\[
\mathcal{S}^{(D)}_{n_p} f = \left( \mathcal{S}^{(1)}_{n_p} \otimes \ldots \otimes \mathcal{S}^{(d)}_{n_p} \right) f
\]

where \( l = (l_1, \ldots, l_d) \) is the quadrature level vector and \( D = (1, \ldots, d) \) is the dimension vector. We can see the first equality is summed over all the 1D quadrature points (A.25) in all dimensions by full tensorized grid.
where the truncation in each dimension is independently defined. Substitute (A.31) into (A.32) yields,

\[ S_{h^p}^l f = \sum_{i_1=0}^{n_1^l} Q_{l_1}^{(1)} (f^{(1)}(\xi^{(1)})) \psi_{i_1} \otimes \cdots \otimes \sum_{i_d=0}^{n_d^l} Q_{l_d}^{(d)} (f^{(d)}(\xi^{(d)})) \psi_{i_d}. \] (A.33)

Essentially speaking, (A.31) is a multidimension accurate set formed by tensor product of 1D accurate set in (A.33).

\[ a(Q_{L}^{(D)}) \supseteq a(Q_{l_1}^{(1)}) \otimes \cdots \otimes a(Q_{l_d}^{(d)}), \] (A.34)

with the basis

\[ \Psi_i \in a_{1/2}(Q_{l_1}^{(1)}) \supseteq a_{1/2}(Q_{l_1}^{(1)}) \otimes \cdots \otimes a_{1/2}(Q_{l_d}^{(d)}). \] (A.35)

This concludes that the full tensor pseudospectral approximation in \( d \) dimension has no internal aliasing \cite{Conrad and Marzouk, 2013}. (A.33) is a useful formula for the following Smolyak’s construction where different quadrature rules are treated in each dimension separately.

**Example A.1.5** Given \( d = 2, l = (3, 4) \) for a CC rule. The accurate basis for the full tensor pseudospectral approximation are the tensor product of the two half accurate sets

\[ a_{1/2}(Q_{l_1}^{(1)}) = \{ \psi_1, \psi_2 \} \] (A.36)

\[ a_{1/2}(Q_{l_2}^{(2)}) = \{ \psi_1, \psi_2, \psi_3, \psi_4 \}. \]

Notice if \( l = (3, 3) \), then \( a_{1/2}(Q_{l_1}^{(1)}) = \{ \psi_1, \psi_2 \} \subset a_{1/2}(Q_{l_2}^{(2)}) \) shows a nested property for the CC rule.
A.1.5.3 Sparse grid method

Also known as Smolyak’s algorithm [Smolyak, 1963]. In order to construct an incremental sparse grid quadrature, it is necessary to define a difference operator,

\[ \Delta_l f = (Q_l^{(1)} - Q_{l-1}^{(1)}) f, \]
\[ \Delta_0 f = Q_0^{(1)} f = 0. \]  \hspace{1cm} (A.37)

The multidimension sparse quadrature rule is constructed as a sparse tensor product,

\[ Q_l^{(D)} f = \sum_{|\mathbf{l}| \leq L + d - 1} (\Delta l_1 \otimes \ldots \otimes \Delta l_d) f \]  \hspace{1cm} (A.38)

where \( L \) is an overall maximum level. The multidimensional level index \( \mathbf{l} \) forms a simplex/triangular truncation following the condition,

\[ |\mathbf{l}| = \sum_{i=1}^{d} l_i \]  \hspace{1cm} (A.39)

**Example A.1.6** Assume \( d = 2 \), \( l = 3 \), and a CC rule. The entire \( l_1 \times l_2 \) grid represents a full tensorization. Whereas the grey lower triangle satisfies \( l_1 + l_2 \leq 4 \), which is the sparse grid.
For computational purpose, reorganize the terms in (A.38) to construct a weighted sum,

\[ Q_l^{(D)} f = \sum_{L \leq |l| \leq L + d - 1} (-1)^{L + d - 1 - |l|} \left( \frac{d - 1}{L + d - 1 - |l|} \right) (Q_{l_1}^{(1)} \otimes \ldots \otimes Q_{l_d}^{(d)}) f \]

\[ = \sum_{l \in I_l} c_l (Q_{l_1}^{(1)} \otimes \ldots \otimes Q_{l_d}^{(d)}) f \]  

(A.40)

where \( c_l \) are the Smolyak coefficients, and \( I_l \) is the Smolyak multidimensional level index set,

\[ I_l = \{ l \in \mathbb{N}^d : L \leq |l| \leq L + d - 1 \}. \]  

(A.41)

which must satisfy the admissibility condition

\[ \text{if for all } l \in I_l, \ l - e_j \in I_l \text{ for } 1 \leq j \leq d, \ l_j > 1, \]  

(A.42)

where \( e_j \) are the unit vectors in \( j \)-th dim and \( l = (l_1, \ldots, l_d) \). This shows the \( l \) grid is smaller in at least one dimension. This condition ensures the validity of the telescope sum expansion of the general sparse quadrature formulas.

The quadrature shall be performed on the sparse grid union

\[ H_{I_l}^{(d)} = \bigcup_{l \in I_l} (\xi_l^1 \times \ldots \times \xi_l^d) \subset [-1, 1]^d \]  

(A.43)

Example A.1.7 From Example A.1.6, the union of the sparse grids quadrature points \( H_{I_l}^{(2)} \) gives

![Graphical representation of quadrature points](image)
which is just the union of the Smolyak multidimensional level index set at the leading surface (union of the diagonal indices in this case). Whereas the union of full tensor quadrature points $\mathcal{H}^{(2)}_{(3,3)}$ is just the (3,3)-grid in example A.1.6.

When performing pseudospectral approximation directly by sparse quadrature rule, the higher order pseudospectral coefficients corresponding to the higher order polynomials are inaccurate [Constantine et al., 2012]. This is due to inclusion of redundant basis without considering the accurate condition of quadrature rules in each dimension for sparse grid rule (i.e., incurring excessive internal aliasing). The accurate sparse grid integration is to include only the basis that are accurate w.r.t. the admissible multidimensional level index $I_l$.

### A.1.5.4 Sparse grid pseudospectral approximation

Follow the same procedure as full tensor pseudospectral approximation derived in (A.33), sparse grid pseudospectral approximation becomes,

$$S(f) = \sum_{i_1=0}^{n_p^{i_1}} \ldots \sum_{i_d=0}^{n_p^{i_d}} Q^{(l)}_l(f\Psi_i)\Psi_i$$

$$= \sum_{i_1=0}^{n_p^{i_1}} \ldots \sum_{i_d=0}^{n_p^{i_d}} \left( \sum_{l\in\mathcal{I}_l} c_t (Q^{(1)}_{i_1} \otimes \ldots \otimes Q^{(d)}_{l_d})(f\Psi_i) \right) \Psi_i$$

$$= \sum_{l\in\mathcal{I}_l} c_t \left( \sum_{i_1=0}^{n_p^{i_1}} Q^{(1)}_{i_1} (f^{(1)}(\xi^{(1)}_{i_1})\psi_{i_1}) \psi_{i_1} \otimes \ldots \otimes \sum_{i_d=0}^{n_p^{i_d}} Q^{(d)}_{l_d} (f^{(d)}(\xi^{(d)}_{i_d})\psi_{i_d}) \psi_{i_d} ) \right)$$

$$= \sum_{l\in\mathcal{I}_l} c_t S^{f^{(l)}}_{n_p^{(l)}} f$$

(A.44)

The last line indicates that the sparse grid pseudospectral approximation is the sum of different full tensor pseudospectral approximation over all admissible multidimensional
level indices. The accurate basis set w.r.t. $l \in \mathcal{I}_t$,

$$\Psi_i \in a_{1/2}(Q^{(D)}_l). \quad (A.45)$$

### A.1.5.5 Dimension Adaptive Sparse Quadrature (DASQ)

The adaptive process is based on some error indicators and quadrature level adapting in different stochastic dimension. The idea is to increase the quadrature level along the dimension which remain under-resolved. Nested quadrature allows level adaption by simple error indicator based on the differential integral of two subsequent quadrature order [Gerstner and Griebel, 1998]. Take a 1D error estimate for example:

$$|E_l^{(1)} f| \approx |(Q_l^{(1)} - Q_{l-1}^{(1)})f| = |\Delta_l^{(1)} f| \quad (A.46)$$

The local error indicator $g_l$ is assigned to each multidimensional level index $l \in \mathcal{I}_t$ by the differential integral

$$g_l = \Delta_l^{(D)} f = (\Delta_{l_1} \otimes \ldots \otimes \Delta_{l_d}) f \quad (A.47)$$

Notice the differential integral are between neighboring level indices for each dimension. Small values of (A.46) indicate smoother solution in that dimension, where increasing level might not be necessary.

The basic algorithm starts by adding indices element-wise by a unit vector set $\{e_1, \ldots, e_d\}$ in all dimensions. Here we define the neighboring multidimensional level index set of a given grid $l$ for the algorithm. The forward neighbors of the grid $l$

$$\{l + e_j : \ 1 \leq j \leq d\}. \quad (A.48)$$
The backward neighbors of the grid $l$

$$\{l - e_j : 1 \leq j \leq d, \ l_j > 1\}. \quad (A.49)$$

The error is evaluated once a forward neighbor satisfy the admissible condition. The largest error grid will become the focus grid $l$ that needed further forward grid build up in order to minimize the overall error.

The adaptive grids have polynomials following the exactness condition. Hence, the PC coefficients associated with the accurate polynomials allowed in the grids increase in order as the grids build up. This is the major difference from the PC coefficients predefined in the direct PCE method without using the exactness condition. Therefore the multidimensional order index set for the PC coefficients is interactively defined as oppose to predefined.

### A.1.5.6 DASQ pseudospectral approximation algorithm

Followed by Gerstner and Griebel [2003]; Huan [2010] with a slight modification to the pseudospectral approach and the quadrature exactness condition

DASQ pseudospectral approximation of the PC terms

$$\left\{ \chi_i(\xi) = f(\xi) \Psi_i(\xi) : i_k \leq n_{\text{per}}^{(k)} \right\},$$

$\mathcal{O} = \emptyset$

$\mathcal{A} = \{(1, \ldots, 1)\}$

$r(1) = \Delta_{l} \chi_{\{0, \ldots, 0\}}$

$g_l = \max(r_l)$

$\eta = g_l$

while $\eta > TOL$

select $l$ from $\mathcal{A}$ with largest $g_l$

$\mathcal{A} = \mathcal{A} \setminus l$

$\mathcal{O} = \mathcal{O} \cup l$

$\eta = \eta - g_l$
for $m = 1, \ldots, d$

\[ j = l + e_m \]

if ( $j - e_q \in \mathcal{O}$ admissible for all $q = 1, \ldots, d$ )

\[ \mathcal{A} = \mathcal{A} \cup \{ j \} \]

\[ \text{determine } \mathcal{P}_j \text{ for the grid } j \]

for $p \in \mathcal{P}_j$

\[ s_p = \Delta_j \chi_i \]

if ( $p$ is an existing PC coefficient in backward neighboring grids )

\[ r(p) = r(p) + s_p \]

else ( $p$ is a new PC coefficient throughout the existing grids )

\[ r(p) = r(p) + Q_j \chi_i \]

end

\[ g_j = \max(s) \]

\[ \eta = \eta + g_j \]

end

end

$\mathcal{O}$ old index set
$\mathcal{A}$ active index set
$\mathcal{P}_j$ multi-index set of accurate PC term for the grid $j$
$Q_l \chi_i$ quadrature $\otimes_{k=1}^{d} Q_{l_k} \chi_i$
$\Delta_l \chi_i$ differential integral $\otimes_{k=1}^{d} \Delta_{l_k} \chi_i$
$g_l$ local error indicator for a grid
$\eta$ global error estimate $\sum_{l \in \mathcal{A}} g_l$ for grids in the active set
$e_k$ unit vector in k-dimension
TOL error tolerance
$s$ differential integral for $\chi_i$
$r$ the accumulated integral $\sum_{l \in \mathcal{O} \cup \mathcal{A}} \otimes_{k=1}^{d} \Delta_{l_k} \chi_i$

Summarize in words:

- Select a grid $l$ with the largest error indicator $g_l$ from all grids in the active set. Save this grid $l$ to the old index set and remove from the active index set. Start working on this single grid $l$.

- Reach out to each dimension by a unit vector from $l$, and assess the admissibility.

- Save the grids to the active set if admissible, and sum the $g_l$ in the active set to obtain a global error $\eta$.

- Repeat the process if the global error $\eta$ were greater than the error tolerance TOL. Otherwise stop the cycle when reaching the TOL.
A.1.5.7 Error estimation

The general error indicator should depend on two factors, which are the differential integral and the quadrature level.

\[ g_l = \max \left\{ \omega \frac{\Delta t \chi_i}{\Delta x} \left( 1 - \omega \right) \frac{1}{\max(l)} \right\} . \]  

(A.50)

The error is expected to decrease monotonically by grid and maximum level increasing. Following the greedy approach by Gerstner and Griebel [2003], set \( \omega = 1 \) and disregard the second term in (A.50). This approach assumes the solution to be very smooth and the error \( \Delta t \chi_i \) will decrease with increasing grids anyway. If the solution is not smooth with spikes on fine scales or large local discontinuities, then the second terms acts to create a buffer for quadrature to neglect capturing such spikes and assign a error by the maximum level. This could end up preventing higher level grids in dimensions with discontinuities.

A.1.5.8 Relative addressing

The multidimensional level index set \( I_l \) for a grid, or grid index for short, \( m \times (d + n_{pc}) \) integer array ( \( m \) is the maximum number of row indices and \( n_{pc} \) is the maximum numbers of PC coefficients indices), has the row values as \( A \cup O \). Each row of the 1 to \( d \)-th columns of \( I_l \) store a single multidimensional level grid. The \( d + 1 \) to \( n_{pc} \)-th columns store the PC coefficient index set \( P_l \) for each grid. \( I_l \) will be kept intact once the grid indices were stored.

The active row index set \( A \) and old row index set \( O \), both are \( m \times 1 \) integer array, stores the row indices of \( I_l \). \( A \) stores the active grids at the leading surface. The
largest error grid in $\mathcal{A}$ are removed to $\mathcal{O}$ for next grid increment.

The error indicator set $\mathcal{G}$, floating point $m \times 1$ array, controls whether to add or remove indices in $\mathcal{A}$ and $\mathcal{O}$. It has the same row order w.r.t. to $\mathcal{I}_t$.

The neighborhood index set $\mathcal{N}$, $m \times 2d$ array, stores the forward and backward neighboring row index of the grid index with the same row order w.r.t. to $\mathcal{I}_t$. It is defined to check the admissibility of an $\mathcal{I}$. The first $m \times d$ stores the forward index set and the 2nd $m \times d$ stores the backward index set of all $\mathcal{I}$.

Use a binary tree technique, namely heap in computer science, to find the hierarchy of error indices. This avoids comparing all the indices with the new input index each time in $\mathcal{A}$ to find the maximum error index. Below highlights how sorting, removing and adding indices in $\mathcal{A}$ works:

- **Sorting rule**: The *father* index $p$ is greater than the *son* index $2p$ and $2p+1$ for all indices.

- **Removing rule**: The maximum error is at the *root* ($1^{st}$ index). Once the root is removed from $\mathcal{A}$ to $\mathcal{O}$, the two sons ($2^{nd}$ and $3^{rd}$ index) with bigger error will be moved up to the root, and leaving an empty father index for the following two sons to recursively fill in until the *leaf*, bottom of the tree, reaches. The leaf index of the process is substituted with the last element $\mathcal{A}$ and using the Adding rule to rearrange.

- **Adding rule**: A new index is put in the end plus one index of $\mathcal{A}$ and compared with the father index according toheap. So suppose the new index is at $p$ el-
element, the father will be at $\text{floor}(p/2)$. If $p$ were greater than $\text{floor}(p/2)$, then swap the values of the indices. Repeat this process until the current father error indicator is greater than the new index.

**A.1.5.9 Reuse nested quadrature function values**

The backtracking algorithm [Huan, 2010] reuses the function value from the previous quadrature points when adaptively increasing $l$ in a dimension for a nested quadrature rule (e.g., CC).

The multidimensional point quadrature index set $I_q$, integer array, stores the entire quadrature indices for each grid (e.g., For a level 2 1D CC quadrature points $[-1.0, 0.0, 1.0]$, $I_q$ stores the multidimensional point indices $[1,2,3]$ respectively). The purpose of storing the indices is to reuse nested quadrature points whenever function values exist in a previous admissible grid (e.g., For a level 3 1D CC quadrature points $[-1.0, -0.7, 0.0, 0.7, 1.0]$, reuse the function values on indices $[1,3,5]$ evaluated on quadrature points $[-1.0, 0.0, 1]$ from previous level 2). Thus, the reuse is always on odd indices (with level 2 on the pointer 2 as an exception). So, the backtracking quadrature point indices are just $\text{ceil}([1,3,5]/2) = [1,2,3]$.

The model function set $F$, floating point array, stores only the function values evaluated on new quadrature points. $F$ is designed for $I_q$ to reuse function values stored in previous grids.
The PC polynomial set $P$, floating point array, stores the polynomial values evaluated on new quadrature points with the same row order w.r.t. $F$. $P$ is also designed for the purpose of reusing polynomial values stored in previous grids. The columns of $P$ is related to new multidimensional order PC.

Here we use a function index at the end+1 column of $I_q$ for the rows of quadrature points so the backtrace reduces to one time in each dimension to find the function value.

\begin{verbatim}
for ( go through the tensorized quadrature points for a given $l$ );
    if ( is a new point )
        Enter a new function index counter;
        Evaluate and store the new function for the new multidimensional point;
    else ( is an old point )
        Backtrace one level by a unit vector in the ascending dimension order
        Find the matching point
        Extract the stored function by the associated function index
        Store the function index to the matching point at the current grid
end
end
\end{verbatim}

\(^a\)A new point satisfies $q(l_i = 1) = \{1\}$, $q(l_i = 2) = \{1, 3\}$, $q(l_i > 2) = \{\text{even number}\}$.

\(^b\)An old point satisfies $q(l_i = 2) = \{2\}$, $q(l_i > 2) = \{\text{odd number}\}$.

\(^c\)The function index will be continually reused as grid increments.

### A.2 Sensitivity analysis

The sensitivity of a parameter is measured by how much variance it contributes to the state output, hence, it is also called variance analysis.
Suppose the state of SST is assumed to be most sensitive to two major parameters controlling CAPE and CMT in a pool of other parameters. Our goal is to use sensitivity analysis to filter out just the fractional variance of these two parameters upon the total variance on SST.

A.2.1 Functional decomposition

Sobol Decomposition

Given a square integrable function \( f(\xi_1, \ldots, \xi_d) \) over the \( d \)-dim hypercube

\[
\xi \in [0, 1]^d, \quad (A.51)
\]

\( f \) has an increasing dimension decomposition of the form

\[
f(\xi_1, \ldots, \xi_d) = f_0 + \sum_{u=1}^{d} f_u(\xi_u) + \sum_{u<v}^{d} f_{u,v}(\xi_u, \xi_v) + \ldots + f_{1,\ldots,d}(\xi_1, \ldots, \xi_d), \quad (A.52)
\]

which can also be written in a compact form

\[
f(\xi) = \sum_{s \subset \mathcal{D}} f_s(\xi_s), \quad (A.53)
\]

where the entire dimension index set \( \mathcal{D} = \{1, \ldots, d\} \). Notice this is not a series expansion as it has a finite number of terms. If each term in the decomposition has zero mean (i.e., \( \int f_s(\xi_s)d\xi_s = 0 \)), then all the terms are mutually orthogonal (i.e., \( \int f_y(\xi_y)f_z(\xi_z)d\xi_yd\xi_z = 0 \)), this unique orthogonal functional decomposition is often called Sobol Decomposition.

Example A.2.1 For \( d = 2 \),

\[
f(\xi_1, \xi_2) = f_0 + f_1(\xi_1) + f_2(\xi_2) + f_{1,2}(\xi_1, \xi_2) \quad (A.54)
\]
A.2.1.1  PCE-based Sobol decomposition

In terms of $|i|$-th order polynomial $\Psi_i$ for PCE, we see immediately a Sobol decomposition w.r.t the desired dimension index set $s = \{s_1, \ldots, s_p\}$ with the corresponding $\xi_s = \{\xi_{s_1}, \ldots, \xi_{s_p}\}$,

$$[\Psi_i(\xi)]_s = \prod_{k \in s} \psi_{i_k}(\xi_k).$$  \hspace{1cm} (A.55)

**Example A.2.2** Suppose we are just interested in $s = \{1\}$, then $[\Psi_i(\xi)]_{\{1\}} = \prod_{k \in \{1\}} \psi_{i_k}(\xi_k) = \psi_{i_1}(\xi_1)$ for all orders of $i$. This would be the subset $\{\psi_1(\xi_1), \psi_2(\xi_1), \ldots, \psi_{n-1}(\xi_1), \psi_n(\xi_1), \ldots\}$ in the infinite PC expansion.

Therefore, each of the Sobol expansion represented in PCE

$$f_s(\xi_s) = \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i(\xi)]_s.$$  \hspace{1cm} (A.56)

The entire Sobol decomposition in terms of PCE

$$f(\xi_1, \ldots, \xi_d) = f_0 + \sum_{u=1}^{d} \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i]_{\{u\}} + \sum_{u<v}^{d} \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i]_{\{u,v\}} + \ldots + \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i]_{\{1,\ldots,d\}}$$  \hspace{1cm} (A.57)

**Example A.2.3** Expand in $d = 2$,

$$f(\xi_1, \xi_2) = f_0 + \sum_{u=1}^{2} \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i]_{\{u\}} + \sum_{|i|=1}^{\infty} \hat{f}_i[\Psi_i]_{\{1,2\}}$$

$$= f_0 + \sum_{|i|=1}^{\infty} \hat{f}_i[\prod_{k \in \{1\}} \psi_{i_k}(\xi_k)] + \sum_{|i|=1}^{\infty} \hat{f}_i[\prod_{k \in \{2\}} \psi_{i_k}(\xi_k)] + \sum_{|i|=1}^{\infty} \hat{f}_i[\prod_{k \in \{1,2\}} \psi_{i_k}(\xi_k)]$$

$$= f_0 + \hat{f}_{10}\psi_1(\xi_1) + \hat{f}_{20}\psi_2(\xi_1) + \ldots + \hat{f}_{01}\psi_1(\xi_2) + \hat{f}_{02}\psi_2(\xi_2) + \ldots + \hat{f}_{11}\psi_1(\xi_1)\psi_1(\xi_2) + \hat{f}_{12}\psi_1(\xi_1)\psi_2(\xi_2) + \hat{f}_{21}\psi_2(\xi_1)\psi_1(\xi_2) + \ldots$$  \hspace{1cm} (A.58)
This shows the Sobol decomposition containing all the PCE terms.

Notice that the summands in Sobol decomposition is in the order of increasing dimensions. Where a single dimension $\xi_j$ of interest could be in multiple summands. This leads to the derivation of Sobol sensitivity index.

### A.2.2 Global sensitivity analysis

The main reason for a Sobol’s decomposition lies in the mutually orthogonal nature

$$\langle f_s, f_{s'} \rangle = \langle f_s^2 \rangle \delta_{s,s'} \quad (A.59)$$

such that the total variance

$$\sigma^2(f) = \langle (f - f_0)^2 \rangle = \sum_{s \subset D} \langle f_s^2 \rangle \quad (A.60)$$

where each term admits a variance

$$\sigma^2(f_s) = \langle f_s^2 \rangle - \langle f_s \rangle^2 = \langle f_s^2 \rangle \quad (A.61)$$

where $\langle f_s \rangle = 0$ renders zero mean by definition. The Sobol sensitivity index

$$S_s = \frac{\sigma^2(f_s)}{\sigma^2(f)} \quad (A.62)$$

There could be a mix of dimensions in the index set $s = \{s_1, \ldots, s_p\}$ (e.g., $S_{\{1\}}$ and $S_{\{1,2\}}$ both are affected by $\xi_1$). Therefore, the fractional contribution of a single dimension $\xi_j$ on the total variance is defined as the total sensitivity index

$$T_{\{j\}} = \sum_{s \subset D, s \ni j} S_s \quad (A.63)$$
Substitute the relationship in (A.56)

$$\sigma^2(f_s) = \left\langle \left( \sum_{|i|=1}^{\infty} \hat{f}_i [\Psi_i]_s \right)^2 \right\rangle = \sum_{|i|=1}^{\infty} \hat{f}_i^2 \left\langle [\Psi_i]_s^2 \right\rangle,$$

we get the PC-based total sensitivity index

$$T_{(j)} = \frac{\sum_{s \subset D \ | |i|=1}^{\infty} \sum_{s \ni j}^{\infty} \hat{f}_i^2 \left\langle [\Psi_i]_s^2 \right\rangle}{\sigma^2(f)},$$

(A.65)

where the total variance from PCE is given in (A.12). The variance terms in $T_{(j)}$ are from all subsets of $D$ (i.e., the power set $\mathcal{P}(D)$ or $2^D$) which includes $j$-th dimension (e.g., suppose $D = \{1, 2, 3\}$ and $j = \{1\}$, the subsets $\{1\}, \{1, 2\}, \{1, 3\}, \{1, 2, 3\}$ are all considered as the $s$ that includes $j$).

A.3 Bayesian inference

For an inverse probability problem, the uninformative prior probability given additional observational data will yield a posterior correction. In the previous section, a closed form prior is designated to the polynomial chaos for orthogonality. Here we use the Bayesian Inference to correct the prior parameter distribution by making use of the measurement data $y$ to infer the posterior distribution.

The Bayes’ rule

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta)p(\theta)d\theta} = \alpha p(y|\theta)p(\theta),$$

(A.66)

where $\alpha = \int p(y|\theta)p(\theta)d\theta$. The posterior density $p(\theta|y)$, the prior density $p(\theta)$, and the observation $y$. 
We are interested in the statistical properties of the model state outputs that depends on the parameters. Such as the expectation of the state under the posterior

\[ E[f] = \int_{\Theta} f(\theta)p(\theta|y)d\theta. \]  

(A.67)

Since the posterior is not a closed form, one seeks to generate samples to obtain an approximation for the integral.

As proposed in Marzouk et al. [2007], the PCE surrogate will be used to speed up the sampling. The general idea is to bring in the surrogate and observations through the likelihood function \( p(y|\theta) \). Where the likelihood of the parameter values given observation is equal to the probability of the observation given the parameter values. (e.g., it assigns low probability to a parameter value if the model is far from capturing the observations).

In order to estimate the likelihood, recall from (4.19), assuming the measurement errors are i.i.d. centered Gaussian random variables \( \epsilon_i \sim N(0,\sigma^2) \) for the entire random field \( y_i = G_i(\theta(\omega)) + \epsilon_i \), where \( i \) is the field index. Since the \( y_i \) is fixed at each index, the randomness comes from \( G_i(\theta(\omega)) \), therefore, \( G_i \) could be seen as a Gaussian random variable centered at the expectation \( y_i \). Hence, \( G_i(\theta) - E[G_i(\theta)] = G_i(\theta) - y_i = \epsilon_i \) is the zero mean centered error Gaussian random variable. The likelihood estimation becomes the multivariate joint distribution of i.i.d. error r.v.

\[ p(y|\theta) = L(\theta) = \prod_i p_{\epsilon_i}(\epsilon_i) = \prod_i p(y_i - G_i(\theta)) \]  

(A.68)
From (A.68), we see the model entering the inverse problem. The posterior for any multidimensional point perturbation $\theta_j$ thus becomes

$$p(\theta_j|y) \propto \prod_i p(y_i - G_i(\theta_j))p(\theta_j) = L(\theta_j)p(\theta_j)$$

(A.69)

Notice pseudospectral method generate samples of $\xi$ instead of $\theta$. $\theta$ is a random vector that contains random variables $[\theta_1, \theta_2, \ldots]$, each could be written in terms of 1D PCE

$$\theta = \sum_{|i|=0}^{np} \hat{\theta}_i \Psi(\xi).$$

(A.70)

Therefore any sample of $\theta_j$ could be generated by $\xi_j$, representing a change of variable. By substituting the (A.69) into (A.67) with this change of variable

$$E[f] = \int_\Theta f(\theta(\xi)) \prod_i p(y_i - G_i(\theta(\xi)))p(\theta(\xi)) d\theta(\xi)$$

$$= \int_\Xi f(\theta(\xi)) \prod_i p(y_i - G_i(\theta(\xi))) | \det D\theta(\xi) | d\xi,$$

(A.71)

where $D\theta(\xi)$ is the Jacobian of $\theta$. This form allows numerical integration by sampling the germ $\xi$. As mentioned in Marzouk et al. [2007], this transformation of $\theta$ needs to be invertible (one-to-one) and the inverse transform must be contained in the prior support of $\Xi$, hence we will restrict to a linear transformation between $\theta$ and $\xi$.

**Example A.3.1** Suppose $\xi \sim U[-1, 1]$ with Legendre polynomial and $\theta$ has a support between $[a,b]$. The linear relationship is

$$\theta = \frac{b + a}{2} + \frac{b - a}{2} \xi,$$

a first order Legendre polynomial expansion.

A Monte Carlo estimation through sampling the prior gives

$$E_{p(\theta)}[f] \approx \frac{\alpha}{n} \sum_{j=1}^n f(\theta_j) L(\theta_j) | \det D\theta(\xi) |.$$  

(A.72)
Although the prior is generally a known function to easily create samples, it is often computationally extensive and excessive to sample through high dimensional parameter space when the probability is focused at a small area. Therefore, it is necessary to use an efficient sampling scheme to sample the posterior directly,

\[ E_{p(\theta|y)}[f] \approx \frac{\alpha}{n} \sum_{j=1}^{n} f(\xi_j) | \text{det} D\theta(\xi) |. \]  

We will drop the two scalar values \( \alpha \) and \( | \text{det} D\theta(\xi) | \) for the sake of simplicity.

### A.4 Markov Chain Monte Carlo (MCMC)

MCMC is a sampling strategy which assumes a stationary Markov Chain with time invariant target distribution \( \pi \) to estimate the population parameters (e.g. \( E_\pi[f] \) or higher moments), while trading off the independence of the samples. In the Bayes’ context, the posterior is the invariant target we concern.

The MCMC estimates \( E_\pi[f] = \frac{1}{n-b} \sum_{i=b}^{n} f(\xi_i) \), where \( b \) is the burn-in steps for the chain to reach the stationary regime of the invariant target (i.e. when samples presumably starts to come from the target). The size of \( b \) is chosen empirically.

#### A.4.0.1 Markov Chain

A random process has the Markov property if the conditional probability distribution of the next state of the process depends only on the current state, not on the sequence of events that preceded it. The sequence of random variable \( X_1, X_2, \ldots \) is called a Markov chain. A sequence of independent events (e.g., a series of i.i.d. fair
coin toss) does not have Markov property. Markov property is formally defined as,

\[ P\{X_{n+1} = x_{n+1} | X_1 = x_1, \ldots, X_n = x_n\} = P\{X_{n+1} = x_{n+1} | X_n = x_n\}. \quad (A.74) \]

The possible values of \( x_i \) form a state space of the chain. The change of states \( x \) to \( y \) of the system are called transitions, and the probabilities associated with various state-changes are called transition probabilities \( P\{X_{n+1} = y | X_n = x\} \).

As mentioned earlier, MCMC focuses on a special kind of Markov Chain, stationary Markov Chain, where the chain generated by a fixed transition probability approaches an equilibrium target distribution. The definition of stationary for Markov Chain is when the transition probability satisfies

\[ P\{X_{n+1} = y | X_n = x\} = P\{X_n = y | X_{n-1} = x\} \quad (A.75) \]

for states values \( x \) and \( y \). The transition probability is independent of \( n \), a fixed distribution independent of where the chain is. Notice \( x \) and \( y \) could be equal state \( x = y \) with non-zero transition probability.

The stationary target distribution \( P^* \) being stationary through this transition probability satisfies

\[ P^*\{X_n\} P\{X_{n+1} = y | X_n = x\} = P^*\{X_n\} \quad (A.76) \]

**Example A.4.1** Suppose given two states, rainy and sunny day, the probability transition kernel of the states is

\[
R = \begin{bmatrix}
0.9 & 0.1 \\
0.5 & 0.5
\end{bmatrix}
\]

\(^1\text{we use } \xi \text{ and } x \text{ interchangeably to represent the uncertainty parameter for demonstration convenience}\)
where the columns and rows are labeled in the order of sunny and rainy. Each index is a transition probability between two states (e.g., $R_{11}$ is the transition probability of sunny day followed by sunny day $P\{X_{n+1} = \text{sunny}|X_n = \text{sunny}\}$, $R_{12}$ is the transition probability of rainy day followed by sunny day $P\{X_{n+1} = \text{rainy}|X_n = \text{sunny}\}$, etc). Notice that the rows of $R$ sum to 1 since $R$ is a probability matrix. The weather prediction starting at a rainy day $0$ predicting the weather state at day $2$ should start with the initial state distribution $P\{X_0\} = [0\%, 100\%] = [0, 1]$

$$P\{X_2\} = P\{X_1\}R = P\{X_0\}R^2 = [0, 1] \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.5 \end{bmatrix}^2 = [0.7, 0.3].$$

Hence, the weather at day $2$ of the chain has $70\%$ of rainy and $30\%$ of sunny day. The weather at large iterations of transition converges to the invariant distribution

$$P^* = \lim_{n \to \infty} R^n = [0.833, 0.167]$$

which is independent of the initial condition. This equilibrium distribution has $83\%$ chance of sunny and $17\%$ of rainy day. Notice that $P^*R = P^*$ shows $P^*$ being invariant.

### A.4.0.2 Detailed Balance condition

In order to generate a chain of samples through a transition kernel, this kernel should satisfy certain conditions to build the invariant distribution.

The fundamental relationship between transition probability, invariant distribution and invariant density is shown as,

$$P^*\{Y \in B\} = \int_{\mathbb{R}^d} P\{Y \in B|X = x\} p(x)dx = \int_B \pi(y)dy. \quad (A.77)$$
Where the invariant distribution $P^*\{Y \in B\}$ of the event $Y \in B$, $B \subset \mathcal{R}^d$, is given by marginalizing the transition probability $P\{Y \in B|X = x\}$ over the entire state space. $\pi(y) = p(y)$ indicates the density being invariant after applying transition probability. The transition probability of $x$ reaching all $Y \in B$ depends on a transition kernel $R(y|x)$ (also written as $R(x, y)$ in some literatures),

$$P\{Y \in B|X = x\} = \int_B R(y|x)dy. \quad (A.78)$$

Since the transition depends on $R(y|x)$, one seeks for the relationship between $R(y|x)$ and $p(y)$. For a stationary Markov chain starting from a point $x$ to reach $Y \in B$ through a move or without a move. Suppose

1. $A$ is the event that stays put at the point $x$ with probability $P\{A\} = r(x)$,

2. $A^c$ is the event that leaves the point $x$ with the probability $P\{A^c\} = 1 - r(x)$.

The transition probability of reaching $B$ thus could be written in the form

$$P\{Y \in B|X = x\} = P\{Y \in B|X = x, A^c\}P\{A^c\} + P\{Y \in B|X = x, A\}P\{A\}. \quad (A.79)$$

To reach $B$ through a move,

$$P\{Y \in B|X = x, A^c\} = \int_B R(y|x)dy. \quad (A.80)$$

To reach $B$ without a move (i.e., already in $B$),

$$P\{Y \in B|X = x, A\} = \delta_{x \in B} = \begin{cases} 1 & x \in B \\ 0 & x \notin B \end{cases} \quad (A.81)$$

Substituting into (A.82) gives,

$$P\{Y \in B|X = x\} = (1 - r(x))\int_B R(y|x)dy + r(x)\delta_{x \in B}. \quad (A.82)$$
Substituting into (A.78),

\[ P^* \{ Y \in B \} = \int_{\mathbb{R}^d} \left( (1 - r(x)) \int_B R(y|x)dy + r(x)\delta_{x\in B} \right) p(x)dx \]

\[ = \int_B \int_{\mathbb{R}^d} p(x)(1 - r(x))R(y|x)dx \, dy + \int_B r(x)p(x)dx \]

\[ = \int_B \left( \int_{\mathbb{R}^d} p(x)(1 - r(x))R(y|x)dx + r(y)p(y) \right) dy \]

\[ = \int_B \pi(y)dy \]  \hspace{1cm} (A.83)

Since \( R(y|x) \) causes \( \pi(y) = p(y) \), the integrands of last two lines of (A.83) thus becomes

\[ p(y) = \int_{\mathbb{R}^d} p(x)(1 - r(x))R(y|x)dx + r(y)p(y) \]

\[ (1 - r(y))p(y) = \int_{\mathbb{R}^d} p(x)(1 - r(x))R(y|x)dx \] \hspace{1cm} (A.84)

\[ (1 - r(y))p(y) = \int_{\mathbb{R}^d} p(x)K(y|x)dx \]

where \( K(y|x) = (1 - r(x))R(y|x) \). Similarly, \( K(x|y) = (1 - r(y))R(x|y) \). By integration over \( x \),

\[ \int_{\mathbb{R}^d} K(x|y)dx = (1 - r(y)) \int_{\mathbb{R}^d} R(x|y)dx \]

\[ = 1 - r(y), \] \hspace{1cm} (A.85)

and substituting into the last line of (A.84) yields the balanced equation

\[ \int_{\mathbb{R}^d} p(y)K(x|y)dx = \int_{\mathbb{R}^d} p(x)K(y|x)dx. \] \hspace{1cm} (A.86)

The integrands results in the detailed balance condition

\[ p(y)K(x|y) = p(x)K(y|x). \] \hspace{1cm} (A.87)

An appropriate transition kernel should satisfy this condition to generate an invariant distribution. This condition serves as the building block for the sampling algorithm.
So far the properties of MCMC shows a preference towards developing an effective algorithm sampler, which provides the desired statistics through sampling the multivariate target distribution, the posterior,

\[
E_{p(\theta|d)}[f] \approx \frac{1}{n-b} \sum_{i=b}^{n} f(\xi^i). \tag{A.88}
\]

### A.4.1 Metropolis-Hastling (MH) sampler

The goal of the Metropolis-Hastling (MH) sampler is to sample the invariant target distribution efficiently by choosing a proposal distribution or candidate generating kernel \( q \) that satisfies the detailed balance condition by some factor.

Suppose \( r(x) = 0 \) so the \( d \)-dimensional point \( x \) is always accepted to make a move, hence \( K(y|x) = (1 - r(x))q(y|x) = q(y|x) \) satisfies the detailed balance condition,

\[
p(y)q(x|y) = p(x)q(y|x). \tag{A.89}
\]

But, this is less likely to be satisfied. It is normally one side being greater than the other, so set

\[
p(y)q(x|y) \leq p(x)q(y|x). \tag{A.90}
\]

Suppose choose an acceptance probability, \( \alpha(y|x) \leq 1 \), to balance the equation

\[
p(y)q(x|y) = p(x)\alpha(y|x)q(y|x). \tag{A.91}
\]

where

\[
\alpha(y|x) = \frac{p(y)q(x|y)}{p(x)q(y|x)} \leq 1. \tag{A.92}
\]

In practice the right hand side might be greater than 1, so

\[
\alpha(y|x) = \min \left\{ 1, \frac{p(y)q(x|y)}{p(x)q(y|x)} \right\}, \tag{A.93}
\]
In summary, we define $K(y|x) = \alpha(y|x)q(y|x)$, and the detailed balance is satisfied when (A.93) holds.

A.4.1.1 MH algorithm

\begin{verbatim}
for ( i = 1, \ldots, N );
    Given $x^i$, draw $y$ using the transition kernel $q(y|x^i)$, where $x^i, y \in \mathcal{R}^d$.
    Calculate $\alpha(y|x^i)$.
    Draw a $u \sim U(0, 1)$;
    if ( $\alpha \geq u$ )
        accept the move to $y$. $x^{i+1} = y$
    else
        stay put at $x^i$. $x^{i+1} = x^i$
end
end
\end{verbatim}

Return the values $\{x^1, x^2, \ldots, x^N\}$

\textsuperscript{a}keeps the chain moving towards higher density area
\textsuperscript{b}allows the chain to move towards higher (lower) density area more (less) frequently

Example A.4.2 Suppose $\alpha = 0.9$, the r.v. $u$ is more likely to be in between $[0, 0.9]$ than $(0.9, 1]$, (i.e., $y$ is more likely to be accepted); if $\alpha = 0.01$, then $u$ is less likely to be in between $[0, 0.01]$ than $(0.01, 1]$ (i.e., $y$ is less likely to be accepted).

The selection of $q$ will determine the ease and efficiency to sample the target. If $q$ is symmetric (e.g., Gaussian, $q(y|x) = q(x|y)$) then $\alpha(y|x) = p(y)/p(x)$. $\alpha$ depends merely on $p$. This is known as the Metropolis algorithm [Metropolis, 1953].

Example A.4.3 Suppose $q(y|x) = q(y - x) = q(\epsilon)$ is a proposal with standard normal density $\mathcal{N}(0, 1)$. The candidate $y = x + \epsilon$ is thus generated by moving away from $x$ with a distance $\epsilon$. 
Under symmetric proposal, the $\alpha$ depends only on the ratio of $p(y)$ and $p(x)$. So, if $x$ jumps to $y$ at a higher density, ‘uphill’, $p(y) > p(x)$, then $y$ is always accepted (i.e., $\alpha(y|x) = 1$); if the jump goes ‘downhill’, it is accepted if $\alpha \geq u$.

Despite the MH sampler being simple and effective, there remains difficulties for some target distributions. When the target includes multiple modes with more correlated samples and differing scales of variability or sharp boundaries, the sampling will be biased and focused locally with less efficient mixing to reach every modes of the distribution. As a result, one should seek for adaptiveness to overcome the difficulties.

A.4.2 Delayed Rejection Adaptive Metropolis (DRAM) sampler

The two quite powerful sampling algorithm, adaptive Metropolis [Haario et al., 2001] and delayed rejection [Green and Mira, 2001], is integrated [Haario et al., 2006] with standard MH sampler to improve efficiency.

A.4.2.1 Delayed Rejection (DR)

Allows multiple proposals to explore the state space in a series of stages. The DR starts from point $x$ and make a “global” move (larger variance proposal) to $y^1$ to explore the state space with potential multi-modality. If $y^1$ gets rejected by flipping the $u$-coin, rather than rejecting right away, it will restart from point $x$ to draw more “local” moves (smaller variance proposal) at higher stages. The stages continue if $y^i$ gets rejected until it got accepted or reaching a predefined numbers of stage. This is
when \( y_i \) gets saved as the chain and the algorithm continues. Suppose starting from \( x \) to \( y^1 \)

\[
\alpha_1(y^1|x) = \min \left\{ 1, \frac{p(y^1)q(x|y^1)}{p(x)q(y^1|x)} \right\} = \min \left\{ 1, \frac{N_1}{D_1} \right\},
\]

(A.94)

and assume \( y^1 \) got rejected after the \( u \)-coin flip

\[
\alpha_2(y^2|x, y^1) = \min \left\{ 1, \frac{p(y^2)q_1(y^1|y^2)q_2(x|y^2, y^1)[1 - \alpha_1(y^1|y^2)]}{p(x)q_1(y^1|x)q_2(y^2|x, y^1)[1 - \alpha_1(y^1|x)]} \right\} = \min \left\{ 1, \frac{N_2}{D_2} \right\}.
\]

(A.95)

The \( i \)th stage continues if previous \( y \)'s got rejected,

\[
\alpha_i(y^i|x, \ldots, y^{i-1}) = \min \left\{ 1, \frac{p(y^i)q_1(y^{i-1}|y^i) \cdots q_i(x|y^i, \ldots, y^1)}{p(x)q_1(y^1|x) \cdots q_i(y^i|x, \ldots, y^{i-1})} \left[ \frac{1 - \alpha_1(y^{i-1}|y^i)}{1 - \alpha_1(y^1|x)} \right] \cdots \left[ 1 - \alpha_{i-1}(y^1|y^i, \ldots, y^{i-2}) \right] \right\} = \min \left\{ 1, \frac{N_i}{D_i} \right\}.
\]

(A.96)

Since all \( y \)'s will be rejected before reaching \( i \)th stage, \( N_j \leq D_j \) for \( j = 1, \ldots i - 1 \), and \( \alpha_j(y^j|x, \ldots, y^{j-1}) = N_j/D_j \). This leads to a recursive relationship,

\[
D_i = q_i(y^i|x, y^1, \ldots, y^{i-1})(D_{i-1} - N_{i-1})
\]

(A.97)

Notice that if \( q_i \)'s are equal and symmetric, the acceptance ratio becomes

\[
\alpha_1(y^1|x) = \min \left\{ 1, \frac{p(y^1)}{p(x)} \right\} = \min \left\{ 1, \frac{N_1}{D_1} \right\}
\]

(A.98)

\[
\alpha_2(y^2|x, y^1) = \min \left\{ 1, \frac{p(y^2)[1 - \alpha_1(y^1|y^2)]}{p(x)[1 - \alpha_1(y^1|x)]} \right\} = \min \left\{ 1, \frac{p(y^2) - p(y^1)}{D_2} \right\} = \min \left\{ 1, \frac{p(y^2) - p(y^1)}{D_1 - N_1} \right\}.
\]

(A.99)
The \( i \)th stage acceptance ratio for symmetric kernel with recursive relationship,

\[
\alpha_i(y^i|x, \ldots, y^{i-1}) = \min\left\{ 1, \frac{p(y^i) - p(y^{i-1})}{D_{i-1} - N_{i-1}} \right\}
\]  

(A.100)

A.4.2.2 Adaptive Metropolis (AM)

For an effective exploration of the target distribution, we need to “tune” a good sampling proposal. The tuning concerns both the “width” and “orientation” of the proposal, which is hard to choose well since the target is unknown. (Gelman et al. 96; Gilks et al 95; 98; Haario et al. 99; Roberts et al. 97). The algorithm automates the tuning process by using the history of the process to build a \( \mathcal{R}^d \) covariance matrix to suit the target.

An adaptive multivariate Guassian proposal is developed

\[
q(X^{n+1}|X^n) \sim N(X^n, \Sigma_n)
\]  

(A.101)

where \( \Sigma_n \) is a covariance matrix build upon the history of \( n - 1 \) saved samples.

Assume the proposal, after some initial steps \( n_0 \), is centered at current point \( X^n \) of the chain. This proposal should be a Gaussian distribution for the chain to remain ergodic [Haario et al., 2006]. Assume the covariance with a prior knowledge (may be quite poor) before \( n_0 \) steps is a fixed value \( \Sigma_0 \). The points after \( n_0 \) steps \( X^0, \ldots, X^{n-1} \) are used to determine a covariance matrix \( \text{Cov}(X^0, \ldots, X^n) \) for the proposal to sample. Together it yields the form,

\[
\Sigma_n = \begin{cases} \Sigma_0 & n \leq n_0 \\ s_d \text{Cov}(X^0, \ldots, X^n) + s_d \epsilon I_d & n > n_0 \end{cases}
\]  

(A.102)
$s_d = 2.4^2/d$ is chosen in terms of optimizing Gaussian proposal and Gaussian target following [Gelman et al., 1996]. $\epsilon$ is a small constant to avoid singularity, but in practice it can be safely set to zero [Haario et al., 2006]. $I_d$ is a $d$-dimensional identity matrix. $\Sigma_0$ is chosen according to a prior knowledge (which may be quite poor). The $\mathcal{R}^d$ covariance matrix is

$$
\text{Cov}(X^0, \ldots, X^n) = \frac{1}{n} \left( \sum_{i=0}^{n} X^i X^iT - (n+1)\bar{X}^n \bar{X}^nT \right)
$$

(A.103)

where $\bar{X}^n = \frac{1}{n+1} \sum_{i=0}^{n} X^i$ and $X^i$ is a $d$-dimension column vector. Substituting (A.103) into line 2 of (A.102) satisfies a recursive formula

$$
\Sigma_{n+1} = \frac{n-1}{n} \Sigma_n + \frac{s_d}{n} \left( n\bar{X}^{n-1} \bar{X}^{n-1T} - (n+1)\bar{X}^n \bar{X}^nT + X^n X^nT + \epsilon I_d \right)
$$

(A.104)

where

$$
\bar{X}^n = \frac{1}{n} \sum_{i=1}^{n} X^i = \frac{n-1}{n} \bar{X}^{n-1} + \frac{1}{n} X^n.
$$

(A.105)

One may choose to update $\Sigma$ every $n_i$ iterations instead of every step.

A.4.2.3 DR+AM

The AM involves with DR in each stages, depending on how the scale factor $s_d$ is. The proposal in DR at first stage is as in AM. The proposal in higher stages are just a scaled version of the first stage variance by $s_d$, normally chosen to reduce the variance at higher stages to explore more locally.
A.4.2.4 DRAM algorithm

```
for ( i = 1, \ldots, N )
    if ( i \leq n_0 )
        \Sigma_n = \Sigma_0;
    else
        \Sigma_n = s_d \text{Cov}(X^0, \ldots, X^n) + s_d I_d;
    end
while ( i_s \leq n_s ) \quad ^a
    given \ x^i, draw \ y \ using \ the \ transition \ kernel \ q(y|x^i) \sim \mathcal{N}(x^i, \gamma \Sigma_n); \quad ^b
    calculate \ \alpha(y|x^i);
    draw \ a \ u \sim \mathcal{U}(0, 1);
    if ( \alpha \geq u )
        \ x^{i+1} = y;
        break \ the \ while \ loop;
    else
        stay \ put \ at \ x^i;
        if ( i_s == n_s )
            \ x^{i+1} = x^i;
            break \ the \ while \ loop;
        else
            set \ \gamma \ to \ a \ smaller \ scale;
            i_s = i_s + 1;
        end
    end
end
Return \ the \ values \ \{x^1, x^2, \ldots, x^N\}
```

\(^a i_s \) is the counter of stages, \(^n_s \) is the maximum allowed stages

\(^b \gamma \) is a scaling factor of the covariance in each stage

A.4.2.5 Mixing efficiency

The stationary Markov Chain is saved after the transient stage, a big enough numbers of steps (i.e., burn in steps). The saved chain represents the samples from target distribution. Despite samples of the chain being serially correlated [Gamerman and Lopes, 2006] as opposed to independent sampling in conventional Monte Carlo
method, the efficient mixing of the chain renders MCMC superior in terms of high dimensional integration.

For a closer look at MCMC mixing efficiency, one assumes central limit theorem for ergodic averages $\bar{f}_n$,

$$\bar{f}_n = \frac{1}{n} \sum_{j=1}^{n} f(\xi_j)$$

(A.106)

$$\sqrt{n}(\bar{f}_n - E_{\pi_\xi}(f)) \xrightarrow{i.d.} N(0, \sigma^2_f)$$

(A.107)

where $\xrightarrow{i.d.}$ means convergence in distribution.

$$\sigma^2_f = \text{Var}_{\pi_\xi} + 2 \sum_{s=1}^{\infty} \text{Cov}_{\pi_\xi}[f(\xi^{(0)}), f(\xi^{(s)})] = \text{Var}_{\pi_\xi} + 2 \sum_{s=1}^{\infty} \Sigma_s.$$  

(A.108)

$$\xi^{(0)} = [\xi^1, \xi^2, \ldots, \xi^i, \ldots, \xi^{n-s}] \text{ for lag-0 samples}$$

$$\xi^{(s)} = [\xi^{1+s}, \xi^{2+s}, \ldots, \xi^{i+s}, \ldots, \xi^n] \text{ for lag-s samples}$$

(A.109)

The asymptotic variance in (A.108) reflects the correlation between successive samples. The sampling method at a fixed n preforms better when the asymptotic variance is smaller with less correlation between samples. The autocorrelation is the autocovariance normalized by the variance (constant for a stationary process),

$$\gamma_s = \frac{\Sigma_s}{\text{Var}(f(\xi^{(0)}))} = \frac{\Sigma_s}{\sigma^2}$$

(A.110)

One could observe the sequence of autocorrelation coefficient $\{\gamma_s\}_{s=1}^{\infty}$ to visualize the evolution of mixing rate. A steeper $\{\gamma_s\}_{s=1}^{\infty}$ when the chain starts means a faster mixing. The autocorrelation decreases as the lag becomes farther. At closer lags, the samples are close enough to produce positive covariance, which sum up to a relatively larger positive value. At farther lags, the samples are mixed with positive and negative values, which sum up to a smaller value.
Bibliography


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