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A DDDAS Framework for Volcanic Ash Propagation and Hazard Analysis

A. Patra¹, M. Bursik^b, J. Dehn^c, M. Jones^c, M. Pavolonis^f, E. B. Pitman^d, T. Singh^a, P. Singla^a, P. Webley^c

^aDepartment of Mechanical & Aerospace Engineering, University at Buffalo

^bDepartment of Geology, University at Buffalo

^cCenter for Computational Research, University at Buffalo

^dDepartment of Mathematics, University at Buffalo

^eGeophysical Institute, University of Alaska, Fairbanks

^fNOAA-NESDIS, Center for Satellite Applications and Research

Abstract

In this paper we will present early work on using a DDDAS based approach to the construction of probabilistic estimates of volcanic ash transport and dispersal. Our primary modeling tools will be a combination of a plume eruption model BENT and the ash transport model PUFF. Data from satellite imagery, observation of vent parameters and windfields will drive our simulations. We will use uncertainty quantification methodology – polynomial chaos quadrature in combination with data integration to complete the DDDAS loop.

Keywords: DDDAS, Volcanic Ash Transport, Uncertainty Quantification

1. Introduction

The dynamic data driven application system paradigm (DDDAS) is formally defined in a series of recent reports [1, 2] and in earlier reports on the subject as systems where data are dynamically integrated into simulation(s) to augment or complement the application model, and, where conversely the executing simulation steers the measurement (instrumentation and control) processes of the application system. The full range of research issues raised by the DDDAS paradigm are many and diverse. We describe here the construction of a framework for DDDAS to target predictions of ash clouds that are produced by explosive eruptions from volcanoes and address primarily questions related to the quantification of uncertainty and a computational strategy for data driven forecasts using large scale computing and analytics. The motivation of the research proposed here will be to develop techniques *that can be completed in a timely fashion to enable the DDDAS control loop* on the simulation and observation, thus, greatly enhancing the quality of the prediction. Recent eruptions of Eyjafjallajökullin Iceland and Puyehue in Chile illustrate the potential of these events to interrupt aviation. Our goal is to provide timely and accurate ash cloud forecasts to minimize these disruptions.

Email address: abani@buffalo.edu (A. Patra)

¹Corresponding author

Our core approach is to use weighted ensembles of a novel coupling of an eruption column model bent and the popular puff tool as our simulation tool inside a DDDAS loop. Infrared and visual satellite imagery can provide data on the position of these clouds. However, both simulation and observation are subject to large error and uncertainty. Thus, we will develop methodology to carefully characterize the error and uncertainties in a timely fashion. Our proposed techniques, if successful will greatly improve the quality of information available on the potential location and concentrations of the ash clouds. In this paper, we provide an overview of the current and planned efforts and preliminary results in implementing a DDDAS approach to this problem domain. In a companion paper [3] we outline in detail one of the critical phases – fast solution of the inverse problem to identify and update the inputs based on observations.

2. Background

2.1. Volcanic Plumes

Long-range volcanic ash transport models [4] have been given the general name Volcanic Ash Transport and Dispersion Models (VATDMs). Numerous VATDMs have been developed by both civil and military aviation or meteorological agencies to provide forecasts of ash cloud motion [5]. The use of these models became well-known following the eruption of Eyjafjallajökull, Iceland, in April, 2010, when the NAME model [6] forecasts were particularly prominent in being used as the basis for an almost complete shutdown of European air traffic. In this paper, we consider a VATDM named puff that is used by the Anchorage Volcanic Ash Advisory Center (VAAC) for real-time civil aviation forecasts. Tanaka [7] and Searcy et al. [8] developed puff for predicting the paths of volcanic clouds at meso- and synoptic scales. puff simplifies the eruption plume to a vertical source, and uses a Lagrangian pseudo-particle representation of the ash cloud in a detailed 3-D regional windfield to determine the trajectory of the cloud. puff and other dispersion models have proven extremely useful in modeling the distal transport of ash for aviation safety [8, 5]. While the work reported here is in the context of puff the statistical and stochastic methodology that will be developed is independent of the puff model, and could be directly applied using other dispersion models. We are in the process of implementing this methodology with the more recently formulated WRF-CHEM tool.

2.2. puff Simulation Model

There are over a dozen operational VATDMs in existence that have been used for ash cloud forecasting and post-event analysis by the world's nine VAACs [9, 5, 10, 11]. puff is one of these VATDMs, and is particularly tied to usage by the Anchorage VAAC. The model is intended to be a rapid response prediction tool of modest complexity, that runs on workstation-class computers. Unlike other VATD models, it is designed solely for predictions of ash-cloud movement in space and time, and it generates displays that can be tailored to user needs at volcano observatories, in a real-time setting during an eruption crisis. For these reasons, puff is necessarily simple by design, but it can be intricate in its implementation. The model takes into account the predominant physical processes that control particle movement, such as winds, dispersion and settling, but it does not account for small scale physical processes that play a lesser role. In some cases we do not understand in detail how these sub-scale process impact the overall cloud movement (e.g. inter-particle interactions), in other cases the required information may not be available in a real-time situation (e.g. precipitation), and in yet other cases inclusion of the process may significantly lengthen model run-time (e.g. radiative heating).

During an eruption crisis, puff predictions have been used to estimate ash cloud movement critical to the assessment of potential impacts – for example, on aircraft flight paths, or on ash fall at airports, or for health concerns. As other more complicated (and thus slower) VATD model results become available they can be incorporated into an impact analysis by volcanologists and atmospheric scientists. Thus, uncertainty analysis and data driven correction of VATD models in general, and of the puff model in particular, is important for appropriate response to the resulting hazards.

puff can be run using one of several numerical weather prediction (NWP) windfields [12–15]. These NWP models are available at differing levels of spatial and temporal resolution; local use of the WRF (Weather Research Forecast) model will allow for customizing the model domains used for verification and validation. puff tracks a

finite number of Lagrangian point particles of different sizes, whose location R is propagated from timestep k to timestep $k + 1$ via an advection/diffusion equation

$$R_i(t_{k+1}) = R_i(t_k) + W(t_k)\Delta t + Z(t_k)\Delta t + S_i(t_k)\Delta t \quad (1)$$

Here $R_i(t_k)$ is the position vector of the i^{th} particle at time $k\Delta t$, $W(t_k)$ is the local wind velocity at the location of the i^{th} particle, $Z(t_k)$ is a turbulent diffusion that is modeled as a random walk, and $S_i(t_k)$ is a source term which models the fallout of the i^{th} particle due to gravity.

Ash loading and plume height are thought to be the most important input variables for volcanic ash transport and dispersion (VATD) modeling, such as that applied to the Eyjafjallajokull plume [16]. Current usage is to derive mass loading from the product of eruption duration and mass eruption rate (MER) (equivalent to mass flux, Q). MER in turn is typically calculated from an empirical relationship derived for strong plumes ($w \gg v$), e.g., $H_T = 1.67Q^{0.259}$ [17], where w is characteristic plume speed (m/s), v is wind speed, H_T is eruption column height (km) and Q is mass eruption rate given as the equivalent volume eruption rate (cu m/s) assuming a magmatic density (for e.g. 3000 kg/cu m for basalt in the case of Eyjafjallajokull). This yields ash loading as a function of cloud height, H_T alone. Plume height, however, is a complex function of source and environmental conditions, so using plume height alone to estimate mass loading can dramatically underestimate mass loading in the case of high wind.

2.3. bent Eruption Column Model

To deal with overdependence on plume height, we can use measurements of several more primitive source variables: vent speeds and vent radii, and ground measurements of ash properties. Using these primitive variables as inputs to suitable models we postulate that we can better sample the uncertain input parameter space for a VATD model rather than the current practice of using plume height conversion.

We thus track ash dispersal using an eruption column, plume rise model bent with uncertain input parameters of vent speed and radius, and mean and variance of grain size, coupled with a radiosonde from near the initiation of the eruption when available to construct a sample space of uncertain input parameters of grain size, mass loading and injection height. The mass loading and height from the plume rise model are then used as input to a VATD model, using NCEP Reanalysis windfields to track the propagation of ash.

The bent integral eruption column model will be used to produce eruption column parameters (mass loading, column height, grain size distribution) given a specific atmospheric sounding and source conditions [18]. bent takes into consideration atmospheric (wind) conditions as given by atmospheric sounding data. Thus plume rise height is given as a function of volcanic source and environmental conditions.

3. DDDAS Workflow Characterization

We begin by laying out the overall workflow and use it to describe the DDDAS framework for this application. Figure 1 describes the overall workflow of the ash plume prediction DDDAS application. Key to workflow are the propagation of uncertainty – in parameters and source terms (wind field) and integration with data from satellites and other observations. We start with a description of the pdf of the concentration of ash at initial time at all points on some grid covering the jurisdiction of interest. As time evolves the concentration pdf is propagated by using the uncertainty described by the wind and input parameters. The wind effect is accounted for by using AGMM (See details below) in the inner loop in lock-step with the bent-puff coupled model. The outer PCQ loop (see Fig. 1) accounts for the input parameter uncertainty. The propagated concentration pdf is updated using data assimilation methodology as described below. After every data assimilation step the input model parameters pdf is updated using the Bayesian framework. Based on the modified pdf a new PCQ based sampling must be redone. Note that we can always start the process at some posterior time if a concentration field and its variability are available. Depending on the uncertainty associated with the posterior pdfs we can use higher fidelity models in the data assimilation loop.

3.1. Uncertainty and Stochastic Variability

There are a number of significant challenges associated with uncertainty characterization and propagation for spatio-temporal varying systems like those encountered in the ash plume transport. Uncertainty arises from several

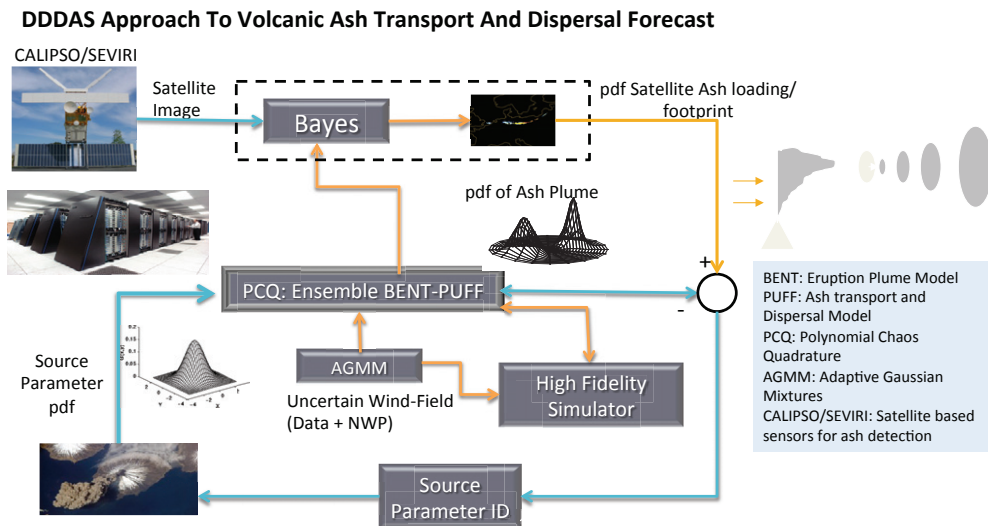


Figure 1: Planned workflow of this DDDAS application as mapped to a set of heterogeneous resources. Blue arrows denote components that have been implemented, while brown arrows denote work in progress.

sources: parameters, initial and boundary conditions, forcing functions, are known only to certain precision. For example, bent-puff input parameters include coefficient of gravity fallout, vent diameter, vent velocity, mean grain size and windfield. *All of these parameters are known only approximately and only to a fixed fidelity.* Despite the potential risk to property and life from inaccurate prediction of ash clouds, *there has never been a thorough quantitative assessment of ash cloud predictions due to parametric and stochastic uncertainties.* Most of the literature[19–23] focuses on tracking the ash material plume while making use of the sensitivity information of plume location to measured material flux or concentration. While a detailed sensitivity analysis can relate the variations in input parameters to ash cloud, *uncertainty analysis casts a much broader net in terms of assessing confidence of predictions based on all available information.* These aforementioned two questions clarify the main outcome of our work here *To provide a prediction of ash cloud motion, together with a quantitative measure of the variability of that prediction, informed by all available data in real time.* [Note: By “real time”, we mean a prediction of cloud motion 12-24 hours in advance, taking no more than 6 hours from initiation to completion.]

A companion paper [3] will provide the technical details of our approach to uncertainty quantification for this problem. We provide here an overview. To discuss uncertainty and its effects in models, we distinguish between parametric uncertainty and stochastic forcing. Mathematically, these two kinds of uncertainty are accounted for differently. However there is not a perfect demarcation between the way we treat these. For example, we cannot know the input windfield perfectly - at every point in the atmosphere at every instant of time and we may choose to model this uncertainty as a stochastic forcing of a given size at each computational location in space-time. Following arguments in [24] that probability theory is the right setting to describe our lack of information, we adopt here a probabilistic framework.

Instead of solving for the ash concentration at a given time and location (based on integration of puff particles) we treat the **concentration at a given location and time as a random variable** \mathbf{x}_k . The time evolution of the vector of \mathbf{x}_k s, is given by a stochastic differential equation (which should be thought of as generalization of Eq. (1) to include the physics of the bent-puff coupling):

$$\mathbf{x}_{k+1} = \mathbf{f}(t_k, \mathbf{x}_k, \Theta) + \boldsymbol{\eta}_k, \quad \mathbf{x}(t_0) = \bar{\mathbf{x}}_0 \quad (2)$$

In this equation, Θ represents uncertain but time-invariant system parameters such as the coefficient of gravity fallout, vent diameter or vent velocity. The random function $\boldsymbol{\eta}_k$ represents stochastic forcing terms, such as turbulent diffusion, or any stochastic effect that might be added to the windfield. These random functions may be modeled as a Gaussian process with specified correlation function \mathbf{Q}_k . The nominal initial position of the center of the particles is given by $\bar{\mathbf{x}}_0$, which may also be uncertain. The total uncertainty associated with the state vector \mathbf{x}_k is characterized by the probability distribution function (pdf) $p(t_k, \mathbf{x}_k, \Theta)$ whose time evolution characterizes our uncertainty. Using the full pdf has many advantages, especially the ability in a DDDAS framework of integrating data and prediction easily using Bayesian approaches.

Several approximate techniques are commonly used to approximate the state pdf evolution [25, 26], the most popular being Monte Carlo (MC) methods [27], Gaussian closure [28], Equivalent Linearization [29], and Stochastic Averaging [30]. In addition, a Gaussian Process approach to solve nonlinear stochastic differential equations has been proposed in Ref. [32]. All of these algorithms except MC methods are similar in several respects, and are suitable only for linear or moderately nonlinear systems, because the effect of higher order terms can lead to significant errors. Monte Carlo methods require extensive computational resources and effort, and become increasingly infeasible for high-dimensional dynamic systems [33] and the limited and time bound response needed in DDDAS settings.

The next two subsections discuss our planned methods for solving the time evolution of state pdf for systems that include stochastic forcing terms and parametric uncertainty.

3.2. Parameter Uncertainty Propagation

The bent-puff model is subject to parametric uncertainty. The propagation of uncertainty due to time-invariant but uncertain input parameters can be approximated by a generalized polynomial chaos (gPC), originally due to Xiu and Karniadakis [34]. Roughly speaking, gPC postulates a separation of random variables from deterministic ones in the solution algorithm for a differential equation. The random variables are expanded as a polynomial, those polynomials being associated with the assumed probability distribution for the input variables (for example, Hermite polynomials for normally distributed parameters, or Legendre for uniformly distribution). Galerkin collocation is used to generate a system of coupled, deterministic differential equations for the expansion coefficients. The gPC collocation step fails when applied to problems with non-polynomial nonlinearities, and can produce non-physical solutions when applied to hyperbolic equations. Non-intrusive spectral projection (NISP) or stochastic collocation methods can overcome these difficulties [35–37]. We will use a different formulation of the NISP idea [38] that we call polynomial chaos quadrature (PCQ). PCQ replaces the projection step of NISP with numerical quadrature. The resulting method can be viewed as a Monte-Carlo-like evaluation of (2), but with sample points selected by quadrature rules.

The bent-puff model contains both stochastic forcing and parametric uncertainty. We assume the parametric uncertainty is independent of the forcing terms, and propose wrapping the PCQ quadrature evaluation around an AGMM solution step. For a fixed value of parameter $\Theta = \Theta_j$, the AGMM provides an output distribution accounting for stochastic forcing. Integration (by PCQ) over the uncertain inputs determines the posterior. Expressed mathematically,

$$\begin{aligned} p(\mathbf{x}_{k+1}) &= \int p(t, \mathbf{x}_{k+1} | \Theta) dp(\Theta) \approx \sum_q \omega_q p(t, \mathbf{x}_{k+1} | \Theta_q) p(\Theta_q) \\ &= \sum_q \omega_q \left(\sum_{i=1}^N w_{k+1}^i \mathcal{N}(\mathbf{x}_{k+1} | \boldsymbol{\mu}_{k+1}^i, \mathbf{P}_{k+1}^i, \Theta_q) \right) p(\Theta_q) \end{aligned} \quad (3)$$

In this expression, ω_q are the PCQ weights assigned to the quadrature points Θ_q .

3.3. Uncertainty Propagation due to Stochastic Forcing

Consider first Eq. (2) for fixed system parameters Θ_0 , and a stochastic forcing η . In the context of the bent-puff model, this assumption is akin to fixing all input parameters but allowing for a random component the windfield. The time evolution of the pdf from time-step k to time-step $k + 1$ is given by the Chapman-Kolmogorov equation (CKE) [39–41]:

$$p(t_{k+1}, \mathbf{x}_{k+1} | \Theta_0) = \int p(t_{k+1}, \mathbf{x}_{k+1} | t_k, \mathbf{x}_k, \Theta_0) p(t_k, \mathbf{x}_k | \Theta_0) d\mathbf{x}_k \quad (4)$$

Here $p(t_{k+1}, \mathbf{x}_{k+1} | t_k, \mathbf{x}_k, \Theta_0)$ is the state transition corresponding to the pdf for the process noise η_k [42]. The CKE is a formidable equation to solve because: (i) the pdf must remain positive, (ii) the pdf must maintain unit volume, and (iii) the domain of p changes in time.

The integral in Eq. (4) is over the state space \mathbf{x}_k , so it is high dimensional. Traditional numerical approaches which discretize the space in which the pdf lies suffer from the “curse of dimensionality”. To overcome this obstacle, we will use a recently developed adaptive Gaussian mixture model (AGMM) in conjunction with information theoretic measures [43, 44] to accurately solve the CKE. The key idea of the AGMM is to approximate the state pdf by a finite sum of Gaussian density functions whose mean and covariance are propagated from one time-step to the next using linear theory. The weights of the Gaussian kernels are updated at every time-step, by requiring the sum to satisfy the CKE [45]. When properly formulated, the mixture problem can be solved efficiently and accurately using convex optimization solvers, even if the mixture model includes many terms. This methodology effectively decouples a large uncertainty propagation problem into many small problems. As a consequence, the solution algorithm can be parallelized on most high performance computing systems. Sec.4 below briefly describes preliminary results, where an ensemble of bent-puff computations were run in parallel. Finally, a Bayesian framework can be used on the AGMM structure to assimilate (noisy) observational data with model forecasts [46, 47].

3.4. Data Assimilation for Reducing Uncertainty

Of course using any sensor data that might become available to correct and refine the dynamical model forecast will reduce the uncertainty of predictions. This model-data fusion process is well documented in meteorology applications where a variety of data assimilation methods are used operationally to improve the quality of the Numerical Weather Prediction (NWP) forecast [48–51]. Several recent studies additionally used conventional filtering approaches to incorporate observations of a chemical species into a dispersion model [52, 53] and discuss how the nonlinearities in T&D models and sparse measurement data cause problems in capturing non-Gaussian state pdf. In general, finding an optimal filter is an infinite dimensional problem [54, 55]. Finite dimensional filters have been derived for a certain nonlinear problems [56–59]. For more general but low-order nonlinear systems, particle filter methods hold promise [60].

Standard Bayesian tools will be employed to incorporate observational data. Given a prediction of the state variable \mathbf{x}_k , standard Bayesian algorithms assume a sensor model \mathbf{h} to obtain the measurement, $\mathbf{y}_k = \mathbf{h}(t_k, \mathbf{x}_k) + \mathbf{v}_k$. Here \mathbf{v}_k is the measurement noise with prescribed likelihood function $p(\mathbf{y}_k | \mathbf{x}_k)$. Using the dynamic state evolution sketched above as a forecasting tool, the state pdf can be updated using the Bayes’ rule and measurement data:

$$p(\mathbf{x}_k | \mathbf{Y}_k) = \frac{p(\mathbf{y}_k | \mathbf{x}_k) p(\mathbf{x}_k | \mathbf{Y}_{k-1})}{\int p(\mathbf{y}_k | \mathbf{x}_k) p(\mathbf{x}_k | \mathbf{Y}_{k-1}) d\mathbf{x}_k} \quad (5)$$

Here, $p(\mathbf{x}_k | \mathbf{Y}_{k-1})$ represents the prior pdf (the computed solution of the CKE), $p(\mathbf{y}_k | \mathbf{x}_k)$ is the likelihood that we observe \mathbf{y}_k given the state \mathbf{x}_k and $p(\mathbf{x}_k | \mathbf{Y}_k)$ represents the posterior pdf of \mathbf{x}_k . For a fixed set of data and underlying probability model, Maximum a-Posteriori (MAP) picks the values of the state estimates that make both the data and model “more likely” than any other values of the state estimates would make them. This may be of considerable use for decision support in situations in which multiple strong and roughly equal modes appear in the posterior estimate. Neither the conditional mean nor the maximum likelihood estimate as the sole reported hypotheses are sufficient to formulate effective decisions in this case [61].

3.5. Model Hierarchy

The use of the modestly complicated puff code and the availability of other models of differing fidelities opens up the possibility of using multiple models with the higher resolution model acting as an effective alternate provider for gaps in the sparse data from observations. We will focus these runs on well defined parameter ranges where the basic puff code's output is deemed to be poor based on observations. Our preliminary work (see below 4) and recent literature[62] indicates that the puff code is sensitive to the choice of number of particles. However, the cost of the computation with very large numbers of particles (10^7 as opposed to the more common 10^5) is very high. We will selectively use a few of these high particle runs to provide a high fidelity source where we notice large discrepancy between the satellite and bent-puff outputs.

3.6. Observation and Testing

We are fortunate to have access to a wealth of data from the 2010 Eyjafjallajokull eruption and the subsequent cloud dispersion. The daily windfields for the important period between April 14 - 20 are known, satellite images tracking the cloud are available, as is plume data (for example, there is Meteosat SEVIRI data on ash loading and plume height, and SEVIRI and CALIPSO data showing the motion of the cloud). This event will provide a rigorous test of the proposed uncertainty methodology, and in particular the sensitivity of simulation results to differing plume and windfield inputs.

Webley et al. [63] suggest the possibility of running VATD models using retrieved ash cloud parameters from satellite remote sensing data. We will assess this potential. We will also generate 'synthetic' satellite imagery from the puff model simulations, using the ash concentrations, optical depths of the clouds and particle sizes to generate equivalent reverse absorptions signals and opaque cloud temperatures. This process is, essentially, an inverse of the volcanic ash retrieval process developed by Wen and Rose [64] and Pavolonis et al. [65]. Here, we will use the VATD concentration maps to determine the effect the ash would have on the temperature of the cloud as seen by the satellite. From this we can compare datasets and examine the satellite retrieval limits and reverse absorption detection capabilities. This synthetic imagery from the puff model will then allow statistical comparisons between the different datasets, to ascertain which parameters have the greatest effect on the model simulation uncertainties.

4. Preliminary Results

A first step in this research effort is reported in [66], where four bent inputs (vent radius, vent velocity, mean grain size, and grain size variance) were considered as uncertain, bent outputs fed into an ensemble of puff simulations, and PCQ was employed as a solution methodology (see additional details in companion paper [?]).

Following runs of bent at Clenshaw-Curtis quadrature points, each bent output is then propagated through puff, which was then run for a real-time period of five days. The outputs from puff were then combined to produce the ensemble by applying the appropriate weight to each deterministic bent-puff run.

Numerical methodology of the type used here must always be tested for consistency, i.e., independence from discretization parameters or sample size. As we seek to develop an ensembling method that could be implemented in a finite computing time, we also need to minimize the number of parcels and runs. For this set of simulations we compared the simulation outputs for 9^4 and 13^4 samples (quadrature points) and the results indicate that 9^4 runs yields substantially the same results as 13^4 runs. The comparison of using 10^5 , 4×10^6 and 10^7 particles in the puff simulation also indicated that the choice of 4×10^6 particles was adequate for our purposes, and consistent with the findings of others [62].

5. Conclusions and Future Directions

Model output was compared with Meteosat-9 retrievals of top ash plume height. Volcanic ash was identified in the satellite data using the methodology described in [67] and [68]. The ash cloud height were retrieved using an optimal estimation approach [69] and [70]. All microphysical assumptions used in the retrieval are described in [71]. In general, plume location is quite close to that shown in the data, with little variance. There are greater divergences between model and data in the eastern portion of the plume where Meteosat-9 data estimate a much smaller plume area than does the model. Estimating probabilities by computing the coefficients in the polynomial approximation of

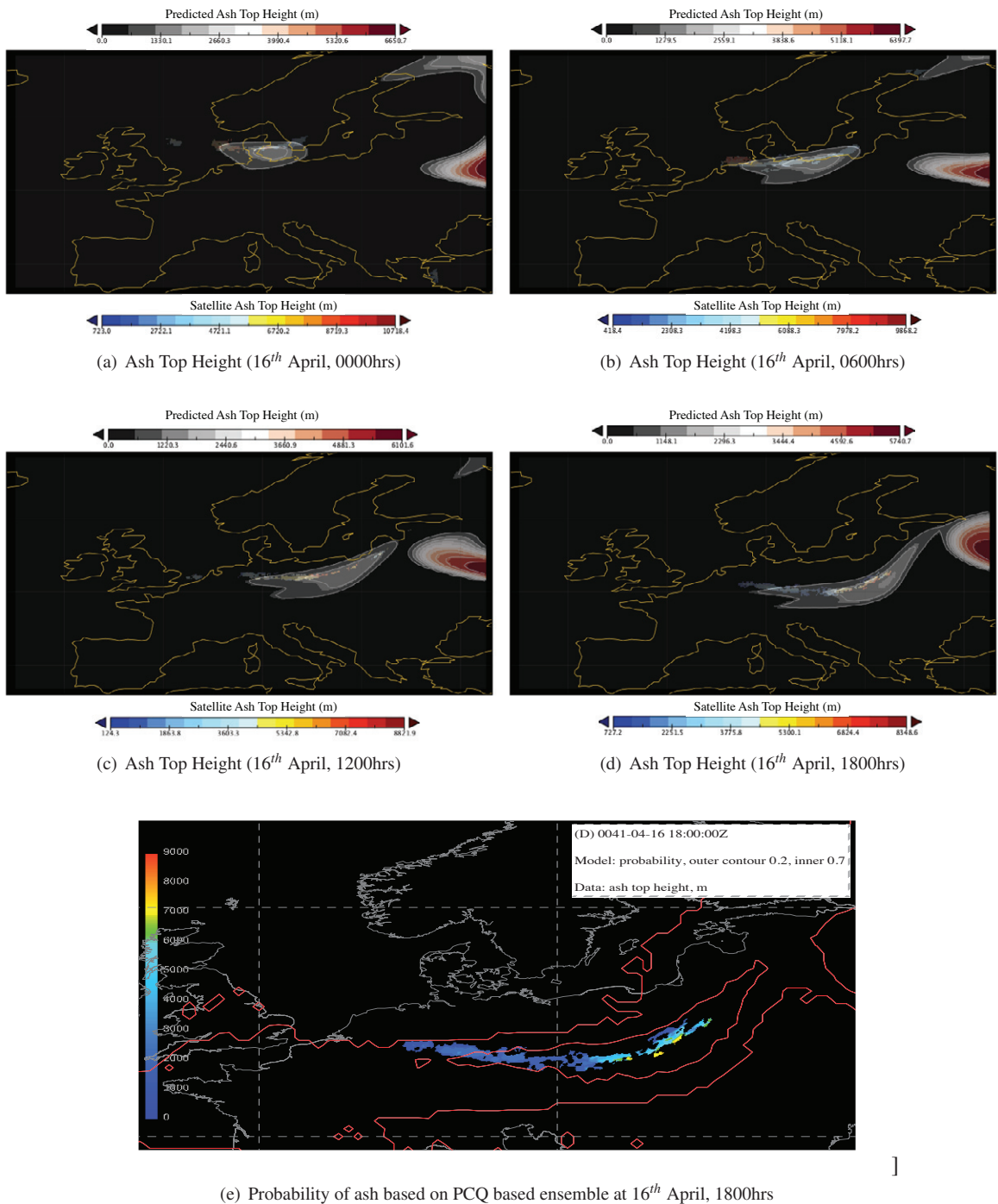


Figure 2: Meteosat-9 SEVIRI ash top height data compared with simulation output for a 9⁴ run implementation of PCQ sampling of the input space. 10⁶ ash particles were used in the simulation. Probability of ash based on PCQ based ensemble at 16th April, 1800hrs from [3]; Inner contour *Prob* > 0.7, outer contour *Prob* > 0.2

the pdf from the PCQ methodology indicates that all observed ash is within the 0.2 probability contours and most is within the 0.7 contour. It appears from the literature that this is the first time such quantitative information has been available from simulation albeit in hind cast mode. In short, preliminary results shows that PCQ scheme yields a valid estimate of mean and standard deviation of ash parameters for a relatively small sample size of order $[9^4]$. The question arises however, whether even PCQ can provide probabilistic estimates useful in Volcanic Ash Advisories in a reasonable time. This question clearly needs to be investigated further.

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