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Analysis of Filesystem Utilization by the"Ensemble of Models" Approach (U)

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Technical Report

Title: Analysis of Filesystem Utilization by the "Ensemble of Models" Approach

Abstract:

In order to execute Uncertainty Quantification (UQ) studies, the number of reads placed on the filesystem will increase. This document works through the file I/O for a climatology UQ study. The utilization of the filesystem for the above discussed will be similar for ICF and Stockpile Stewardship applications.

Introduction

The current state of the art for the quantification of uncertainty of a multi-physics simulation code is the utilization of an ensemble of models approach. As an overview of the ensemble of models approach, a set of uncertain input parameters is identified along with an identified set of observational and output parameters. The model is computed *n* number of times with each ensemble simulation using a unique set of parametric combinations of input parameters thereby creating an ensemble of simulations. Response surface models (also known as statistical emulator models, surrogate models, or meta models) are trained using the ensemble results. The response models are then convolved with observational data to further constrain input parameters and to create uncertainty bounds on the model outputs.

Using the Community Climate System Model (CCSM) specifically the atmospheric component of CCSM, the Community Atmospheric Model (CAM), as the model of interest, this document provides a rough model of the demands on a filesystem that is needed to execute a UQ study on CAM. Each ensemble simulation consists of 12 simulation years and uses 384 processors on the Atlas machine. The LLNL UQ Pipeline is LLNL's standard tool to execute UQ studies. The UQ Pipeline possesses the capability to execute the ensemble simulations on LLNL's diverse set of HPC environments, produce response models, generate uncertainty bounds, and analyze the results. The process executing the LLNL UQ Pipeline is run on a different compute node from the set of concurrent, executing ensemble simulations.

Filesystem Utilization of a Single CAM Ensemble Simulation:

The numbers that are provided in this section were done in collaboration with Dr. Donald Lucas, AEED Physicist. The data files do not include all of the files that are produced in a UQ study, but provide an idea of what is required of the filesystem in order to execute a UQ study.

The studies currently in progress involving CAM use a resolution of 1.9° x 2.5° x 26 levels. This equates to (NX x NY x NZ) = (96 x144 x 26) = 360,000 grid cells. In the near future, it is expected that CAM will be run with a 50km x 50km x 50 levels resolution. As an extreme example, if 1 meter resolution is desired, $2*\Pi*6{,}500\text{x}10^3 = 20\text{x}10^6$ y grid cells and $40\text{x}10^6$ x grid cells will be required, where $6{,}500\text{x}10^3$ is the approximate circumference of the equator.

Different metrics (temperature, mass, energy, etc.) are tracked in each cell.

Each cell currently tracks 100 variables.

Therefore, there are 360,000 grid cells * 100 = 36M values

Current timestep employed employed is 30 minutes/1,800 seconds. A restart file is created at the end of each timstep.

Integration time is 12 simulation years

A restart file is periodically written to the filesystem. The periodicity is set by the discretion of the scientist.

CAM produces a series of history files that are written to the filesystem at a rate of 1file per simulation month. For a 12 year study, a total 12 yrs * 12 months/year = 144 history files are produced. Each field in a history file is monthly averaged. Each value uses single precision (4 bytes). The size of a history file is described by the following equation:

[n3d*96*144*26 + n2d*96*144] * nb, where n3d is the number of 3D outputs, n2d is the number of 2D outputs, and nb is the number of bytes per number stored.

From above n3d = 41, n2d = 84, and nb = 4 to store single precision numbers. Thus, [41*96*144*26 + 84*96*144] * 4 ~= 64MB.

After each ensemble simulation completes, a diagnostic file is also created. The diagnostic file possesses the observational data that will be used to constrain the response models. The storage requirements for the diagnostics file is can be described by the equation describing the size of the history file. This equation assumes that there is an observational data point for every data point located in the history file.

During the process of a study, the history files is compared and contrasted with the diagnostics file. Different sets of metrics like RMS error might be computed during the course of analyzing the history and the diagnostics file. The data produced from the analysis could go into the training data file and for other UQ Pipeline functions.

In order for the UQ Pipeline to produce a response model, a training data file is needed to be created. The training data file consists of a set of rows that is equal to the number of completed ensemble simulations. Each row in the training data file represents the output of an individual simulation associated with the unique set parametric values applied to the identified set of uncertain input variables. The size of the training data file is described by the equation:

#EnsembleSimulations*(4bytes(#InputVariables+#OutputVariables))

To generate the training data file, 120 history files are read from disk and a subset of the values read from the history file are averaged to create the value of the specific output variable that is written to the training data file. The first 2 simulated years (24 history files) are not included in the calculation.

Once the training data file is computed, the set of response models are then computed. An equation that describes the disk requirements to store the size of the response model is not provided. A set of writes are needed to store the response surface.

Using the above provided grid cells sizes, a single run of the CAM study produces ~11.6GB of data. This number is also influenced by the physics packages being utilized in the simulation.

Uses of a filesystem to execute an "Ensemble of Models" UQ study:

A key question to consider when executing a UQ study is have enough training data points (ensemble simulations) been generated that adequately represent the response function? If not, then more ensemble simulations need to be generated. The next question that needs to be addressed of which sample points need to be selected that not only represent the topologically interesting regions of the mult-dimensional response surface with the minimum number of sample points but also produces response surfaces that are not subject to significant statistical variation. This question is important because of the computational cost in running an ensemble simulation.

Current sampling technologies allow for the simultaneous variation of input variables of less than 10. With this technology, 100s of ensemble simulations are generated. 1000s of ensemble simulations will need to be executed if higher numbers of uncertain input dimensions are to be studied. Given the numbers provided above, it will be intractable for a user to analyze all of the produced data to make an informed decision about in the sample space where new sample points should be selected in order to produce adequate response surfaces and to intelligently employ a HPC machine to execute UQ studies. As part of a LLNL Strategic Initiative entitled, "*The Advance of UQ Science with Application to Climate Modeling,Inertial Confinement Fusion Design, and Stockpile Stewardship Science"* (Klein, Garaizar, *et al.*, 2009), adaptive sampling techniques are being developed and will be integrated into the UQ Pipeline. These methods along with the development of automated decision analysis methods will provide the UQ Pipeline the necessary technology to decide where in the sample space the next set of ensemble simulations will be run, if needed. From the perspective of the filesystem, the adaptive sampling methods will analyze the response surfaces. Using the information provided by the methods, the UQ Pipeline will read the diagnostics file for each ensemble simulation and the training data file in order to make those decisions.

The UQ Pipeline concurrently executes the set of ensemble models and the UQ Pipeline will be analyzing the output of the ensemble simulations as new data becomes available to the UQ Pipeline. Hence, the creation of history files, the creation of diagnostics files, the creation of training data files, the generation of response surfaces, and the analysis of the files will be conducted concurrently. The filesystem must therefore possess the capability for concurrent writes and reads where the number of reads has significantly increased in order to execute a UQ study. In fact, it seems the number of reads will equal the number of writes. While this analysis is not completely rigorous, for the data files discussed for every write, there is a corresponding read of that file.

This document shows that the number of reads increases with UQ applications, and the read will not be initiated not only by the scientist but by the UQ Pipeline. The size of the produced files will significantly increase as the resolution of the simulation increases, and the number of the ensemble simulations needed to produce accurate response models will increase the number of produced data files. The utilization of the filesystem for the above discussed will be similar for ICF and Stockpile Stewardship applications.

<u>Key Questions:</u>

Will current filesystem technology scale to higher resolution UQ studies that require more ensemble simulations?

What is the read/write throughput of a HPC filesystem?

What are the architectural details that influences the throughput of a HPC filesystem?