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# Scaling the Science Using Adaptivity and Uncertainty Quantification – Case Study of Volcanic Hazard Analysis using HPC

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## ABSTRACT

The recent emergence of new classes of architectures for high end computing at the PetaFlop scale and beyond is driven by new generation processors with multiple cores. This requires us to rethink how applications can make use of these machines. For simulations of physical systems modeled by partial differential equations (PDE) the traditional approach of just growing grid sizes to improve numerical accuracy is problematic since scaling complex numerical codes on such architectures and the extremely large numbers of available processing elements is difficult and often rules out the use of efficient computing procedures like adaptive mesh refinement. A simple application of Amdahl's law indicates that to scale to hundreds of thousands processors we need almost perfect parallel efficiencies that are perhaps unobtainable in the classical data parallel paradigm on realistic problems. Load balance can never be perfect and synchronization times can never be completely hidden. In this paper we will explore alternate paradigms focussed on making the fullest possible use of the machine to deliver computations that are useful. We argue in essence that simple scaling of the numerical simulation tool while useful may be increasingly difficult and unproductive given the uncertainties in model and data. A better return may be obtained by exploring these uncertainties and means for delivering not a simple simulation but a useful scientific insight.

We will present in this paper our recent experience in using a complex PDE based model of volcanic flows to analyze hazard at several sites. For constructing a hazard map that indicates areas with higher probability of inundation by a flow, suitably chosen ensembles of numerically accurate simulations have to be conducted. We will focus in this talk on running these ensembles in a timely fashion efficiently on large scale hardware. We will use ensembles of runs of a parallel adaptive finite volume simulator called TITAN [1] designed to construct these hazard maps. Even with access to very high end resources the O($10^6$) simulations required to run simplistic Monte Carlo type ensembles is still unaffordable since each simulation uses up hours of time on $O(10^2)$ processing elements. We focus rather on using the simulations to create a surrogate statistical model (also called an emulator) of the hazard. The construction of this emulator with desired accuracy and minimal computation requires the use of Bayesian principles that are again "adaptive" and inherently sequential. We will discuss suitable strategies for adaptive sampling of the input parameter space to drive the construction of these emulators in parallel.

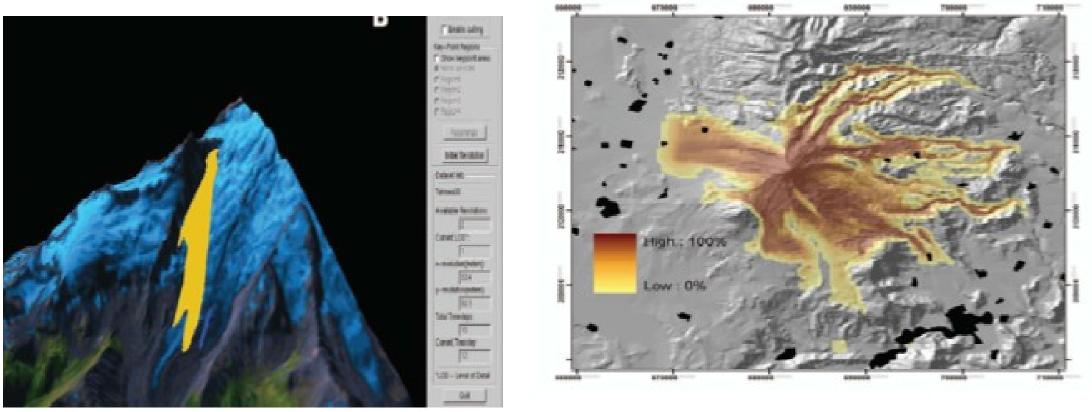


Figure 1: Figure on left shows a snapshot of hazardous mass flow simulated by the TITAN tool. Figure on right shows hazard maps constructed using ensembles of these computations. Darker colors indicate larger probability of inundation due to flow.

Thus, we explore parallelism and adaptivity at two levels – first each simulation uses an adaptive grid as it tracks the flows over time and second the ensemble of computations used to construct a Bayesian emulator for constructing a hazard map is adaptive and parallel. We argue that this hierarchical use of parallelism and adaptivity delivers efficient use of modern HPC resources.

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