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Title: Extreme Scale Infrasound Inversion and Prediction for Weather Characterization and Acute Event Detection

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Overview Description and Impact: Accurate and timely weather predictions are critical to many aspects of society with a profound impact on our economy, general well-being, and national security. In particular, our ability to forecast severe weather systems is necessary to avoid injuries and fatalities, but also important to minimize infrastructure damage and maximize mitigation strategies. The weather community has developed a range of sophisticated numerical models that are executed at various spatial and temporal scales in an attempt to issue global, regional, and local forecasts in pseudo real time. The accuracy however depends on the time period of the forecast, the nonlinearities of the dynamics, and the target spatial resolution. Significant uncertainties plague these predictions including errors in initial conditions, material properties, data, and model approximations. To address these shortcomings, a continuous data collection occurs at an effort level that is even larger than the modeling process. It has been demonstrated that the accuracy of the predictions depends on the quality of the data and is independent to a certain extent on the sophistication of the numerical models. Data assimilation has become one of the more critical steps in the overall weather prediction business and consequently substantial improvements in the quality of the data would have transformational benefits. This paper describes the use of infrasound inversion technology, enabled through exascale computing, that could potentially achieve orders of magnitude improvement in data quality and therefore transform weather predictions with significant impact on many aspects of our society.

Traditional data acquisition consists of spatially and temporally limited measurements from a range of sources, such as satellites, balloons, ground sampling, and flight sensors. This is an extensive process resulting in voluminous data but yet the overall information content is limited because the sampling is spatial and temporally sparse in addition to being heterogenous. For instance, satellites provide averaged quantity of interests over some spatial area at a certain temporal rate. Ground samples and balloon measurements provide highly accurate data at specific point locations but at a slower and mostly inconsistent temporal rate. In the context of the complex dynamics, these data acquisitions provide sparse information and cannot provide continuity that would eliminate the spatial and temporal uncertainty associated with atmospheric material properties. If somehow atmospheric material properties, such as density, temperature, humidity, and wind velocities, could be measured in a continuous spatial and temporal manner, the quality of the calibrated models realized would potentially revolutionize weather forecasting.

For the last decade, geophysical full waveform inversion (FWI) technology has matured to provide quality reconstructions of subsurface material properties by acquiring data from systematic explosion-based experiments and solving a large scale optimization problem in which the difference between data and numerical predictions are minimized. The numerical predictions are generated by sophisticated simulations of the wave propagation physics. This full waveform inversion provides the foundational technology to reconstruct material properties in the atmosphere through similar mechanics. The instantiation of a source generates acoustic waves which transmit and reflect as a result of changes in properties in the atmosphere. By recording the reflected waves through sensors, a large scale inverse problem can be solved that reconciles the differences between observations and numerical predictions. The study of sound in the atmosphere is known as infrasound and typically operates in a low frequency range below 20 Hz. Sources occur through natural events such as volcano eruptions, earthquakes, acute weather systems and through man-made events, such as explosions, rocket launches, aircraft induced

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shock waves. The culmination of FWI technology, the study of sound wave in the atmosphere known as infrasound, and the prospect of exascale computers can provide a paradigm shift in data quality for weather models.

System Requirements: We estimate that a single deterministic inversion of atmospheric material properties will require approximately 24 hours of simulation on an exascale computer. This estimate is based on a three dimensional mesh (1E12 cells) to resolve wave propagation around the globe at a frequency of 0.3 Hertz. Since the instantiation of a source will generate traveling waves in both direction, the wave front only need to be simulated half-way around the globe. The resource estimate also assume 10 percent processor efficiency, 100 optimization iterations and 10 forward solutions to calculate adjoint, gradient, globalization metrics per optimization iteration. A global inversion with these specifications would potentially be sufficient to resolve 1 km variations in the atmosphere. More detailed resolution would be potentially beneficial but dictates corresponding increases in computational resources. Furthermore, managing uncertainties in the infrasound inversion problem would also improve the material property reconstruction, but the computational requirements would far exceed even the exascale capability.

Code and Tools: Sandia has invested considerable effort into the development of large scale inversion of engineering and geophysical applications. Existing large scale inversion capabilities for wave propagation can be applied to the infrasound problem today for simplistic atmospheric conditions at coarse resolutions. Our software leverages the Trilinos framework which is a component-based design, offering software flexibility and extensibility. In particular, the software is uniquely positioned to address exascale computing issues.

Models and Algorithms: To realize a complete and accurate capability suitable to address general weather conditions, a moving media capability would need to be incorporated into the wave propagation dynamics and corresponding adjoint calculations. Furthermore, target inversion parameters such as temperature, humidity, and wind velocities, would require development of algorithms to connect to existing inversion parameters (density and wave speed).

End-to-End Requirement: Interfaces will be required to automatically communicate updates of atmospheric properties and quality metrics between infrasound and weather models.

Related Research: In addition to the impact on weather predictions, infrasound information is currently used to help detect nuclear detonations in combination with seismic and trace-gas measurements, in support of the comprehensive nuclear test-ban treaty. These approaches however use simplistic algorithms and although capable of determining locations, the quality of the source reconstruction is not sufficient to conclusively determine the type of explosion. FWI technologies applied to both seismic and infrasound measurements will drastically improve the quality of the reconstruction by simultaneously inverting for material properties (in the subsurface and atmosphere) and source terms. Although the infrasound inversion in this case can now be limited to a smaller region, the frequency of the source will encompass a much larger range and therefore require finer mesh resolutions, which consequently will increase the computational requirements. In combination with seismic inversion, we estimate a similar order of magnitude computational requirement would be required in comparison to the global infrasound inversion. The FWI-based infrasound technology can also provide accurate characterization of initial conditions for chemical, biological, and nuclear plant disasters where a malfunction causes a catastrophic failure and nuclear, chemical, or biological fallout need to be tracked in real time. Not only could infrasound reconstruct the initial conditions to provide more accurate forecasts (using a transport model) but subsequent infrasound inversions could determine atmospheric density changes and help track the plume, the quality of which is critical for evacuation and mitigation purposes.

10-year Problem Target: The 10 year target would be to achieve a 10 fold improvement in weather predictions spatially and another 10 fold improvement in temporal improvement, solely due to infrasound data acquisition and FWI inversion. Additionally the target would be to significantly reduce overall damage, injuries, and cost from acute events.