DDDAS APPROACHES TO WILDLAND FIRE MODELING AND CONTAMINANT TRACKING

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ABSTRACT

We report on two ongoing efforts to build Dynamic Data Driven Application Systems (DDDAS) for (1) short-range forecasting of weather and wildfire behavior from real time weather data, images, and sensor streams, and (2) contaminant identification and tracking in water bodies. Both systems change their forecasts as new data is received. We use one long term running simulation that self corrects using out of order, imperfect sensor data. The DDDAS versions replace codes that were previously run using data only in initial conditions. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process. Jonathan D. Beezley Jan Mandel

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1 INTRODUCTION

We describe the current state of a dynamic data driven application system (DDDAS) for simulating wildland fires and identifying and tracking contaminants.

DDDAS is a paradigm whereby application (or simulations) and measurements become a symbiotic feedback control system. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process. Such capabilities promise more accurate analysis and prediction, more precise controls, and more reliable outcomes. The ability of an application to control and guide the measurement process and determine when, where, and how it is best to gather additional data has itself the potential of enabling more effective measurement methodologies. Furthermore, the incorporation of dynamic inputs into an executing application invokes new system modalities and helps create application software systems that can more accurately describe real world, complex systems. This enables the development of applications that intelligently adapt to evolving conditions and that infer new knowledge in ways that are not predetermined by the initialization parameters and initial static data.

The motivation for our research is the following:

- The obvious societal value of an accurate forecast compounded with the inherent challenge in modeling nonlinear, rapidly changing phenomena.
- The difficulty in obtaining remote or in situ data.
- The challenges of communicating the on site, out of sequence data of unknown quality to remote supercomputers and using it to steer simulations.

The work necessarily extends beyond data assimilation work in progress in atmospheric or ocean sciences due to the specific application challenges: the model is strongly nonlinear and irreversible, the data arrives out of sequence from disparate data sources, and error distributions cannot be considered Gaussian. Our two DDDAS eamples are built upon previously existing models and codes.

Components have been developed and added to the coupled atmosphere-wildfire model which

- save, modify, and restore the state of the model,
- apply ensemble data assimilation algorithms to modify ensemble member states by comparing the data with synthetic data of the same kind created from the simulation state,
- retrieve, process, and ingest data from both novel ground-based sensors and airborne platforms in the near vicinity of a fire, and
- provide computational results visualized in several ways adaptable to user needs.

Components have been developed and added to the contaminant-ocean model which

- apply multiscale interpolation to a hydrodynamic and some contaminant transport models,
- correct incorrect earlier forecasts and initial guesses,
- retrieve, process, and ingest data from novel sensors in water bodies that can be on buoys or on a drone, and
- provide computational results visualized in several ways adaptable to user needs.

DDDAS requires sensors capable of dynamically supplying data to a simulation. An ideal sensor would be sensitive, selective, and able to communicate high level spatial and chemical information to the simulation rapidly using negligible bandwidth. Integrated Sensing and Processing (ISP) aims to replace current sensor designs with such DDDAS optimized sensor system architectures, comprising interdependent networks of functional elements, each of which may span the roles and functions of multiple separate subsystems in present generation sensor systems. ISP simplifies sensing in DDDAS through spanning those multiple roles and functions. ISP research is developing mathematical tools that facilitate the design and global optimization of systems that interactively unite usually independent functions of sensing, signal processing, communication, and exploitation. ISP achieves diminution of crucial degrees of freedom in sensing system design and operation without regard to traditional subsystem limits and interconnect structures. This reduction is realized by applying modern systematic methods from physics based computational modeling and fast data adaptive representations to discover and take advantage of structure present in the data across every stage of the sensor system. In many instances, ISP enables an instantaneous dimensionality reduction to a tractable optimization problem that is far more deferential to the end to end structure of the problem than the traditional sensing approach.

One such ISP sensor is the Solid-State Spectral Imager (SSSI). The SSSI is a lens-free optical sensor with no moving parts that is configurable by a simulation, which chooses specific Integrated Sensing and Processing (ISP) light pulse sequences designed to probe and to resolve chemical uncertainties in the system being simulated. The sequences selected by the simulation are downloaded into the SSSI sensor to enable location and quantification of specific chemical analytes. The SSSI has been used to study water quality when outfitted with conventional LEDs (light-emitting diodes) of various wavelengths. By substituting laser diodes for the LEDs the SSSI becomes a multivariate DIAL (differential absorption LIDAR, or Light Detection And Ranging) for analyses of airborne particulates and gases like oxygen and carbon dioxide.

Data that come into the data center must go through a process consisting of up to six steps.

- 1. *Retrieval*: Get the data from sensors. This may mean receiving data directly from a sensor or indirectly through another computer or storage device (e.g., a disk drive).
- 2. *Extraction*: The data from some sensors may be quite messy in raw form, thus the relevant data may have to be extracted from the transmitted information.
- 3. *Conversion*: The units of the data may not be appropriate for our application.

- 4. *Quality control*: Bad data should be removed or repaired if possible. Missing data (e.g., in a composite satellite image) must be repaired.
- 5. *Store*: The data must be archived to the right medium (or media). This might mean a disk, tape, or computer memory, or no storage device at all (or only briefly) if data is not being archived permanently or only temporarily.
- 6. *Notification*: If a simulation is using the data as it comes into the data center, the application needs to be informed of the existence of new data.

ISP simplifies DDDAS by performing data extraction and data conversion at the detector in the sensor, eliminating steps 2 and 3 in the previous paragraph. ISP also presents the data as high-level information tokens that require very little communication bandwidth. Bad data may be edited or removed as data are tokenized, potentially eliminating step 4 in the data center as well.

In Sections 2 and 3, we describe the wildland fire model, the identification and tracking of contaminant model, and and their DDDAS components, respectively. In Section 4, we draw some conclusions about the commonality of DDDAS components in these two examples.

2 WILDLAND FIRE MODEL

The original modeling system is composed of two parts: a numerical weather prediction model and a fire behavior model that models the growth of a wildfire in response to weather, fuel conditions, and terrain (Clark, Coen, and Latham 2004, Coen 2005). These models are two way coupled so that heat and water vapor fluxes from the fire are released into the atmosphere, affecting the winds in particular, while the fire affected winds feed back upon the fire propagation. This wildfire simulation model can thus represent the complex interactions between a fire and the atmosphere.

The meteorological model is a three-dimensional nonhydrostatic numerical model based on the Navier-Stokes equations of motion, a thermodynamic equation, and conservation of mass equations using the anelastic approximation. Vertically-stretched terrain-following coordinates allow the user to simulate in detail the airflow over complex terrain. Gridded national weather forecasts are used to initialize the domain and update lateral boundary conditions. Two-way interactive nested grids capture the outer forcing domain scale of the synoptic-scale environment while allowing the user to telescope down to tens of meters near the fireline through horizontal and vertical grid refinement. Weather processes such as the production of cloud droplets, rain, and ice are parameterized using standard treatments.

In the original model, local fire spread rates depend on the modeled wind components, fuel properties, and terrain slope through an application of the semi-empirical Rothermel fire spread formula (Rothermel 1972). We are replacing the Rothermel model with a simple physics and PDE based model (Mandel, Chen, Franca, Johns, Puhalskii, Coen, Douglas, Kremens, Vodacek, and Zhao 2004). This PDE model uses the reaction-convection-diffusion equation for the temperature T and fuel supply S,

$$c\frac{\partial T}{\partial t} = -\nabla d\nabla T - av \cdot \nabla T + e\frac{\partial S_k}{\partial t} - b\left(T - T_a\right), \quad (1)$$
$$\frac{\partial S}{\partial t} = -f(T)S. \quad (2)$$

(1) is the balance of heat. The term $-\nabla d\nabla T$ models the heat diffusion, $-av \cdot \nabla T$ is the convection by wind with speed v, $e\frac{\partial S_k}{\partial t}$ is the heat generated by burning the fuel, and $-b(T - T_a)$ is the heat lost to the ambient environment with temperature T_a . (2) is the balance of fuel. This simple model is capable of producing a reasonable fire behavior with an advancing fire front. A more advanced version of this model is under development, which will include several species of fuel, radiative heat transfer between fuel species, and evaporation of moisture. It is anticipated that this model will replace the empirical fire model and it will be coupled to the atmospheric model. For related physics based fire models in the literature, see, for example, Linn, Reisner, Colman, and Winterkamp (2002), Serón, Gutiérrez, Magallón, Ferragut, and Asensio (2005).

Forecasting with the coupled atmosphere fire model is achieved using the Ensemble Kalman Filter (EnKF). Ensemble filters work by advancing in time a collection of simulations started from randomly perturbed initial conditions. When the data is injected, the ensemble (called *forecast*) is updated to get a new ensemble (called *analysis*) to achieve a least squares fit using two conditions: the change in the ensemble members should be minimized, and the data *d* should fit the ensemble members state u,

$$h(u) \approx d,\tag{3}$$

where h is called the *observation function*. The weights in the least squares are obtained from the covariances of the ensemble and of the data error. For comprehensive surveys of EnKF techniques, see Evensen (2003), Evensen (2004), Tippett, Anderson, Bishop, Hamill, and Whitaker (2003). In general, *EnKF works by forming the analysis ensemble as linear combinations of the forecast ensemble*.

We are using filters based on the EnKF with data perturbation (Burgers, van Leeuwen, and Evensen 1998). But, even with the simple wildfire model (1)-(2), the data assimilation produces an ensemble with nonphysical solutions causing the simulations to break down numerically. Therefore, we have proposed a regularization by adding a term involving the change in the spatial gradient of ensemble members to the least squares (Johns and Mandel rint). Existing ensemble filter formulas assume that the observation function is linear, h(u) = Hu, and then compute with the observation matrix H. To simplify the software, we have derived a mathematically equivalent ensemble filter that only needs to evaluate h(u) for each ensemble member.

For the issue of assimilating of out-of-order data we will use system states that combine states at several times (Mandel, Chen, Franca, Johns, Puhalskii, Coen, Douglas, Kremens, Vodacek, and Zhao 2004). The parallel computing framework we have developed was designed with this in mind.

Data comes from fixed ground sensors that measure temperature, radiation, and local weather conditions (Kremens, Faulring, Gallagher, Seema, and Vodacek 2003). These systems will survive burn-over by low intensity fires and are intended to supplement other sources of weather data derived from permanent and portable automated weather stations. The temperature and radiation measurements provide the direct indication of the fire front passage and the radiation measurement can also be used to determine the intensity of the fire.

Data also come from images taken by sensors on either satellites or airplanes. The primary source of image data is the Wildfire Airborne Sensor Project (WASP) (Li, Vodacek, Kremens, Ononye, and Tang 2005). This three wavelength digital infrared camera system is carried on an airplane that is flown over the fire area. Camera calibration, an inertial measurement unit, GPS, and digital elevation data are used in a processing system to convert raw images to a map product with a latitude and longitude associated with each pixel. The three wavelength infrared images can then be processed using a variety of algorithm approaches (Li, Vodacek, Kremens, Ononye, and Tang 2005, Dozier 1981) to extract which pixels contain a signal from fire and to determine the energy radiated by the fire (Wooster, Zhukov, and Oertel 2003, Smith, Wooster, Drake, Perry, Dipotso, Falkowski, and Hudak 2005).

The data are related to the model by the observation equation (3). The observation function h maps the system state u to synthetic data, which are the values the data would be in the absence of modeling and measurement errors. Knowledge of the observation function, the data, and an estimate of the data error covariance is enough to find the correct linear combinations of ensemble members in the ensemble filter. The data assimilation code also requires an approximate inverse q of the observation function. For a system state u and data d, q(h(u) - d) is the direction in which the system state can change to decrease a norm of the data residual h(u) - d. For an observation function that is simply the value of a variable in the system state, the natural choice of approximate inverse can be just the corresponding term of the data residual, embedded in a zero vector.

Building the observation function and its approximate inverse requires conversion of physical units between the model and data and conversion and interpolation of physical coordinates. In addition, synthetic data at instants of time between the simulation time of ensemble members need to be interpolated to the data time. The data injection itself is done by updating the ensemble to minimize a weighted sum of the data residual and the change in the ensemble.

The data items enter in a pool maintained by the data acquisition module. The assimilation code can query the data acquisition module to determine if there are any new data items available, request their quantitative and numerical properties, and delete them from the pool after they are no longer needed.

3 CONTAMINANT MODEL

The DDDAS contaminant tracking system consists of sensors, a hydrodynamic and contaminant transport models, a data assimilation system, and computers, network and software to integrate the capabilities of the various components into a unified system for disaster management and mitigation. Here we give a brief overview of the different components while highlighting their most pertinent features.

The new ISP sensor is a Solid-State Spectral Imager (SSSI) designed to gather, among other things, hydrological and geological data, and to perform chemical analyses. The sensor is suitably small and light enough to be mounted on various roving platforms to be used in remote-sensing situations, and can scan ranges of 10-100 meters in distance. Using a laser-diode array, photodetectors, and on-board processing, the SSSI combines innovative spectroscopic integrated sensing and processing with a hyperspace data analysis algorithm (Lowell, Ho, and Lodder 2002).

The SSSI detects and identifies contaminants in water using near-infrared, visible, and ultraviolet light. Absorption, fluorescence, and even Raman spectrometry can be implemented, but absorption spectrometry is the most common. Virtually every organic compound (e.g., polycyclic aromatic hydrocarbons, paraffins, carboxylic acids, and sulfonic acids) has a near-IR spectrum that can be measured, including two classes of terrestrial biomarkers, lipids, and amino acids. Near-infrared spectra consist of overtones and combinations of fundamental mid-infrared bands, giving near-infrared spectra a powerful ability to identify organic compounds while still permitting some penetration of light into samples (Dempsey, Davis, R. G. Buice, and Lodder 1996).

The SSSI uses Walsh-Hadamard or CRISP (Complementary Randomized Integrated Sensing and Processing) encoding sequences of light pulses to further increase the signal-to-noise ratio. In a Walsh-Hadamard sequence multiple laser diodes illuminate the target at the same time, increasing the number of photons received at the photodetector and the signal-to-noise (S/N). The Walsh- Hadamard sequence can be demultiplexed to individual wavelength responses with a matrix-vector multiply operation (Silva and Pasquini 2001). CRISP encoding uses orthogonal pseudorandom codes with unequal numbers of on and off states. The duty cycle of each code is different and the codes are selected to deliver the highest duty cycles at the wavelengths where the most light is needed and lowest duty cycle where the least light is needed to make the sum of all of the transmitted (or reflected) light from the samples proportional to the analyte concentration of interest.

The hydrodynamic model consists of the Spectral Element Ocean Model (SEOM) in its two-dimensional shallow water version. The spatial discretization relies on the spectral element method, an h-p type finite element discretization, which relies on relatively high degree (5-8th) polynomials to approximate the solution within each element. The main features of the spectral element method are: geometric flexibility due to its unstructured grids, dual paths to convergence: exponential by increasing polynomial degree or algebraic via increasing the number of elements, dense computational kernels with sparse inter-element synchronization, and excellent scalability on parallel machines. The model can be forced through winds, tides, and lateral injection of mass at inflow boundaries (e.g., river input). The model is supplemented with an advection-diffusion equation to simulate the trajectory of contaminants as they are carried along by the simulated flow.

The initial deployment of the sensor and model will focus on estuarine regions where water quality monitoring is critical for human health and environmental monitoring. The authors will capitalize on an existing configuration of the model of the Hudson-Raritan Estuary to illustrate the model's capabilities. A sample tidal calculation is performed using a grid that encompasses the Newark/New York bays regions, the Long-Island sound, and a substantial portion of the Hudson River. The model is forced with tidal elevation obtained from tide gauges located on the eastern edge of the Long Island Sound in Montauk, NY and in Sandy Hook, NJ. Runs without data assimulation have shown good comparison with observation (Figure 1) and previous modeling results. However, for DDDAS the use of data assimilation is imperative to inject observational data in the model while accounting for model and observational errors.

The data assimilation reduces the computational errors associated with initial data, essentially the solution at previous time step, and improves the predictions. Using the first set of measurements, the approximation of the initial data is recovered. As new data are incorporated into the simulator, the initial data are updated using an objective function. We note that the formulated problem is ill-posed because there are fewer sensors than the finite dimensional space describing the initial data. The objective function is set up based on both a measurement error as well as



Figure 1: Comparison of Tidal Elevation in Bridgeport, CT

a penalization term that depends on the prior knowledge about the solution at previous time steps (or initial data). The prior information is refreshed using the updated initial data. The penalization constants depend on time of update and can be associated with the relative difference between simulated and measured values. In the simulations, both the prior and penalization constants change in time.

To account for the errors (uncertainties) associated with sensor measurements, we consider an initial data update within a Bayesian framework. The posterior distribution is set up based on measurement errors and prior information. This posterior distribution is complicated and involves the solutions of partial differential equations. We could use a Metropolis-Hasting Markov chain Monte Carlo (MCMC) method to generate samples from the posterior distributions. However, a sampling with MCMC is expensive since it requires iterative steps and the acceptance rate is typically low. We developed an approach that combines least squares with a Bayesian approach that gives a high acceptance rate. In particular, we can prove that rigorous sampling can be achieved by sampling the sensor data from the known distribution, thus obtaining various realizations of the initial data. Our approach has similarities with the Ensemble Kalman Filter approach, which can also be adapted to an initial data update.

The SSSI is reprogrammable in the field. When an interesting chemical trace is discovered, the reaction from the application overseeing the SSSI is two-fold: (a) invoke an appropriate application, and (b) request that the SSSI look for specific other chemical traces using other specific

pulse sequences. There is a symbiotic relationship between the sensor network and the application simulation that is typical in a DDDAS.

Consider finding hydrocarbon fuel in a body of water. Gasoline can be a sign of innocuous pollution from a small boat. Heavier fuel oils could be an indication that a larger boat leaked or sank recently nearby. Jet fuel could come from a downed aircraft. The SSSI needs to be reprogrammed in the latter case and a search and locate application must be invoked to find the accident and rescue any people that may be in danger. Emergency services, the coast guard, and the news media may need to be automatically informed of progress.

The SSSI has a modest amount of memory and computing capacity on board. USB2 and Ethernet will be put onto the SSSI over time, thus reducing the amount of time needed to reprogram the device.

A programmable, portable low-cost sensor and network for DDDAS in extreme aqueous environments must be able to perform chemical analyses to be effective in terrorist attack and accident scenarios. Most oil sensing in the oceans is already done by remote sensor systems (Fingas and Brown 2000).

Once the spectrum of a sample has been collected, it must be classified to determine the substance present. The Bootstrap Error-adjusted Single-sample Technique (BEST) (Dieter, Lodder, and James E. Lumpp 2006) is the analytical basis of SSSI, and the foundation for the chemical library. Spectra recorded at n wavelengths are represented as single points in a n-dimensional hyperspace. In this scheme, similar samples produce similar spectra that project as "probability orbitals" or "clusters" into similar regions of hyperspace. The BEST metric is a clustering technique for exploring these distributions of spectra in hyperspace.

Oil droplets can travel nearly anywhere in the ocean. The droplet size exerts a major effect on droplet motion (OSB 2005). The rise velocity of oil droplets extends from about 2.5×10^{-7} m/s for a diameter of 2 μ m to 4.3×10^{-3} m/s for a diameter of 260 μ m. Droplets traveling at 2.5×10^{-7} m/s will ascend only 0.001 m and 0.02 m, over periods of 1 hour and 24 hours, while over equivalent periods, droplets ascending at 4.3×10^{-3} m/s will climb 15 m and 370 m. In the meantime, a vertical diffusivity of 51 cm²/s will distribute oil droplets (equally upward and downward) about 6 m and 30 m over the same time. Therefore, the smallest oil droplets act as though they are neutrally buoyant (transported only by diffusion), while the largest droplets are advected largely by their buoyancy.

Using multiple linear regression the BEST classification algorithm can be performed in situ, allowing a rover to classify many samples, only notifying the simulation when an interesting substance is found. An initial library can be computed based on substances likely to be found in the target environment. When a substance unknown to the BEST library is found, the sensor can sample nearby points with similar spectra to create a new library entry for the new substance. Scientists can determine the type of substance present by further analyzing raw spectra of the substance provided by SSSI and by using data from their other instruments, apply these data to update the simulation. The SSSI chemical library will comprise substances expected to be in the environment in which the SSSI operates.

4 CONCLUSIONS

The two DDDAS applications described in this paper have many things in common:

- The correct sensor needs to be chosen to get the right data at a given time.
- The sensors must be placed in the right locations
- Data is not necessarily accurate nor does it arrive on time in the correct order. Hence, data must be filtered before use and error distributions in the data must be known.
- The sensors should be reprogrammable in some sense by the application.
- The potential for rapid error growth without data steering.
- The application's models, numerical methods, and major item to be tracked may need to be changed as a result of the incoming sensor data or a human in the loop.
- Long term simulations are possible using dynamic data instead of having to run many short term ones with incoming, but static initial guesses.

In the future, we hope to apply both projects to environmental issues arising in the Amazon region. Flooding of parts of the Amazon occurs for up to ten months in a year. Numerous nutrients and contaminants are transported long distances during the flooding of the várzeas. There are substantial petroleum deposits in the region that leak into the rivers. We hope to apply the SSSI concepts to each of these problems.

In addition, 90% of the population in the region lives in the várzeas. The method of choice to clear land for building is to burn the jungle. While the fire model is different for a mountainous wildland fire than a flat surface jungle fire, we hope to extend our DDDAS to this case.

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