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Objectively Optimized Earth Observing Systems

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1. Introduction

In this chapter we discuss an approach to making Earth Observing Systems autonomous by integrating the situational awareness provided by our theoretical and observational knowledge of the system being observed. Our theoretical understanding of the system is encapsulated in a deterministic model. The observational knowledge is integrated via a data assimilation system. We will start by surveying what has been done to date, then outline our contribution to the field, and finally suggest some future areas of development.

2. Current Observing Systems and Autonomy

Modern observing systems are typically composed of a variety of components, or assets, that are interconnected to form a 'Sensor Web' (Botts et al., 2007). The communications fabric of the Sensor Web is a vital component that links the sensors and control systems and allows coordinated data transmission and instrument control. Effective autonomous control of individual sensors and/or the overall Sensor Web is highly desirable, maybe even indispensable, if the observing system is to be able to respond in real time to the evolving state of the environment.

The current Earth observing capability depends primarily on spacecraft missions and ground-based networks to provide the critical on-going observations necessary for improved understanding of the Earth system. Aircraft missions have played an important role in process studies but are often limited to relatively short-duration flights. However, for over a decade, it has been recognized that autonomous aerial observations can make an important contribution to Earth observing systems (Coronado et al., 1998; Sandford et al., 2004). The ability of the observing system to respond in real time to an evolving situation can, in some cases, be critical. An example would be robotic reconnaissance operations in extreme environments that are potentially hazardous (such as volcanic gas sampling, mine fields, battlefield environments, enemy occupied territories, terrorist infiltrated environments, or areas that have been exposed to biochemical agents or radiation) (Caltabiano et al., 2005; Chen et al., 2006; Fink et al., 2007). In other cases autonomy is necessary as the vehicles are operating in inaccessible locations, such as remote planetary atmospheres (Ippolito et al., 2005; Young et al., 2005; Morrow et al., 2006).

Observing platform autonomy is a relatively new field (Davis et al., 1992; Schiller et al., 1993). The nature of the autonomy depends in part on the type of asset. For space based orbital assets the autonomy could be directing the real time instrument pointing, or

instrument mode (e.g. zoom in, global survey, step and stare, etc). For sub-orbital assets such as aircraft or unmanned aerial vehicles (UAVs) the autonomy is generally much more developed and typically includes automated route planning for a single UAV (Sullivan et al., 2004; Kunchev et al., 2006; Ceccarelli et al., 2007; Pehlivanoglu et al., 2007; Pehlivanoglu and Hacıoglu, 2007) and coordinated route planning for a fleet of UAVs (Bellur et al., 2002; Dargar et al., 2002; Mahler and Prasanth, 2002; McInnes, 2003; Zelinski et al., 2003; Gilmore and Garbarino, 2004; Hope et al., 2004; King et al., 2004; Maddula et al., 2004; Chen et al., 2005; Jin et al., 2006; King et al., 2006; Sinha et al., 2006; Smith and Nguyen, 2006c;b;a; Fink et al., 2007; Lamont et al., 2007; Smith and Nguyen, 2007; Yuan et al., 2007). When we are dealing with a fleet of distributed autonomous systems there can also be an element of decentralization, so that in addition to concerted action, each member may exhibit some degree of individual autonomy (Richards and How, 2004; Smith and Nguyen, 2005). The UAV targets may be a set of fixed locations or mobile targets (Rafi et al., 2006).

Autonomy can even be used to improve mission-level functional reliability through better system self-awareness and adaptive mission planning (Valenti et al., 2007). The flight duration of UAVs is continually improving; some UAVs are now capable of continuous flight over many days (Noth et al., 2006), for such vehicles autonomy is again a benefit. Presently, the UAVs come in all shapes and sizes, from palm top micro UAVs, to helicopters, to giant strategic UAVs that can loiter over targets for extended periods of time (Natarajan, 2001). Unmanned aerial vehicles also include blimps (Elfes et al., 2001; Elfes et al., 2003; Hygounenc et al., 2004). A blimp is a small airship that has no metal framework and collapses when deflated (Beji and Abichou, 2005). In some cases the blimp can only control its vertical position by ascent or descent, with the surrounding wind field controlling its horizontal location. For conventional balloon borne observations the autonomy could be in directing the optimal time and location for launch.

Autonomous direction is not limited to orbital and sub-orbital platforms; they can include unmanned ground vehicles (UGV) (Kamsickas and Ward, 2003; Kelly et al., 2006; Li and Cassandras, 2006), unattended ground sensors (UGS) (Roberts et al., 2003), and subsea and surface (UUV and USV) vehicles (Davis et al., 1992; Hansen et al., 2006; Steinberg, 2006) operating together with minimal human oversight.

UAVs (aircraft or helicopter) are advanced and complex robotics platforms used for a variety of tasks. For example, UAVs can be used in applications for environmental monitoring (weather and/or pollution), traffic monitoring (Dudziak, 1998; Chung and He, 2007), surveillance (Persson, 2002; Ryan et al., 2007), intelligence gathering (Stottler et al., 2007), terrain mapping (Templeton et al., 2007), emergency services assistance (Ryan and Hedrick, 2005; Beard et al., 2006; Onosato et al., 2006; Snarski et al., 2006; Fabiani et al., 2007), studying the movement of agricultural threat agents, pollen, plant pathogens, and other biological particles (Wang et al., 2007), crop condition (Herwitz et al., 2004; Johnson et al., 2004; Furfaro et al., 2007), photogrammetry, and surveying (Schmale et al., 2008).

UAV autonomy is accomplished by a complex interconnection of systems related to a wide range of topics, e.g., flight low level control, navigation and task-based planning, elaboration of sensor signals, software architecture for reactive behaviors, communication (Zingaretti et al., 2008). In some applications the UAVs will be working in a cooperative network with other autonomous agents, such as UGVs (Unmanned Ground Vehicles) and UGSs (Chandler et al., 2002; Murphey and O'Neal, 2002; Roberts et al., 2003; Zingaretti et al., 2008) to accomplish specific tasks that may, or may not, have been defined a priori.

The autonomy has to be based on objective criteria that can be evaluated in real time via methodologies such as optimization, information theory, computer vision, mixed integer linear programming, fuzzy logic, genetic algorithms, artificial cognition, geographic information systems (GIS), set partition theory, vehicle health status, and/or threat assessments (Atkins et al., 1998; Chandler and Pachter, 1998; Sinopoli et al., 2001; Chandler et al., 2002; Levin et al., 2002; Cruz et al., 2003; Flint et al., 2003; Miller and Larsen, 2003; Nikolos et al., 2003; Lee et al., 2004; Ertl and Schulte, 2005; Kamal et al., 2005; KrishnamurthyGopalan et al., 2005; Vachtsevanos et al., 2005; Pettersson and Doherty, 2006; Pongpunwattana et al., 2006; Skoglar et al., 2006; Yang et al., 2006; Smith, 2007; Smith and Nguyen, 2007). Autonomy is often implemented using multi-layer hierarchical control architectures (Boskovic et al., 2002). The autonomous operation can include features such as the Cognitive Emotion Layer (CEL) that uses dynamical emotional response mechanisms to model response to continuous stimuli and provides adaptive decision making and control capabilities for the exploration platform (Ippolito et al., 2005). A given control system may provide more than one autonomous mode, for example, (Sasiadek and Duleba, 2000) outline an approach where the motion planning problem is split into two stages: a decision mode and a trace mode. In the decision mode, the vehicle selects its current direction of motion on the basis of the current value of a performance index. In the trace mode vehicle traces boundary and edges of obstacles using its on-board sensors.

Alternatively, an operator can issue the commands remotely. For example, an operator in a manned aircraft can issue mission level commands to an autonomous aircraft in real time (Sandewall et al., 2003; Schouwenaars et al., 2006). The open source movement has had a radical impact on the software Architecture for Autonomy (Brotten et al., 2006) open source frameworks can reduce the cost and risk of systems engineering.

Hybrid UAVs also exist, for example, the McDonnell Douglas Bird Dog, where a semi-autonomous UAV has been coupled with a manned ground vehicle (Kolding and Pouliot, 1997). In addition to making observations and delivering payloads UAVs can facilitate communications by acting as routing nodes (Francel, 2000). This is a role that may be increasingly important.

3. Situational Awareness via Theory and Observation

A valuable addition can be made to the studies described above, a situational awareness that comes from directly coupling our theoretical and observational understanding of the specific system being observed. The disciplines of numerical weather prediction and oceanography have long benefited from coupling a theoretical understanding as encapsulated by a deterministic model with a wide variety of observations through the mathematical formalism of data assimilation (Pielke et al., 1992; Swinbank and O'Neill, 1994; Kalnay et al., 1996). The use of data assimilation has dramatically improved forecast accuracy (Simmons and Hollingsworth, 2002).

3.1 Data Assimilation

Data assimilation is the term given to recursive Bayesian estimation in the geosciences (Wikipedia, 2008a). Data assimilation proceeds by analysis cycles. In each analysis cycle, observations of the current (and possibly, past) state of a system are combined with the results from a deterministic mathematical model (the forecast) to produce an analysis, which

is considered as 'the best' estimate of the current state of the system. This is called the analysis step. Essentially, the analysis step tries to balance the uncertainty in the data and in the forecast. The model is then advanced in time and its result becomes the forecast in the next analysis cycle.

The analysis and forecasts are best thought of as probability distributions. The analysis step is an application of the Bayes theorem. Advancing the probability distribution in time would be done exactly in the general case by the Fokker-Planck equation (Wikipedia, 2008b), but that is unrealistically expensive, so various approximations operating on simplified representations of the probability distributions are used instead. If the probability distributions are normal, they can be represented by their mean and covariance, which gives rise to the Kalman filter (Kalman, 1962).

More recently the use of data assimilation has also been extended to cover chemically reactive atmospheric systems relevant to issues such as ozone depletion and air quality (Fisher and Lary, 1995; Elbern et al., 1997; Menard et al., 2000; Lary et al., 2003).

It is current practice for today's forecasts for weather, air-quality, fire likelihood etc. to be generated on a fixed time schedule. However, new technologies and improved numerical model physics are enabling on demand forecasts in response to particular events (Plale et al., 2006). These forecasts ingest global and regional data in real time and can consume large computational resources. It is now timely to couple these concepts and take the next step of creating a coupled prediction and observation system. Such a coupled system can provide improved forecast accuracy and efficient collaborative adaptive sensing to make best use of the suite of observational assets. This synergistic approach offers distinct benefits to the respective user communities, and when used together, promise a paradigm shift in atmospheric science research.

As a growing volume of data is now freely available, it is a powerful approach where the incorporation of existing data into the analysis can be used to guide the optimal collection of new data. Large volumes of data are routinely provided by governmental organizations including in situ observations, geospatial data sets, remote sensing products, and simulation model output. Increasingly these data are being made available as web-services. Web services offer a means for sharing data more openly by providing a standard protocol for machine-to-machine communication. An example of the use of web-services in this manner is the machine accessible interface for the National Water Information System (NWIS) (Goodall et al., 2008), an online repository of historical and real-time stream-flow, water-quality, and ground water level observations maintained by the United States Geological Survey (USGS). These services provide a middle-layer of abstraction between the NWIS database and hydrologic analysis systems, allowing such analysis systems to proxy the NWIS server for on-demand data access. The services are intentionally designed to be generic and applicable to other hydrologic databases, in order to provide interoperability between disparate data sources.

3.2 Autonomous Observation for Atmospheric Chemistry

Our research effort has been focused on incorporating such situational awareness provided by coupling theory and observation. Our specific case study has been creating a software infrastructure for an autonomous observing system for atmospheric chemistry. The system works on generic principles that should be easily transferable to other scenarios. The observing system consists of many elements, orbital (several satellite instruments), sub-

orbital (aircraft, UAVs and balloons), and ground-based assets. The satellite assets include those with fixed pointing for which autonomy is not relevant and those with flexible pointing and multiple modes for which autonomy are most useful. The software infrastructure needs to be aware of all the observational elements and their capabilities at any given time *and* to be aware of the state of the system we are observing and the precision with which we know its current state.

Such an autonomous Objectively Optimized Observation Direction System is of great utility for NASA's observation and exploration objectives. In particular, it is useful to have a fleet of smart assets that can be reconfigured based on the changing needs of science and technology. Our project integrates a modeling and assimilation system within a Sensor Web. This enables a two-way interaction between the modeling/assimilation system and the sensing system to enhance Sensor Web performance and usage. Our aim is to develop a key technology currently missing in Sensor Web implementations, an autonomous Objectively Optimized Observation Direction System (OOODS). The OOODS will objectively optimize the workflow management of a set of assets, i.e. plan, monitor, and control the resources. This workflow management will involve a high level of situation awareness.

An important concept in such a system is the direct two-way feedback between the distributed Sensor Web and an autonomous OOODS (involving a numerical prediction and assimilation system). The project concentrates on the principles of how such an OOODS would operate, its architecture, and development as a plug-in for a Sensor Web simulator/controller. Two scenarios have been chosen to show the relevance of the technology to both current and future objectives of NASA Earth science. The project leverages technology that has already won five NASA awards and is currently being used in several NASA Aura validation and earth system science projects.

The goal of the Sensor Web OOODS described is to employ an objectively optimized data acquisition strategy for integrated Earth observation that is responsive to environmental events for both application and scientific purposes. Such an OOODS Sensor Web can achieve science objectives beyond the abilities of a single platform by specifically directing observations of high scientific value. This will be achieved by using objective criteria for the observation direction enabling a high degree of collaboration among the sensing and analysis assets. Once such a framework is in place, what the objective criteria are can readily be changed for other applications, depending on the desired science or application goals.

A Sensor Web with such a goal oriented OOODS can be of particular use for decision support systems. For example, in the scenarios we have chosen here, an obvious application would be for air quality decision support systems and in responding to a large hazardous release of atmospheric contaminants.

3.3 Key Principles

Metrics of what we do not know (state vector uncertainty) are used to define what we need to measure and the required mode, time and location of the observations, i.e. to define in real time the observing system targets. Data assimilation provides us with the state vector uncertainty. Below we will consider in detail how we construct the state vector uncertainty. Metrics of how important it is to know this information (information content) are used to assign a priority to each observation. The metrics are passed in real time to the Sensor Web observation scheduler to implement the observation plan for the next observing cycle. The same system could also be used to reduce the cost and development time in an Observation

Sensitivity Simulation Experiment (OSSE) mode for the optimum development of the next generation of observing systems.

4. Implementation

Now that we have considered the principles behind the autonomy let us move to the details of the two key components that we have used. The first component is a Sensor Web simulator. The second is our data assimilation system. Figure 1 shows an engineering diagram for our system.

4.1 Sensor Web Simulator

The Sensor Web simulator describes the capabilities and locations of each sensor as a function of time, whether they are orbital, sub-orbital, or ground based. The simulator has been implemented using Analytical Graphics Incorporated (AGI) Satellite Tool Kit (STK). STK makes it easy to analyze and visualize optimal solutions for complex space scenarios (www.agi.com). STK performs complex analysis of land, sea, air, and space assets, and shares results in one integrated solution. The STK functionality enables us to calculate the position and orientation of each asset, to evaluate inter-visibility times, and to determine quality of dynamic spatial relationships.

STK can be used for real time monitoring of operations with live feeds from sensors or for mission concept design and visualization. The Sensor Web data assimilation system feeds multivariate objective measures to an STK Matlab plug-in (e.g. information content for observation priority and system uncertainty for target definition). The target definition and priority are then passed to the STK Scheduler plug-in (our smart scheduler) that is aware of each assets capability and then constructs an optimal observation schedule for each asset in the Sensor Web. The STK Scheduler is a fully integrated add-on module for STK that provides a powerful scheduling and planning application to mission designers and operations engineers alike. Users can define tasks and related resource requirements, request schedule solutions, and analyze the results through a user-friendly graphical user interface (GUI) or via the Application Program Interface (API). The STK Scheduler is powered by a scheduling engine from Optwise Corporation that finds better solutions in a shorter amount of time than traditional heuristic algorithms. The global search algorithm within this engine is based on neural network technology that not only outperforms traditional scheduling engines, but can find solutions to larger and more complex problems. STK Scheduler allows system planners to maximize the value of limited resources. Examples of other uses of STK for UAV systems in real-time operations and post-mission analysis can be found online at <http://www.agi.com/solutions/specializedAreas/uav/>.

Some complementary work in building Earth Observing simulators for meteorology is also underway (Higgins et al., 2005; Kalb et al., 2005; Halem et al., 2007; Seablom et al., 2007). The end product of these studies will be a “sensor web simulator” (SWS) that would objectively quantify the scientific return of a fully functional model-driven meteorological sensor web.

4.2 Chemical Assimilation System

The chemical modeling and assimilation system provides situational awareness by supplying the time evolution of uncertainty and information content metrics that are used to tell us what we need to observe and the priority we should give to the observations.

State Vector Uncertainty for Target Definition

We use the state vector uncertainty to define our targets. As the state vector uncertainty is a product of the modeling and assimilation system let us consider the mathematical formalism that we use.

In the case considered here the model consists of a system of coupled ordinary differential equations (ODEs). Each ODE describes the time evolution at a given location of a chemical constituent. In our standard configuration we consider fifty-eight atmospheric constituents cast in Lagrangian coordinates. The fifty-eight constituents give a comprehensive description of the reactive oxygen, hydrogen, nitrogen, chlorine, bromine and methane chemistry of the atmosphere. We use the extensively validated AutoChem model described (Fisher and Lary, 1995; Lary et al., 1995; Lary, 1996). The model is explicit and uses an adaptive time-step, error monitoring time integration scheme for stiff systems of equations (Stoer and Bulirsch, 2002; Press, 2007). AutoChem was the first model to ever have the facility to perform 4D variational data assimilation (4D-Var) (Fisher and Lary, 1995) and now also includes a Kalman filter (Khattatov et al., 1999; Lary et al., 2003). AutoChem can also autonomously provide analyses of the results from the Sensor Web assets to the users. An example of the analysis AutoChem can provide can be found at www.CDACentral.info.

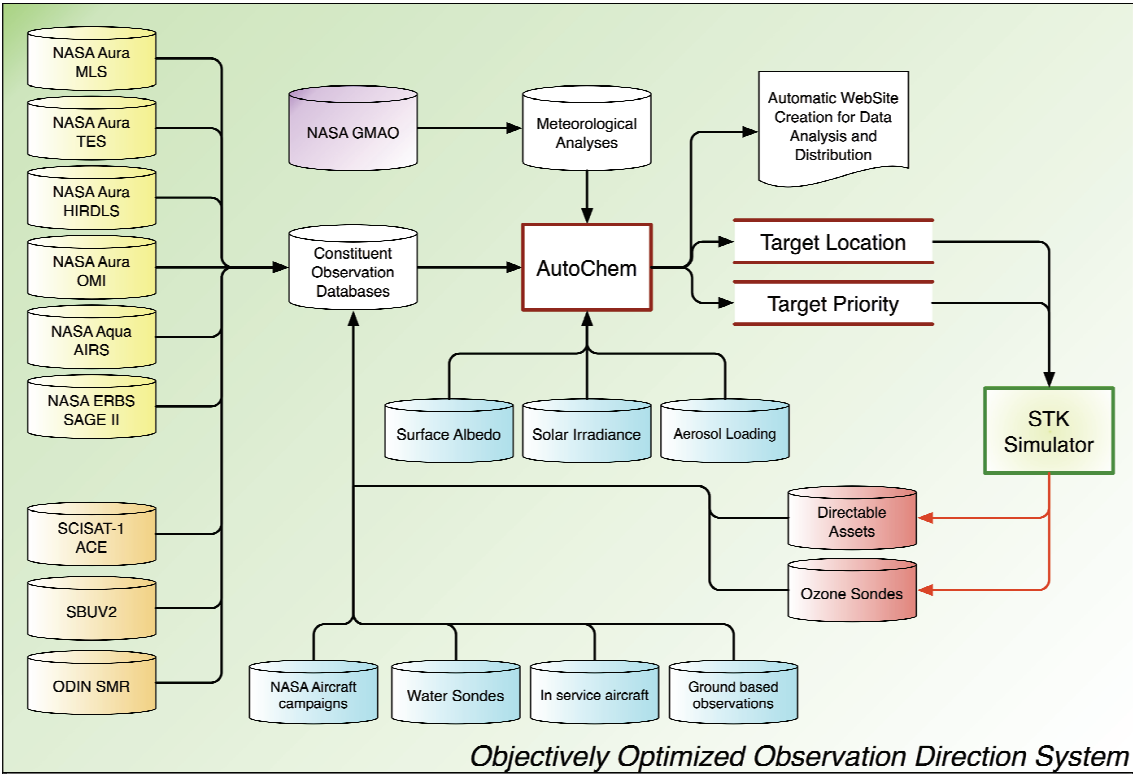


Figure 1. Modeling and Assimilation System Engineering Diagram

AutoChem is NASA release software constituting an automatic code generation, symbolic differentiator, analysis, documentation, and web site creation tool for atmospheric chemical modeling and data assimilation. Figure 1 is a schematic of the system and how the AutoChem plug-in fits into the Sensor Web. AutoChem is a suite of Fortran90 and Matlab programs. The code written by AutoChem is in Fortran90, the documentation is written in LaTeX and then converted to PDF files, the websites are written in HTML and JavaScript.

Given databases of reactions (unimolecular, bimolecular, trimolecular, photolysis, heterogeneous and cosmic ray ionization) AutoChem automatically selects the reactions involved in a user-defined constituent list. AutoChem can use online XML reaction databases maintained by NIST. AutoChem then constructs the time derivatives and symbolically differentiates them to give the Jacobian, and then symbolically differentiates the Jacobian to give the Hessian. All the Fortran90 code and ancillary files for the forward model, its adjoint and a full Kalman filter are automatically generated. The code and documentation generation is extremely fast, typically taking less than a second. When the code generation is complete all that is required is compilation with the supplied makefile. AutoChem is very flexible and has already been used in a wide variety of kinetic applications. It has also been adapted for use within the Earth Science Modeling Framework (ESMF). It could also be used for a variety of other applications such as combustion modeling, interstellar chemistry and modeling of metabolism. AutoChem is also enabled for the machine learning of ODEs to accelerate the solution of the stiff ODEs.

The chemical Kalman filter allows the optimal combination of model simulations and measurements taking into account their respective uncertainties. Consider a model of a physical system represented by operator (generally nonlinear) M , and let vector x with dimension N_x be a set of input parameters for the model. These input parameters are used to predict the state of the system, vector y with dimension N_y :

$$y = M(x) \quad (1)$$

Assume that vector x represents the state of a time-dependent numerical photochemical model, i.e., concentrations of modeled species at model grid points in the atmosphere. In the case of a box model that includes N species, the dimension of vector x would be N . We will now limit the discussion to the case when M is used to predict the state of the system at some future time from past state estimates. Formally, in this case

$$x = x_t, y = x_t + \Delta t \quad (2)$$

$$\text{and } x_t + \Delta t = M(t, x_t) \quad (3)$$

Let vector y_o contain observations of the state. Usually, the dimension of y_o is less than N_y , the dimension of the model space, since not all model species are usually observed. The connection between y_o and y can be established through the so-called observational operator H :

$$y_o = H(y) \quad (4)$$

Combining the above two equations, we get

$$y_o = H(M(x)) \quad (5)$$

We now assume that the probability density functions associated with x and y can be satisfactory approximated by Gaussian functions:

$$\text{PDF}(y) \approx \exp\left(-\frac{(x-x_t)^T C^{-1}(x-x_t)}{2}\right) \quad (6)$$

where \mathbf{x}_t is the true value of \mathbf{x} and \mathbf{C} is the corresponding error covariance matrix. Its diagonal elements are the uncertainties (standard deviations) of x , and the off-diagonal elements represent correlation between uncertainties of different elements of vector \mathbf{x} . The covariance matrix \mathbf{C} is defined as

$$\mathbf{C} = \langle (\mathbf{x} - \mathbf{x}_t)(\mathbf{x} - \mathbf{x}_t)^T \rangle \quad (7)$$

where angle brackets represent averaging over all available realizations of \mathbf{x} .

For most practical applications we need to introduce the linear approximation. In the linear approximation we assume that for small perturbations of the parameter vector $\Delta \mathbf{x}$ the following is approximately true:

$$M(\mathbf{x} + \Delta \mathbf{x}) = M(\mathbf{x}) + L\Delta \mathbf{x} \quad (8)$$

Formally, L is a derivative of M with respect to \mathbf{x} :

$$L = \frac{dM}{d\mathbf{x}} \quad (9)$$

For small variations of \mathbf{x} one can show that the evolution of error covariance matrix \mathbf{C}_t is given by:

$$\mathbf{C}_{t+\Delta t} = L\mathbf{C}_tL^T + \mathbf{Q} \quad (10)$$

Matrix \mathbf{Q} is the error covariance matrix introduced to take into account uncertainties of the model calculations. The Kalman filter equations are

$$\mathbf{x}_t + \Delta t = M(t, \mathbf{x}_t) \quad (11)$$

$$\mathbf{C}_t + \Delta t = L\mathbf{C}_tL^T + \mathbf{Q} \quad (12)$$

$$\hat{\mathbf{x}}_t = \mathbf{x}_t + \mathbf{C}_t\mathbf{H}^T(\mathbf{H}\mathbf{C}_t\mathbf{H}^T + \mathbf{O})^{-1}(\mathbf{y}_o - \mathbf{H}\mathbf{x}_t) \quad (13)$$

$$\hat{\mathbf{C}}_t = \mathbf{C}_t + \mathbf{C}_t\mathbf{H}^T(\mathbf{H}\mathbf{C}_t\mathbf{H}^T + \mathbf{O})^{-1}\mathbf{H}\mathbf{C}_t \quad (14)$$

At the end of each analysis period the model value (\mathbf{x}_t) and the corresponding observation (\mathbf{y}_o) are 'mixed' (see (13)) with weights inversely proportional to their respective errors to produce the analysis, $\hat{\mathbf{x}}_t$. Then the model is integrated forward in time starting from the obtained analysis. Once an observation has been incorporated in the model, the analysis error covariance is updated to reflect this (see (14)). In the absence of observations, the model state is updated using (5), while evolution of the error covariance is obtained from the linearized model equations as in (12).

If no observations are available, then

$$\hat{\mathbf{x}}_t = \mathbf{x}_t \quad (15)$$

$$\text{and } \hat{\mathbf{C}}_t = \mathbf{C}_t \quad (16)$$

The diagonal elements of C_t are our state vector uncertainty providing us with an objective measure of “what we don’t know” and are used to define our targets.

Information Content for Target Priority

A basic postulate of information theory is that information can be treated like a measurable physical quantity, such as density or mass. Consequently we can construct an optimization method for use in observing systems where there is an objective optimization for information content. This allows the best return of information for a given investment in measuring systems. Based on information content and level of uncertainty we can create a dynamic observation control system that adapts what measurements are made, where they are made, and when they are made, in an online fashion to maximize the information content, minimize the uncertainty in characterizing the system’s state vector.

As a dynamic system evolves with time not all of the state variables within the state vector contain equal amounts of information (information content), and not all state variables are known to the same precision. It is therefore clearly desirable that the observations made of a system both contain the maximum information content possible with a given observing platform capability *and* allow the systems state to be characterized with a minimum uncertainty. Information content is a broad term that could be quantified in any number of ways depending on the system or problem being studied. Therefore, although we describe some specific measures of information content for the atmosphere’s chemical system, these measures could easily be substituted with alternative measures that may be more suitable depending on the given objectives of an investigation. Although we describe a specific example here from atmospheric chemistry, the principle is clearly more general. It is suggested that the concepts of information content and uncertainty could be used generically to determine: what should be measured, when and where. Thus providing a cost effective strategy for using resources and minimizing the data storage required in characterizing a system with a given level of precision.

It is valuable to have objective measures of chemical information content, for example, to assist in the best use of our earth observing systems. This is particularly true as many recently launched and soon to be launched remote sensing instruments have high spectral resolution. The high resolution often enables individual spectral lines to be resolved. Consequently we are about to experience a dramatic increase in the total capacity with which to observe the atmosphere. However, this will not be accompanied by the corresponding increase in human resources to process (retrieve) the data and produce constituent profiles. So any assistance in directing our attention will be useful.

Information theory has been widely applied by communication engineers and some of its concepts have found application in psychology and linguistics. The ideas of information content and uncertainty are closely related and their application to atmospheric composition have been rather lacking to date. There are many conceivable measures of chemical information content that could be used. The most appropriate will depend on the purpose of a given investigation. Claude Shannon (Shannon and Weaver, 1949; Shannon, 1997) provided a framework for engineers to approach problems related to transmitting information content through communications channels. In chemical systems we would like to ask what are the key chemical players?

Ranking the Key Chemical Players

To make best use of any observing system it is useful to construct a ranked list of variables/constituents that characterizes their chemical information content. This list is

obviously a function of the question asked as well as time and location. Such an index could be based on answering the question in going from time t to time $t+\Delta t$ what are the key chemical players?

Let vector x represent the state of a time-dependent photochemical box model, i.e., concentrations of all modeled species in a parcel of air at a given instant. In the case of a box model that includes N species, the dimension of vector x would be N . The photochemical box model M describes the transformation of vector x from time t to time $t+\Delta t$. Formally,

$$x_{(t+\Delta t)} = M(t, x_t)$$

(17)

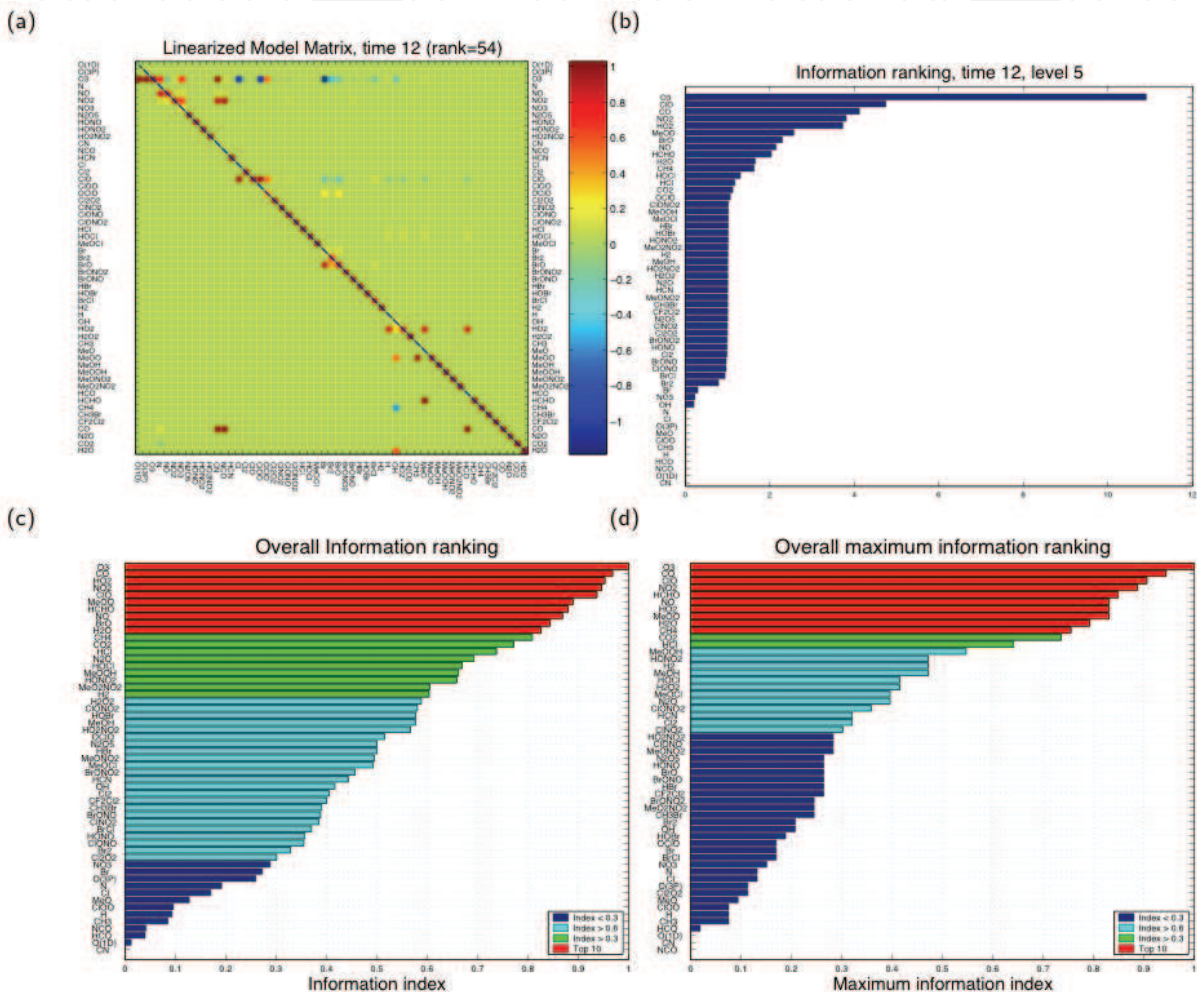


Figure 2 (a) shows the linearized model matrix for a local solar time 12:15 at a potential temperature of 426 K (≈ 18 km) on 30 March 1992 at 38°S . (b) shows the chemical information content index, I_c . (c) shows the information index $TotI_c$. (d) shows the corresponding index based on the maximum value of elements of M . In (c) and (d) the values have been normalized by the maximum value of $TotI_c$ so that the values range from zero to one.

An example of the model matrix is shown in Figure 2 (a). The figure shows the linearized model matrix for a local solar time 12:15 at a potential temperature of 426 K (an altitude of approximately 18 km) on 30 March 1992 at 38°S . The photochemical model was carefully initialized from a Kalman filter chemical data assimilation analyses of measurements made by the Atmospheric Trace Molecule Spectroscopy Experiment (ATMOS) instrument (Atlas-

1). This model simulation simultaneously agreed with ATMOS Atlas-1 observations of O_3 , NO , NO_2 , N_2O_5 , HNO_3 , HO_2NO_2 , HCN , $ClONO_2$, HCl , H_2O , CO , CO_2 , CH_4 , and N_2O to within the observation and model uncertainties. The analyses and its reliability was described in detail in (Lary et al., 2003).

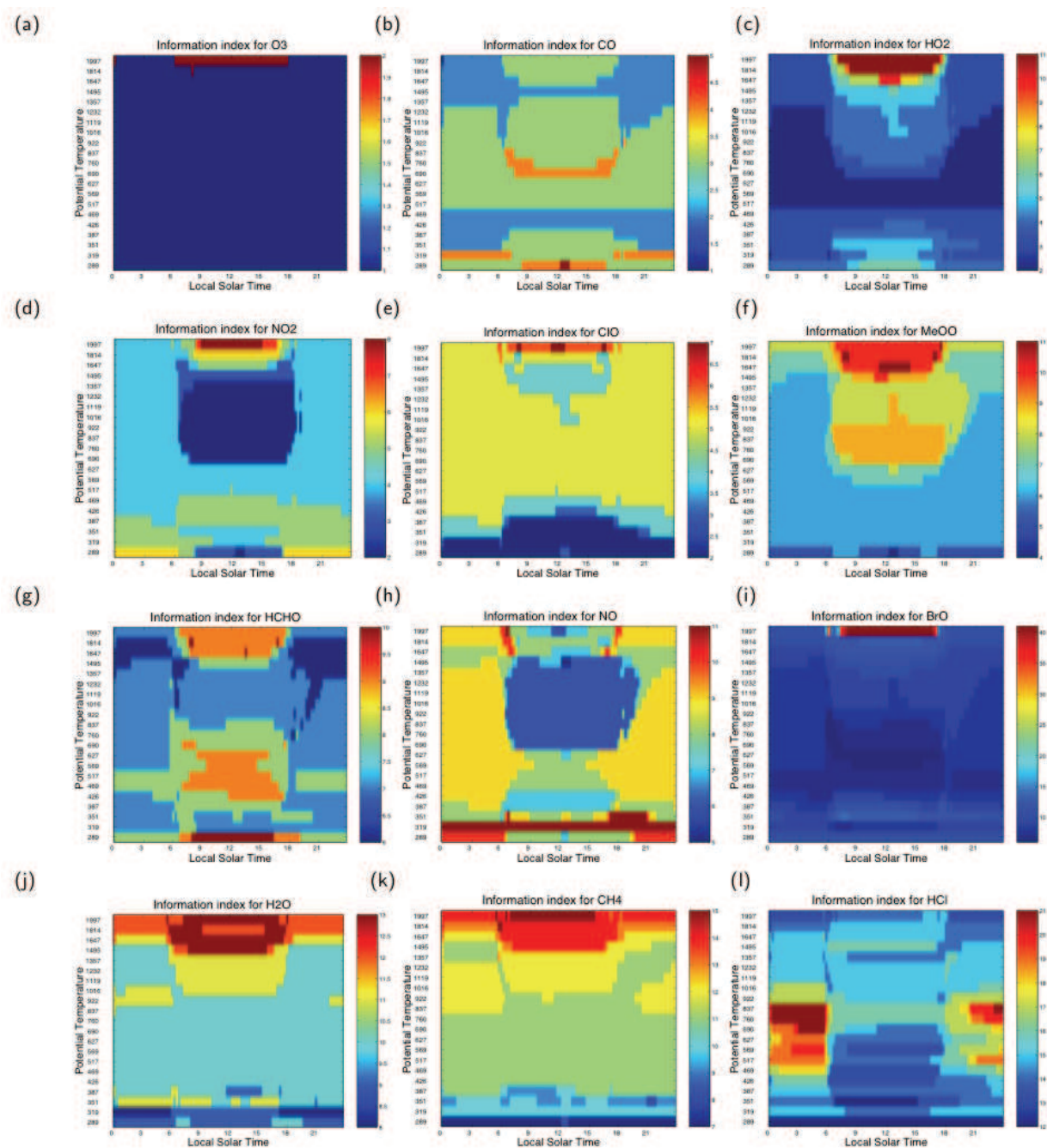


Figure 3. The chemical information content changes with time and location. The panels show some examples of how the information index changes with time (at 15 minute intervals) and location in a vertical profile at 38°S

It can be seen that some rows of M (an example is in Figure 2 (a)) such as the one for O_3 have many more significant elements than others, i.e. highlighting the fact that it is currently a

key player in the dynamically evolving system. We can use this to construct an information content index, I_c .

$$I_c = \sum_i M(i, j) \quad (18)$$

where i and j refer to the rows and columns of M . An example of this information content index, I_c , is shown in Figure 2 (b) corresponding to the model matrix, M , shown in Figure 2 (a). As one would expect O_3 comes out at the top of the list. The order of this list is a rather strong function of time and location.

If we now sum the index I_c at each grid point in a vertical profile and at each time throughout a diurnal cycle we get a composite index of the species role throughout the day.

$$TotI_c = \sum I_c \quad (19)$$

An example of this is shown in Figure 2 (c). The values have been normalized by the maximum value of $TotI_c$ so that the values range from zero to one. One being the greatest information content, zero being the least. For some species their importance is shorter lived (i.e. not so persistent, they are important for just a short while, for these species using a definition based on the maximum value of elements of M is more suitable. An example of this is shown in Figure 2 (d).

The ranking of species provided is sensible, when sorted in order of maximum $TotI_c$ the top 10 species are O_3 , HO_2 , NO_2 , ClO , CH_3OO , $HCHO$, NO , BrO , and H_2O . We see key representatives of carbon, nitrogen, hydrogen, and bromine species reminding us how coupled atmospheric chemistry is. It is interesting that two of the top ten are peroxy radicals, number three is HO_2 and number six is CH_3OO . Figure 3 shows how the chemical information content changes with time and location for ten of the species with the highest information content. The panels show some examples of how the information index changes with time (at 15 minute intervals) and location for a vertical profile at 38°S.

It is interesting to note that both the uncertainty used to define the targets and the information content used to define the priorities can be a strong function of altitude. This emphasizes that real time diagnosis of these metrics is more advantageous than a priori prescription.

A Hybrid Approach

We noted earlier that an autonomous system could have multiple modes of operation. So it is quite conceivable that the metrics used above for target selection and priority based on uncertainty and information content could be used in different ways. For example, during the validation campaign of a new instrument we may want to target regions where we know the state of the system with the highest precision for our validation. In this case we would use targets defined by the minima in our state vector uncertainty. Conversely, during routine operation we would like the observing system to be adaptively reducing the total uncertainty, so would use targets defined on the maxima in our state vector uncertainty.

Taking this one step further, it may be of use to have feature recognition as part of the targeting. For example, we may be focusing on ship tracks, or jet streaks in the weather systems. In this case we can combine the approaches by choosing, for example, the ship tracks where we have the highest information content and uncertainty.

5. Future Directions

As data volumes increase communication bandwidth becomes an increasingly important consideration. This can be made part of the multi-objective optimization. It is conceivable that the distributed sensor web also becomes part of the communications network for the system.

6. Conclusion

We have described how situational awareness can be integrated into an autonomous observing system by incorporating our theoretical and observational knowledge of the system. Metrics of what we do not know (state vector uncertainty) can be used to define what we need to measure and the required mode, time and location of the observations. The mathematical formalism of data assimilation provides us with the state vector uncertainty. Metrics of how important it is to know this information (information content) are used to assign a priority to each observation. A basic postulate of information theory is that information can be treated like a measurable physical quantity, such as density or mass. Consequently we can construct an optimization method for use in observing systems where there is an objective optimization for information content. This allows the best return of information for a given investment in measuring systems. Based on information content and level of uncertainty we can create a dynamic observation control system that adapts what measurements are made, where they are made, and when they are made, in an online fashion to maximize the information content, minimize the uncertainty in characterizing the system's state vector. The metrics are passed in real time to the Sensor Web observation scheduler to implement the observation plan for the next observing cycle.

7. References

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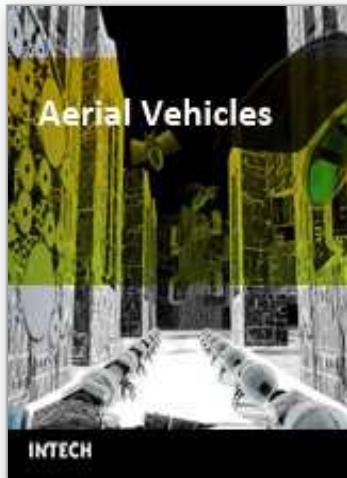
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This book contains 35 chapters written by experts in developing techniques for making aerial vehicles more intelligent, more reliable, more flexible in use, and safer in operation. It will also serve as an inspiration for further improvement of the design and application of aerial vehicles. The advanced techniques and research described here may also be applicable to other high-tech areas such as robotics, avionics, vetronics, and space.

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