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Multi-Platform Atmospheric Sounding Testbed (MAST)

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1. Introduction

NASA's Earth atmospheric science missions study the physical properties of Earth's atmosphere (such as pressure, temperature, wind, humidity, aerosols, and trace gases) by employing a wide range of atmospheric sounding systems. An emerging new paradigm in Earth science missions addresses the interplay between observing systems and Earth system models where observations are assimilated to validate the models and simulated experiments are performed to optimize future observations. The new paradigm provides a bridge between scientists and engineers allowing them to collaboratively explore many questions such as

- What needs to be measured?
- When and where?
- How often and how long?
- How accurately & how precisely?

Multi-platform Atmospheric Sounding Testbed (MAST) is an end-to-end simulation environment at Jet Propulsion Laboratory that enables the new paradigm. The MAST allows scientists to formulate the exploration space parametrically, simulate observing systems realistically, and validate science impacts quantitatively. The parametric formulation of the exploration space addresses interactive design of sampling strategies and measurement quality ranges that can be represented as a sensor-web operation composed of multiple instruments and multiple platforms. The realistic observing system simulation addresses integration of numerical models of sensor-specific measurement physics, sampled atmospheric phenomena, and measurement noise. The quantitative validation of science impact addresses retrieval sensitivity as a function of measurement precision and accuracy and assimilation sensitivity as a function of sampling duration, frequency, and measurement type.

The MAST team is composed of the investigators of three independent research tasks, Observing System Simulation Experiment (OSSE) (Lee et al, 2007), and GEOS-Chem-Adjoint (GCA) (Sandu et al., 2003, Henze et al.,2007)], and Sensor-web Operations Explorer (SOX) (Lee et al., 2008). The OSSE team researches forward modeling and inverse methods for atmospheric sounding system design and validation. The GCA team researches 4D-variational assimilation methods and full-chemistry sensitivity analysis methods for the Goddard Earth Observing System-Chemistry GEOS-Chem) community. Finally the SOX team researches advanced information system technologies for an integrated air-quality

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campaign that involves multiple sensors and multiple platforms. The capabilities developed in the three research tasks are seamlessly integrated to achieve the end-to-end simulation environment by developing three collaborative systems. As shown in Figure 1, scientists explore measurement scenarios primarily interacting with the SOX framework. The SOX system performs the requested exploration by interfacing with the OSSE system and the GSA system for observing system simulation and science impact validation. The heterogeneous computational environments required by the three systems (including operating systems, programming languages, processor types, and file systems) are integrated employing a two-layer network topology (Figure 2) and client-server protocols.

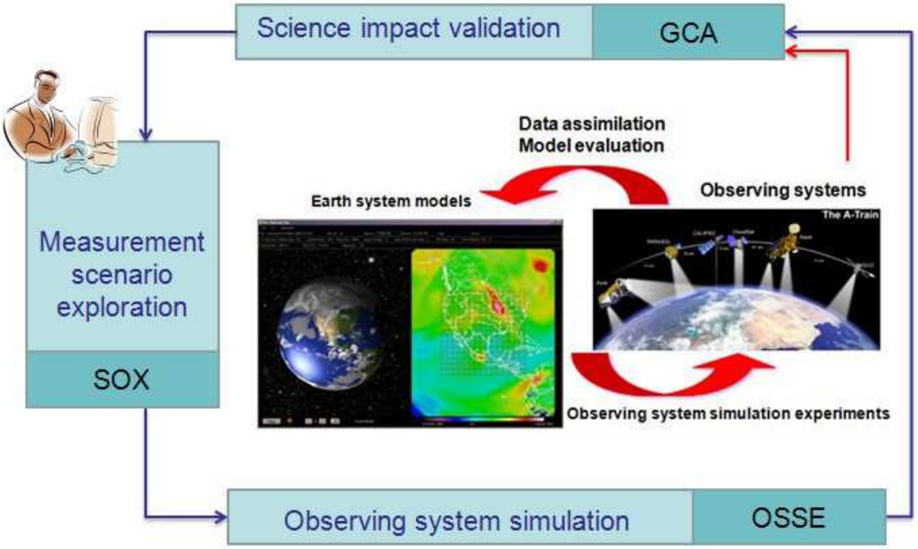

Fig. 1. New Paradigm for Earth Atmospheric Science Mission Concept Design

2. OSSE System

The OSSE System simulates an atmospheric sounder by integrating three types of models, a forward model for the physical properties of the atmosphere, an instrument model for measurement quality, and an inverse method for retrieving the atmospheric state variables. In the OSSE system, a radiative transfer function (Clough et al., 2005) is used as a forward model to simulate atmospheric chemistry missions, which generally exploit the spectral range between unltraviolet (UV) and mid infrared (IR). The forward radiative transfer function computes ideal signal radiance as an input to the instrument system. The instrument model distorts the ideal signal into a noisy measurement data by introducing spatial, spectral, and radiometric distortion properties of the instrument system (Figure 3). The distortion properties of an instrument system are addressed by three generic components, an imager, a spectrometer, and a radiometer. The inverse method retrieves an unknown atmospheric state variable (e.g., vertical profile of Ozone) from the noisy measurement data. The inverse method estimates the state variable employing the Tangent-Linear of the forward model function (i.e., analytic Jacobian) and a priori knowledge.

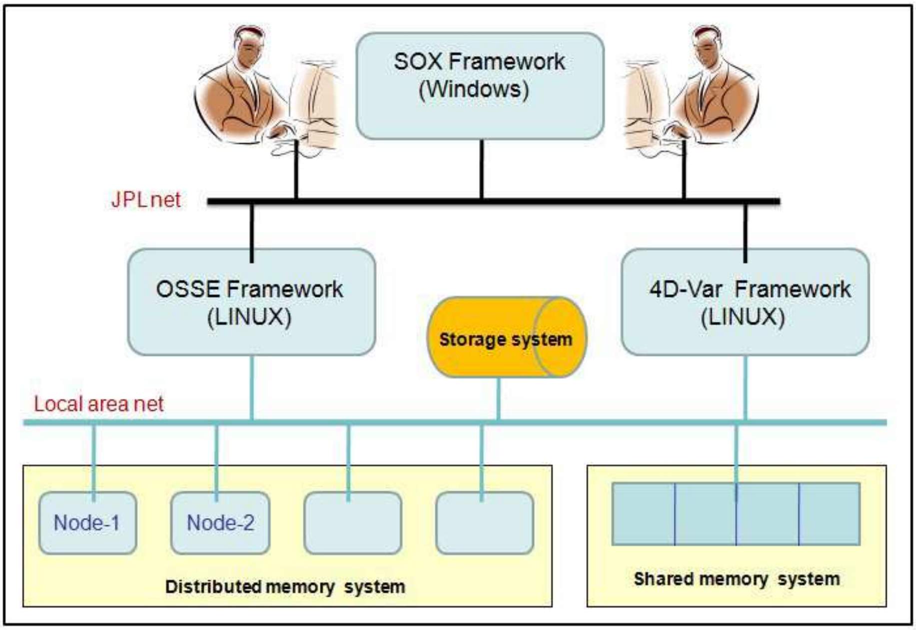

Fig. 2. The MAST System Architecture

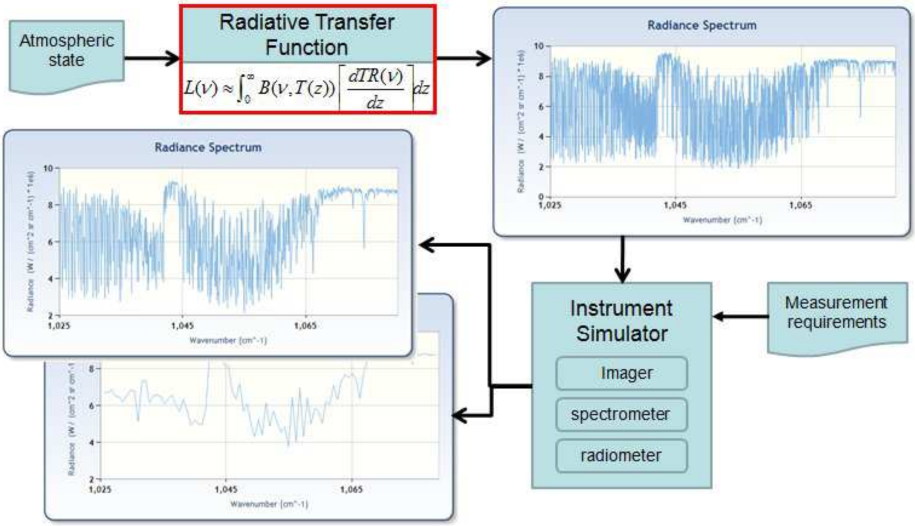

Fig. 3. Ideal Signal Radiance and Measured Radiances

The OSSE process starts with a reference atmospheric state and a measurement requirement as shown in Figure 4. The atmospheric state describes vertical profiles of temperature, humidity, pressure, and trace gas density; and the measurement requirement specifies the range of the instrument's response properties to be explored. The atmospheric state may also include surface emission, surface reflectance and scattering, and cloud contribution when the spectral range includes the visible wavelength range. The forward radiative transfer function transforms the reference atmospheric state into a signal radiance spectrum. The instrument model simulates a set of noisy measurements where each measurement represents the output of a specific instrument response property. The inverse method estimates the atmospheric state variables from the noisy measurements and analyzes the retrieval error sensitivity with respect to instrument response properties.

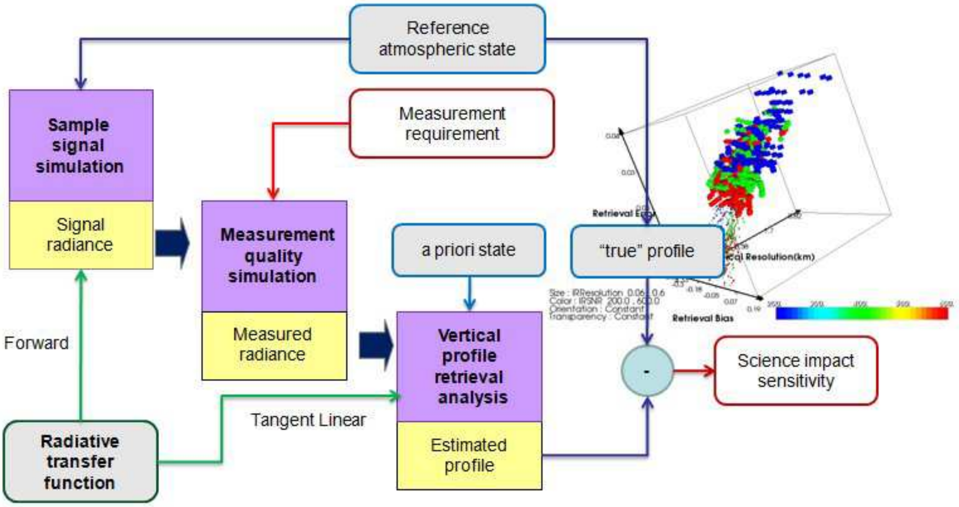

Fig. 4. Observing System Simulation Experiment Framework

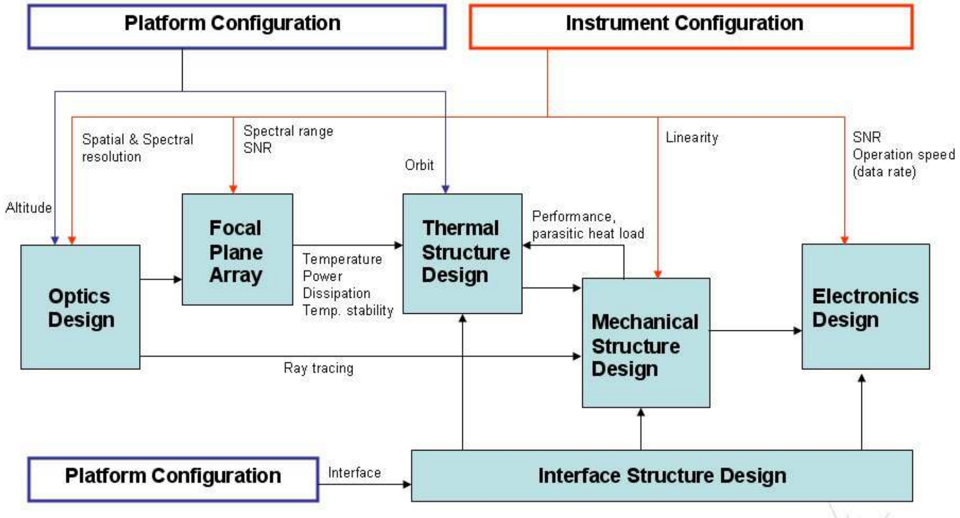

Fig. 5. Relationship between Measurement Requirements and Instrument Subsystems

The retrieval error sensitivity (Rogers, 2000) with respect to the measurement requirements provides a quantitative evaluation of science impact during the conception phase of an instrument enabling scientists to answer "what to measure", "how precisely, and how accurately". In order to establish a bridge between science and engineering, the measurement requirements is formulated as a trade space whose coordinate axes include science impacts and instrument design drivers. Figure 5 illustrates the rationale behind the instrument response properties that are represented in the measurement requirements. The platform altitude and orbit drive optics design and thermal design. The instrument signal-to-noise ratio (SNR) and spectral range requirements drive the focal-array design. The spectral linearity requirement drives mechanical design, which indirectly drives thermal design. The operation speed and date rate drives electronics design.

"Exploration" of an instrument concept refers to population of the trade space defined above where the science objective coordinate is represented with the retrieval error and retrieval error bias for a specific atmospheric component, and the instrument response property coordinate is represented with spatial and spectral resolution, SNR, spectral range, linearity, and operation speed. The evaluation of science impact, taking sampling strategies into consideration, requires a comprehensive coverage of the atmospheric states and global data assimilation.

3. GCA system

The GEOS-Chem-Adjoint (GCA) research team develops a standardized adjoint of the GEOS-Chem for global data assimilation and a full chemistry sensitivity analysis (Sandu et al., 2007). GEOS-Chem is a global 3D model of atmospheric composition driven by assimilated meteorological observations from the Goddard Earth Observing System (GEOS) of the NASA Global Modeling and Assimilation Office. The global data assimilation optimizes the combination of three sources of information: an a priori state, a forward model of physical and chemical processes, and observations of some state variables. The observations in this case refer to the retrieved vertical profile of the trace gas components, generally known as level-2 mission data products.

Adjoint models are powerful tools widely used in meteorology and oceanography for applications such as data assimilation, model tuning, sensitivity analysis, and the determination of singular vectors. The **GCA** System (Figure 6) provides adjoint models for chemistry, advection, convection, and deposition/emission. The adjoint model computes the gradient of a cost function with respect to control variables. Generation of adjoint code may be seen as the special case of differentiation of algorithms in reverse mode, where the dependent function is a scalar. Developing a complete adjoint of global atmospheric models involves rigorous work of constructing and testing adjoints of each of the complex science processes individually, and integrating those adjoints into a consistent adjoint model.

The mathematical formulation for calculating gradients of a model output using the adjoint method can be derived from the equations governing the forward model analytically or discretely. The GCA system employs the discrete adjoints. This provides exact resulting gradients of the numerical cost function for easier validation and allows application of automatic differentiation tools (e.g., Tangent-linear Adjoint Compiler Model (TAMC)). The Kinetic Pre Processor (KPP) module provides very effective sparse matrix computational kernels, which lead to high computational efficiency (Sandu et al., 2005).

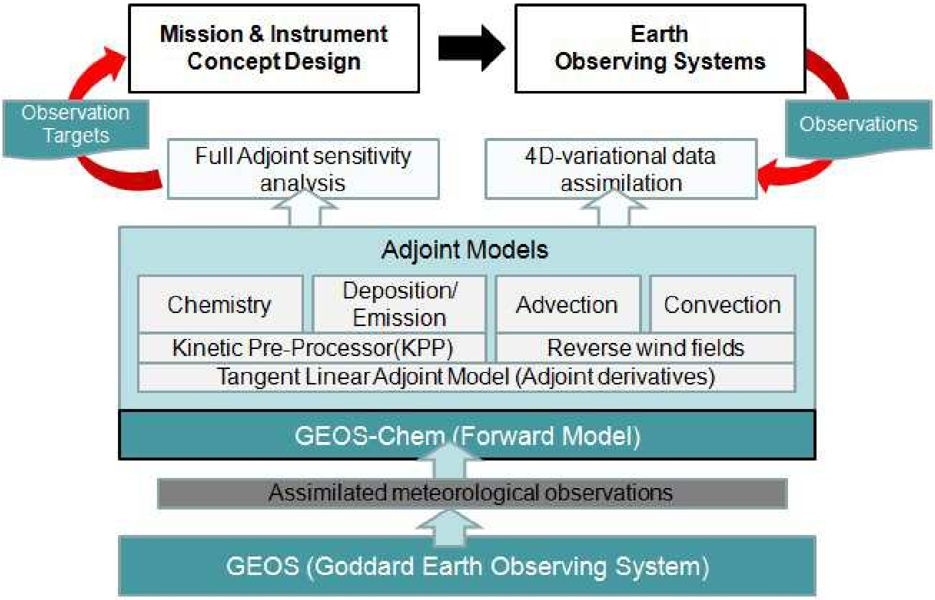

Fig. 6. GEOS-Chem-Adjoint System

The adjoint sensitivity analysis approach is receptor-oriented, and it traces backward in time for the cause of a perturbation in an output variable contrast to the forward sensitivity analysis, which propagates the initial perturbation forward in time. The sensitivity mode allows collaborative observation planning between air-borne and space-borne missions as well as targeted observation planning. Figure 7 illustrates two types of sensitivity analysis results. The top three charts show the sensitivity of an ozone profile over the **Tropospheric Emission Spectrometer** (TES) (Kulawaik et al., 2006) orbit track with respect to surrounding chemical content such as NOx, CO, and Ox. The bottom three charts show the sensitivity of ozone density in New York with respect to past presence of NOx, 7 days earlier, 0.5 day earlier, and the same day. The exploration of the sampling strategies and measurement quality ranges requires a system that integrates the OSSE and GCA capabilities.

4. SOX system

The SOX system enables measurement scenario exploration in collaboration with the OSSE system and the GCA system by developing complex phenomena visualization, community model integration, process streamlining, collaborative design environments, experiment database management, and computational load balancing. For exploring the measurement scenarios on multiple platforms, a set of design tools has been implemented to interactively manipulate and visualize the sampling strategies on geostationary Earth orbit (GEO), low-Earth-orbit (LEO), and air-borne platforms. The measurement scenarios are translated into a list of sample locations and times of observation, and into a list of instrument performance specifications. Each sample list represents a sampling strategy on a specific platform, while each instrument list represents the performance ranges of a single type of instrument. The

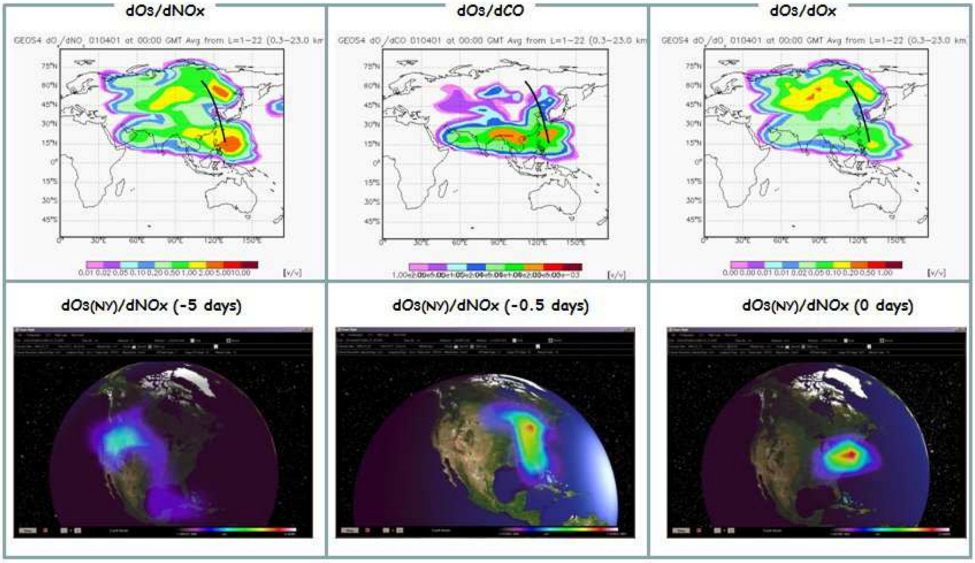

Fig. 7. Sensitivity Mode of GEOS-Chem Adjoint

sample lists can be combined to represent a sampling strategy on multiple platforms, multiple sampling strategies on a single platform, or multiple sampling strategies on multiple platforms. Similarly, the instrument lists can be combined to represent multiple sensors of varying performance ranges.

The SOX system performs the exploration by organizing the end-to-end process into four stand-alone stages, sampling strategy, instrument property, retrieval analysis, and data assimilation as shown in Figure 8. At each stage, the resulting datasets are stored in the respective database along with the request information. A sample list is submitted as an input to the sampling strategy exploration, while an instrument list is submitted as an input to the measurement quality exploration along with a signal-radiance database previously generated. The SOX on-line service facilitates the collaborative design environment among the distributed teams at JPL.

In order to manage the on-line requests, balance computational loads, and integrate community models, the SOX system has implemented four types of services, a request handler, a load distributor, an application dispatcher, and a status monitor (Figure 9). The request handler checks for the new on-line requests in the SOX database and alerts the load distributer with a list of items to be explored. The load distributer divides the list into multiple sub-lists, assigns one sub-list per available processor, and starts the application dispatcher. For example, a sample list of 1024 samples will be divided among 8 processors by composing eight sample lists with 128 samples, one per processor. Within each processor, the application dispatcher performs the exploration task activating an application-specific interface module for input dataset preparation, command script composition, and output dataset conversion. The status monitor checks the run status of the application on each processor and updates SOX database with the completion status so that it can be accessed via the on-line service. The SOX system utilizes MySQL relational database manager for distributed database service and Mono for execution of the .NET framework on Linux platforms. A set of standard services has been also utilized including international information service (IIS), .NET framework, Active server page (ASP), Asynchronous Java script, and active XML (AJAX).

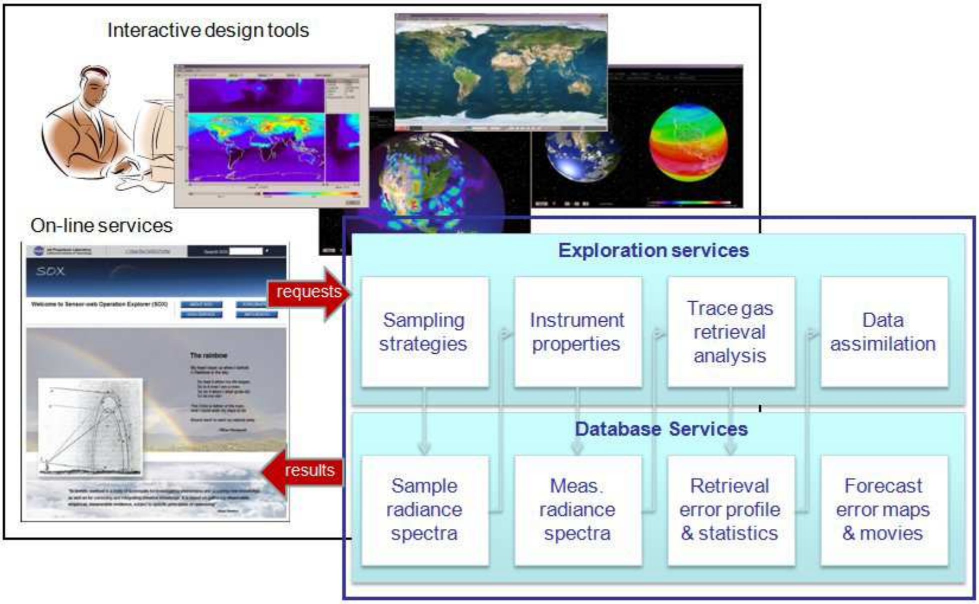

Fig. 8. Design Tools and On-line Services of SOX Framework

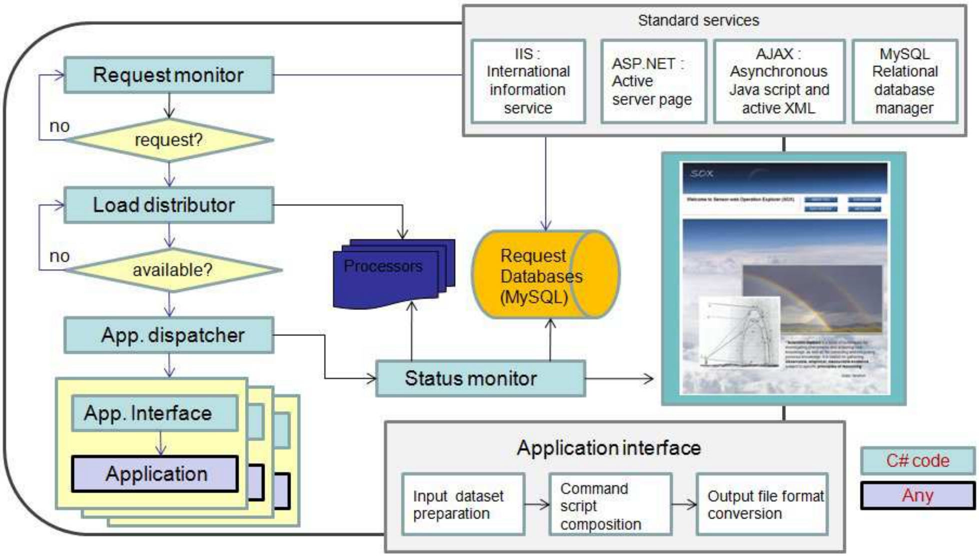

Fig. 9. On-line Service Process Flow

5. Conclusion

The MAST has successfully demonstrated an end-to-end simulation process that can quantitatively evaluate the science impacts of instrument concepts and sampling strategies by integrating the OSSE system, the GCA system, and the SOX system (see Figure 10). The end-to-end process is organized with four stages of (1)observation scenario exploration, (2)measurement quality exploration, (3)measurement quality evaluation, and (4)observation scenario evaluation employing forward models, system performance simulations, and inverse methods. The first two stages enable scientists to formulate and explore measurement requirements while the last two stages enable scientists to validate and optimize them against science objectives and design processes. The four stages are streamlined by infusing a wide range of information technologies including on-line services, distributed database management, and parallel computing.

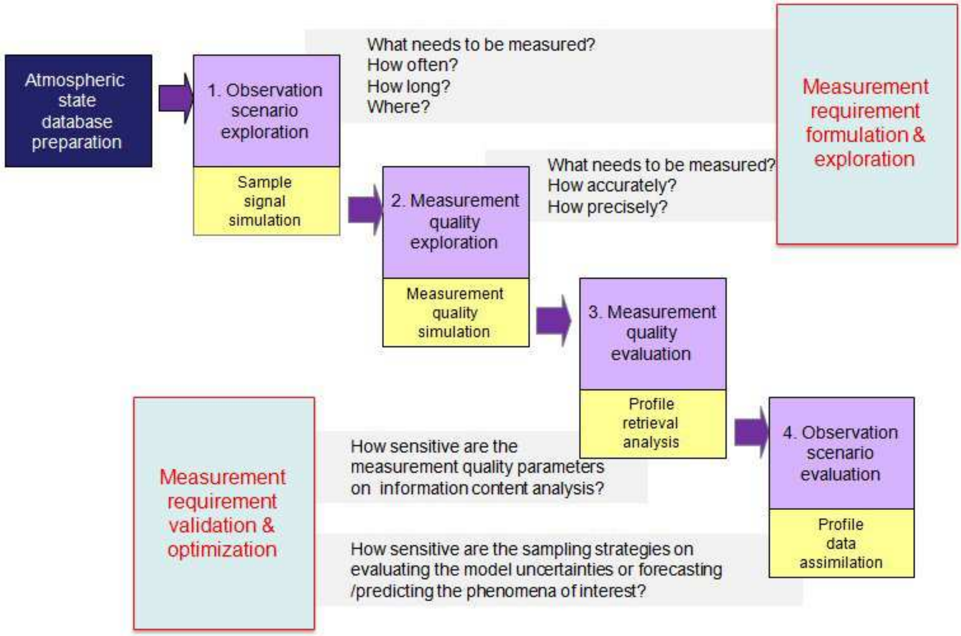

Fig. 10. End-to-end Process of the MAST and Measurement Requirements

The MAST currently supports GEOCAPE (Geostationary Coastal and Air Pollution Events) concept study (lead: Dr. Annmarie Eldering/JPL), part of Tier-2 missions recommended by the NRC decadal survey (http://nasascience.nasa.gov/earth-science/decadal-surveys). The MAST is being utilized to evaluate the advantage of geostationary orbit over low-Earth orbit and to explore the detailed science return from improved measurement capabilities including spectral coverage (IR, UV, IR+UV), spectral resolution, and signal-to-noise ratio. The science impact evaluation is with respect to chemical data assimilation for improved air quality forecasts, pollutant emission monitoring, and regional-scale to intercontinental-scale pollution transport.

The MAST capabilities will be extended to support the CLARREO (Climate Absolute Radiance and Refractivity Observatory) concept study part of Tier-1 missions recommended by the NRC decadal survey, for mission design and virtual observation for climate model uncertainty evaluation. The largest source of uncertainty for climate prediction is climate feedbacks that are coupled radiative response of the hydrological cycle to anthropogenic forcing. The MAST will be employed to evaluate the sensitivity of the climate feedbacks which are manifested at unresolved scales for contemporary climate models and the proposed CLARREO footprint.

The future research areas of interest include a web-based model integration infrastructure that provides a dynamic coupling of global and regional phenomena models, a model-based system engineering process that comprehensively validates and verifies instrument design and mission planning, and a heterogeneous data assimilation method that can rapidly assimilate observations from multiple sensors on multiple platforms. The research described in this paper was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the Advanced Information System Technology (AIST) program under the Earth Science Technology Office (ESTO) of the National Aeronautics and Space Administration (NASA).

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