

NASA/GSFC Contract NASW-99032

Photochemical Phenomenology Model for the New Millennium

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**ABSTRACT**

The "Photochemical Phenomenology Model for the New Millennium" project tackles the issue of reengineering and extension of validated physics-based modeling capabilities ("legacy" computer codes) to application-oriented software for use in science and science-support activities. While the design and architecture layouts are in terms of general particle distributions involved in scattering, impact, and reactive interactions, initial Photochemical Phenomenology Modeling Tool (PPMT) implementations are aimed at construction and evaluation of photochemical transport models with rapid execution for use in remote sensing data analysis activities in distributed systems. Current focus is on the Composite Infrared Spectrometer (CIRS) data acquired during the CASSINI flyby of Jupiter. Overall, the project has stayed on the development track outlined in the Year 1 annual report and most Year 2 goals have been met. The issues that have required the most attention are: implementation of the core photochemistry algorithms; implementation of a functional Java Graphical User Interface; completion of a functional CORBA Component Model framework; and assessment of performance issues. Specific accomplishments and the difficulties encountered are summarized in this report. Work to be carried out in the next year center on: completion of testing of the initial operational implementation; its application to analysis of the CASSINI/CIRS Jovian flyby data; extension of the PPMT to incorporate additional phenomenology algorithms; and delivery of a mature operational implementation.

**1. YEAR 2 ACCOMPLISHMENTS**

The stated goals from the Year 1 annual report are here discussed in terms of the progress made in achieving these goals and what if any technical issues arose in the process of working towards these goals.

**1.1 Application Goals & Tasks**

1.1.1 Complete development of initial implementations (1-D photochemical transport modeling of planetary stratospheres using empirical atmosphere models and the Newton-Raphson algorithm) (1<sup>st</sup> & 2<sup>nd</sup> quarters)

We have succeeded in developing an initial, partially tested, implementation of the 1-D transport modeling code employing the Newton-Raphson algorithm but were unable to meet the target goal of 2<sup>nd</sup> quarter for completion of the initial implementation. The initial version has been tested successfully only for a simplified Chapman ozone chemistry scheme. In addition, the coupling between the PPMT GUI (client code) and the PPMT photochemistry implementation (servers)

was not completed due to delays in development of the PPMT GUI. The principle cause of the delay in completing the GUI was a steeper than expected learning curve for the eXtensible Markup Language (XML) and the Mathematics Markup Language (MathML). Both XML and MathML play substantial roles in the communication of data between the GUI and the photochemistry code. Finally, although we did complete an initial implementation of the 1-D transport code, the initial version has not yet been fully integrated into a compliant CCM framework because of unexpected delays in the availability of an open source Java implementation of the CCM. As a result of unexpected changes in the Information Technology sector some companies that had previously committed to development of a CCM platform changed direction and delayed their CCM implementation. Consequently, we needed to redirect some effort to solidifying our “partial” implementation of the CCM. We still support our initial decision to base the PPMT architecture on a CCM framework and we are excited to be at the forefront of the CCM maturity process (we are now an Influencing member of the Object Management Group (OMG), actively participating in the Finalization Task Force (FTF) for the CCM, and developers of the most advanced CCM implementation known to the CCM FTF).

#### 1.1.2 Validation and testing of initial implementations via detailed analysis of CASSINI/CIRS Jupiter flyby data (e.g., CIRS/JUPITER Far-IR Composition Study data, CIRS/Jupiter Mid-IR Composition Map data) (2<sup>nd</sup> & 3<sup>rd</sup> quarters)

Prior to validation and testing of the PPMT implementation, a number of databases needed to be constructed: reference solar flux spectra, photoabsorption cross sections and branching ratios, identification of chemical species relevant to the Jovian atmosphere and corresponding lists of relevant chemical reactions, and pertinent atmosphere models. Mapping existing data formats to XML and MathML was not trivial and required additional effort than expected. The database files were completely defined by the early part of the 4<sup>th</sup> quarter and rigorous testing of the PPMT implementation commenced soon after. We are still in the process of validating and testing the implementation and expect to complete this task early next quarter.

Regarding analysis of CASSINI/CIRS data, calibrated data sets with required meta-data suitable for scientific analysis are expected to be available no sooner than mid-September, 2001.

#### 1.1.3 Delivery of a completed, validated “official” PPMT Jupiter version to NASA/GSFC Code 693 (end of 2<sup>nd</sup> quarter) [Also: 1.1.6 Delivery of the next “official” PPMT version . . . (end of 4<sup>th</sup> quarter)]

The obstacles described in the previous subsections and described in following sections have resulted in failure to meet this goal. Delivery of a completed, validated, “official” PPMT implementation with “default” database files for Jupiter is expected early next quarter (provided the CASSINI/CIRS Jovian flyby data are released soon).

#### 1.1.4 Construction (i.e., re-coding of legacy algorithms) and implementation of photon transport algorithms . . . (3<sup>rd</sup> & 4<sup>th</sup> quarters)

This was an obviously ambitious goal. After delivery of the Year 1 annual report, we recognized that elementary particle transport phenomenology went well beyond the role(s) captured in the PPMT architecture. It was decided that it would be beneficial not only to the PPMT project but to the aeronomy community at large if we “spun off” the implementation of elementary particle transport under a separate AISR proposal. We subsequently submitted a proposal and were awarded a contract several months ago. Therefore, implementation of photon (as well as electron and possibly hydrogen and proton) transport has begun under the follow-on contract

entitled “Transport Phenomenology Modeling Tool” (TPMT, Dr. Douglas Strickland, P.I.). We hope photon transport algorithms will be available for use in the PPMT within six months; however, design and architecture layout modifications or extensions may be required.

#### 1.1.5 Begin extension of photochemical modeling methods to the thermospheric/ionospheric region with addition of methods for calculating corresponding emissions at UV and visible wavelengths (3<sup>rd</sup> & 4<sup>th</sup> quarters)

This task cannot be commenced until a validated PPMT implementation is completed. This task in particular entails close coupled between the PPMT and TPMT software, hence potential design and architecture conflicts (*e.g.*, those stemming from performance issues) need to be resolved quickly. We expect to begin work on this task in the 2<sup>nd</sup> quarter of Year 3.

### **1.2 Software Development Goals & Tasks**

#### 1.2.1 Complete implementation of Graphical User Interface (GUI) for the PPMT that satisfies the Use Cases needed to support detailed analysis of the CASSINI/CIRS Jupiter flyby data sets

We succeeded in developing a functional Graphical User Interface for the PPMT that satisfies most (but not all) of the use cases associated with analysis of the CASSINI/CIRS Jupiter flyby data sets. Specifically, the PPMT GUI currently supports a client/server distributed processing scenario using validated XML (and MathML) as the means of data transport between the Java GUI and the PPMT servers. (There are many potential servers depending on how a user deploys the PPMT system on one or more computer hosts). The GUI allows users to specify: the model atmosphere, the external solar flux spectrum (and make adjustments), the chemical species involved (transient, transported, bath, and end-product — these can be selected or deleted but currently can not added except through editing of XML configuration files), the reaction scheme and associated reaction rate coefficients (allowed reactions can be constructed using the identified species but reaction rates are currently limited to certain functional forms), and eddy mixing profile layers. The GUI reads a “default” Jupiter configuration XML file from a remote server and then allows the user to modify specific contents of the configuration in a graphical manner. Plotting capabilities have also been added via the freeware Java plotting tool from the Berkeley Ptolemy project. Use cases that are not currently satisfied by the GUI include: addition of new species (and all required information such as cross sections, branching ratios, *etc*), specification of general expressions for reaction rates and eddy mixing coefficients, saving and loading of local configuration files, and support for construction of “custom” model atmospheres (*e.g.*, for use in extra-solar planet modeling).

We have decided to implement a relatively simplistic equation editor in Java that will allow a user to specify one or more mathematical expressions for reaction rate coefficients, eddy mixing coefficients, and any other future use cases that require specification of mathematical expressions. The math equation editor will generate MathML context and will be limited to only those functions and operations that are deemed necessary for the PPMT. Unfortunately, there are no robust, freeware implementations of a Java equation editor that we can reuse. There are, however, several free Java equation editors that are available that are extensible and will serve as the basis for the PPMT equation editor.

1.2.2 Incorporate type definitions and use of the CORBA Persistent State Service (PSS) to enable archiving of phenomenology inputs as well as post-processing outputs

We have just recently incorporated the PSS into our CCM implementation so we will be able to take advantage of the PSS once the PPMT is ported to our CCM implementation (expected in the next quarter).

1.2.3 Incorporate use of XML to maintain disconnect between the PPMT GUI and the PPMT server and for standardized configuration of CCM component "Homes"

This goal has been reached.

1.2.4 Establish test suite for automated component and integration tests of the PPMT

This goal has been reached although we need to continue to maintain the test suite as we add additional functionality to the PPMT.

1.2.5 Develop web pages for deployment platform that provides access to GUI, PPMT servers, compiled middleware products (ORB and CORBA Services), Application Programmers Interface (API), and documentation

We have not yet created a web site for accessing the PPMT. This task will be completed once the PPMT "official" version is ready for release.

1.2.6 Port PPMT to open source CCM implementation (when available)

As discussed in section 1.1.1, there are no robust CCM implementations available. Consequently, we have developed our own robust CCM implementation that will serve as the framework of the PPMT. We expect to port the PPMT to our CCM implementation in the early part of the next quarter.

1.2.7 Port PPMT to Linux/Intel platform

This goal has not yet been reached. We will port the PPMT before we release it (expected next quarter).

1.2.8 Implement security measures in the PPMT by incorporating use of the CORBA Security Service and the CORBA Firewall specification. These security measures are needed primarily by users and developers that work within a network that is protected by a firewall or IP packet filter.

This goal has not been reached. However, we will be adding security features to our CCM implementation (as defined in the CCM specification) and these features will be available to the PPMT once we port it to the CCM framework.

## 2. YEAR 3 GOALS & TASKS

### 2.1 Application Goals & Tasks

- Completion of testing and optimization of the initial implementation for 1-D photochemical transport modeling of planetary stratospheres using empirical atmosphere models and the Newton-Raphson algorithm (1<sup>st</sup> quarter)
- Delivery of a completed, validated “official” PPMT Jupiter version to NASA/GSFC Code 693 (1<sup>st</sup> quarter)
- Validation and testing of initial implementations via detailed analysis of CASSINI/CIRS Jupiter flyby data (*e.g.*, CIRS/Jupiter Mid-IR Composition Map data) (1<sup>st</sup> & 2<sup>nd</sup> quarters)
- Initial expansion of recognized phenomenology for condensation loss processes (3<sup>rd</sup> & 4<sup>th</sup> quarters)
- Begin extension of photochemical modeling methods to thermospheric/ionospheric region and addition of methods for calculating corresponding emissions at UV and visible wavelengths (3<sup>rd</sup> & 4<sup>th</sup> quarters)
- Delivery of the next “official” PPMT version including basic photon transport algorithms (MUV stratospheric photodissociation and IR molecular band spectral radiances) to NASA/GSFC Code 693 (end of 4<sup>th</sup> quarter)

### 2.2 Software Development Goals & Tasks

- Update and maintain test suite for automated component and integration tests of the PPMT (all quarters)
- Implement a simple MathML equation editor and MathML evaluator (1<sup>st</sup> quarter)
- Port PPMT to our open source CCM implementation (1<sup>st</sup> quarter)
- Test PPMT on Linux and SGI platforms (1<sup>st</sup> quarter)
- Add additional plotting capabilities to the GUI (1<sup>st</sup> quarter)
- Add post-processing capabilities to the GUI (2<sup>nd</sup> – 4<sup>th</sup> quarters)
- Continue work on CCM implementation to enhance deployment and configuration and to add security features (1<sup>st</sup> & 2<sup>nd</sup> quarters)

### **3. ANTICIPATED PPMT-BASED STUDIES & SOME LESSONS LEARNED**

We are becoming especially eager to carry out analysis of the CASSINI/CIRS Jovian flyby data, now that an operational implementation of the PPMT is nearing completion. The various obstacles that have arisen, described in previous reports and in this document, demonstrate the genuine research aspect of this project – the risks and challenges have at times been very frustrating – but now the advances accomplished on the software front can be utilized in scientific studies. One study of considerable intrinsic interest, to be carried out with Dr. Paul Romani (NASA/GSFC), is investigation of the chemical pathways responsible for the ubiquitous presence of benzene in the Jupiter atmosphere, seen in ISO and CASSINI/CIRS data; the initial study in this direction will likely focus on methylacetylene and allene abundances and chemistry. Another anticipated study involves utilization of the latitudinal distributions of observed hydrocarbons (*e.g.*, C<sub>2</sub>H<sub>2</sub> and C<sub>2</sub>H<sub>6</sub>) to infer the distributions of unobserved species and the magnitudes of vertical *vs* horizontal dynamical mixing responsible for these distributions. Phosphine chemistry is also of interest, but investigation of the distribution of phosphine compounds in the Jovian atmosphere will require the extension of PPMT to incorporate condensation-related processes. In anticipation of the CASSINI tour of the Saturnian system, PPMT will be applied in predictive studies of photochemistry on Saturn and Titan, for which relevant reference databases will need to be constructed; the design and architecture, GUI, and computational capabilities of the PPMT are of particular advantage in this sort of study, allowing rapid and thorough comparative analysis of photochemical schemes proposed by competing groups. From a scientific viewpoint, this will be a very active, exciting year.

#### **3.1 *The impact of architectural design decisions and distributed computing on performance***

As discussed in previous quarterly reports in the first year, most modern software processes or methodologies (especially the Unified Process subscribed to by us) promote an iterative process that attempts to minimize long-term risk and maximize robust designs and implementation productivity. We have attempted to follow the recommendations of the Unified Process as deemed relevant to the PPMT project and we have been fairly successful to date. Several issues that we have encountered with respect to the software development process deserve to be mentioned. Specifically, in following an iterative scheme for developing an architecture, implementing architectural designs, and testing implementations we failed in two important ways:

1. Assessing the impact of chosen algorithms on a domain model
2. Consideration of the overall scalability of our design and implementation

In the first case, through the typical cycle of domain modeling, analysis and design, implementation, and testing, it is important during the analysis and design phases of a development cycle to ensure that the requirements of an algorithm can be satisfied by a corresponding domain model. In other words, the implementation of a design must fit within the constraints defined by a domain model; since a domain model defines the types or classes of objects in a system, the behavior of the objects, and the interaction between the objects, an algorithm is constrained to use the constructs (*i.e.* classes, packages, attributes, operations, associations, *etc*) defined by the domain model (except when dealing with the specifics of a particular behavior of an object). Whenever an algorithm does not “fit” within the constraints of the domain model then the domain model must be improved or generalized to accommodate the algorithm (this may appear backwards but of what use is a domain model without some form of software to justify it?). To illustrate the issue, we encountered a problem with our domain model because it did not properly support the computation of Jacobian elements that are required by the Newton-Raphson algorithm. The problem arose because the Jacobian elements contain

contributions from both photodissociation and chemical reactions, yet there was no “placeholder” in the domain model for these Jacobian elements (they were assumed to be local “behavior” and therefore not important from a domain perspective). The Jacobian problem was temporarily resolved but needs to be revisited from a domain perspective to ensure that the domain model does not expose what are otherwise artifacts of a particular algorithm.

Our initial test framework for the PPMT implementation was based on a simplified Chapman ozone chemistry that included about six chemical species involved in about six chemical reactions with an artificial atmosphere model that contained ten altitude points. The performance of the PPMT code when tested in this case was relatively quick and did not indicate that our decisions to use Java and CORBA were faulty. After our initial tests we produced detailed input configuration files that consist of many more chemical species and reactions and atmosphere models containing up to 200 altitude points. When we executed the PPMT code with the more realistic inputs, we were surprised to find that our algorithms did not scale well and that performance was significantly degraded. After some investigation we determined that a false assumption about the performance of certain key parts of the PPMT architecture (namely, the access of remote, *i.e.* CORBA, particle distribution “fields” via an iterator approach) had resulted in poor performance and lack of scalability. Fortunately, we had anticipated (but, unfortunately, not tested) the possibility of performance problems in accessing remote particle distribution fields and had designed the field iterator to provide alternative behavior that enhances performance. We are presently making improvements to the PPMT software to utilize the performance-oriented behavior of the design and we are achieving significant improvements in performance as a result.

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