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LAWRENCE LIVERMORE NATIONAL LABORATORY

High Performance Parallel Processing (HPPP) Global Atmospheric Chemisty Models on Massively Parallel Computers Final Report CRADA No. TC-0824-94-D

D. Rotman, S. Baughcum

February 23, 2018

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DISCLAIMER

High Performance Parallel Processing (HPPP) Global Atmospheric Chemistry Models on Massively Parallel Computers

Final Report
CRADA No. TC-0824-94-D

Date: October 16, 1998 Revision: 3

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL) and The Boeing Company.

University of California
Lawrence Livermore National Laboratory
PO Box 808, L-795
Livermore, CA 94550

The Boeing Company
Atmospheric Physics Group
Physics Organization
PO Box 3707, MS 6H-FC
Seattle, WA 98124

B. Project Scope

This project was a multi-partner CRADA with nine industrial partners. During this portion of the CRADA; the Global Radiation, Chemical and Dynamical Interactions group at LLNL worked with the Atmospheric Chemistry Group of Boeing. LLNL took responsibility for the general model development and implementation on the massively parallel computer while Boeing took the lead in establishing the primary emission scenarios. Both parties analyzed and attempted to understand and evaluate the model results.

This project was to be done in three phases, each lasting approximately a year. The first phase entailed the development and implementation of the computer code and any needed physics specific to the aircraft emission problem. This was to include the complete three-dimensional chemical transport model of the troposphere and stratosphere and the needed input and chemistry files. Phase two was to establish the background atmosphere and investigated any climate effects from an initial set of aircraft scenarios. Phase three used the results of phase two to obtain a new and updated aircraft design fleet and emissions and understand the effects of that improved aircraft.

The main deliverable of this project was to be a three dimensional chemical transport model implemented on the T3D for use in the analysis of the Boeing subsonic and supersonic aircraft fleet. That milestone was never met during the extent of the project. Computer issues were partly the cause of not attaining this goal. The T3D was a small memory (per node) machine, thus portions of the model needed to be re-done to adjust to this constraint. In addition, computing speed we attained from the T3D was lower than hoped making full implementation and testing of the chemistry difficult. However, under estimation of the effort to implement the complete model and linkages to a climate model were the primary reasons all milestones were not completed.

However, while the complete chemistry model was not delivered under this project, progress towards understanding possible ozone effects from aircraft was accomplished through the use of a tracer transport model. Our effort was done in three phases, each lasting approximately a year. The first phase included the development and implementation of the tracer transport code needed physics specific to the aircraft emission problem. Phase two worked on validating the tracer model against measurements and against simulations from other models (i.e., for idealized tracer tests). Phase three used knowledge gained in phase two and tracer studies of emission distributions to estimate impact on global ozone from aircraft.

Phase 1
LLNL and Boeing developed and implemented a three-dimensional tracer transport model of the troposphere and stratosphere on the T3D parallel computer. This model incorporated an upstream biased advective scheme for accurate modeling of sharp gradients. Additional physics, such as land emissions and convection, were added. The primary task was the implementation of the model and Boeing derived emission scenarios on the T3D.

Phase 2
The transport model was validated through comparison to observations for atmospheric species with long lifetimes and known loss mechanisms (i.e., N_2O and CO_2). In addition, model results of standard/idealized transport test cases were compared to other model results (i.e., "NO_y-like" aircraft exhaust, transport of sine functions, etc. etc.). These calculations were done using the T3D.

Phase 3
Tracers that mimic the emissions of stratospheric aircraft were simulated using the 3-D model. Multiple simulations were accomplished, each representing a different scenario of aircraft flight patterns. Knowing the background ozone distribution, these emission simulations were then used to assess possible ozone impacts.

The main deliverable of this project was the three dimensional tracer transport model implemented on the T3D for use in the analysis of the Boeing subsonic and supersonic aircraft fleet. The parties provided reports to assess progress and a final report at the conclusion of the project. Implementation and model details were also published as a book chapter.

C. Technical

The project between Boeing and LLNL was to implement a 3-D chemical transport model interactively linked to a 3-D global climate model on a massively parallel T3D computer. It had the following milestones,

<u>LLNL Milestones</u>

- task Description	<u>Month</u>
- implement model on T3D	0- 6
- add land surface interactions	6-12
- link chemical transport model to climate model	6-12
- initial calculations to establish background atmosphere	12-18
- while linked to GCM, examine climactic effects of aircraft emissions	18-24
- perform added complete analysis of ozone and climatic effects	24-36

<u>Boeing Milestones:</u>

- develop needed chemistry set and parameters	0- 6
- provide all subsonic and supersonic emissions scenarios	6-12
- continue the development of chemistry packages	6-12
- assist in the evaluation of the ozone perturbation calculations	12-18
- assist in the evaluation of the climatic effects of emissions from aircraft	18-24
- provide updated and improved emission scenarios	24-36

These milestones were not completed. However, in attempting these milestones, accomplishments were made. This project between Boeing and LLNL implemented a 3-D tracer transport model on a massively parallel T3D computer. Accurate and efficient algorithms for advection were implemented on the T3D. These algorithms provided the interactions between the aircraft emissions and atmosphere parameters such as temperature, pressure and meteorological data.

D. Expected Economic Impact

The completion of this project guided the industry in developing an environmental analysis of products through better understanding of the possible environmental consequences.

E. Partner Contribution

As part of this project, Boeing provided the emission scenario for testing and establishment of a "standard" distribution of engine exhausts. In addition, Boeing provided possible flight scenarios for possible future fleets. The parties provided reports to assess progress and a final report at the conclusion of the project.

F. Documents/Reference List

a) Subject Inventions disclosed by LLNL: None

Subject Inventions disclosed by Participant: None

b) Licensing status:

CRADA Article XIV Reporting Inventions

The Parties agree to disclose to each other each and every Subject Invention that may be patentable or otherwise protectable under the Patent Act. The Parties acknowledge that The Regents will disclose Subject Inventions to the DOE within two (2) months after the inventor first discloses the invention in writing to the person(s) responsible for patent matters of the disclosing Party.

These disclosures should be in such detail as to be capable of enabling one skilled in the art to make and use the invention under 35 USC 112. The disclosure shall also identify any known, actual, or potential statutory bars (i.e., printed publications describing the invention or a public use or on sale of the invention in this country). The Parties further agree to disclose to each other any subsequent known actual or potential statutory bar that occurs for an invention disclosed but for which a patent application has not been filed. All invention disclosures shall be marked as confidential under 35 USC 205.

<u>Book Chapter:</u>
Title of Book: Industrial Strength Parallel Computing: Programming Massively Parallel Processing Systems
Title of Chapter: Global Atmospheric Chemistry and Aircraft Impacts
Publisher: Morgan Kaufmann Publishers
Authors: Douglas A. Rotman, John R. Tannahill and Steven L. Baughcum

G. Acknowledgment

Participant's signature of the final report indicates the following:

1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that:
   a) all reports either completed or in process are listed;
   b) all subject inventions attributable to the project have been disclosed or are included on a list attached to this report; and
   c) appropriate measures have been taken to protect intellectual property attributable to this project.
4) The Participant certifies that if tangible personal property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.

[signature] 4/12/99
Steve Baughcum — Date
Boeing Company

[signature] 5/4/99
Douglas Rotman — Date
Lawrence Livermore National Laboratory

Attachment I - Final Abstract
Attachment II - Project Accomplishments Summary
Attachment III - Final Quarterly Report

High Performance Parallel Processing (HPPP) Global Atmospheric Chemistry Models on Massively Parallel Computers

Final Abstract
Attachment I
CRADA No. TC-0824-94-D

Date: October 16, 1998 Revision: 1

This project was a multi-partner CRADA with nine industrial partners. During this portion of the CRADA, the Global Radiation, Chemical and Dynamical Interactions group at LLNL worked with the Atmospheric Chemistry Group of Boeing. The objective of this project was to improve the understanding of the atmospheric chemical and climatic impacts, particularly on ozone in the troposphere and stratosphere, that may occur from future projected fleets of supersonic aircraft. This effort involved a close collaboration between LLNL and The Boeing Company. The primary tool used in these atmospheric chemistry transport studies was the LLNL IMPACT three-dimensional tracer-transport model of the troposphere and stratosphere. A significant fraction of this project was aimed at further development, testing, and validation of this model on the Cray T3D parallel computer to meet the needs for aircraft assessment. LLNL took responsibility for the general model development and implementation on the massively parallel computer while Boeing took the lead in establishing the primary emission chemistry and scenarios. Both parties analyzed and attempted to understand and evaluate the model results.

High Performance Parallel Processing (HPPP) Global Atmospheric Chemistry Models on Massively Parallel Computers

Project Accomplishments Summary (Attachment II)
CRADA No. TC-0824-94-D

Date: October 16, 1998 Revision: 3

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL) and The Boeing Company.

University of California
Lawrence Livermore National Laboratory
PO Box 808, L-795
Livermore, CA 94550

The Boeing Company
Atmospheric Physics Group
Physics Organization
PO Box 3707, MS 6H-FC
Seattle, WA 98124

B. Background

Atmospheric chemistry and constituent transport are important aspects in the understanding of climate and climate change. Chemical processes influence the distributions of many of the greenhouse gases and the aerosols that determine the radiative forcing on the climate. Many of the greenhouse gases undergo atmospheric chemical and photochemical transformations that alter the natural balance of other important atmospheric constituents. For example, the resulting effects on ozone in both the troposphere and stratosphere are of serious concern (WMO, 1989, 1991, 1994). The strong relationship between methane, carbon monoxide and the hydroxyl radical is also of concern because of the importance of the hydroxyl radical in determining the oxidizing capacity of the atmosphere. Such chemical interactions also influence the time dependent predictability of global climate change on scales extending from regional to global.

Key elements in atmospheric chemistry models are the boundary conditions and emissions. Carbon dioxide, methane, carbon monoxide, nitrous oxide, chlorofluorocarbons, bromine compounds, sulfur dioxides and a host of other compounds and aerosols are emitted by human activities such as power generation, chemical production, fire extinguishing, mining as well as activities such as biomass burning. All these chemical compounds have potential impacts on the environment and climate.

Of these activities, our work relates directly to the emission of oxides of nitrogen into the stratosphere from a fleet of supersonic aircraft. Some of the questions that need to be addressed by chemical-transport modeling include:

-What are the important chemical processes and reaction channels, both in the gas, aerosol, and aqueous phase that can influence the distribution of important chemical species? What is their dependence on atmospheric conditions?

-What is the potential impact of changing ozone concentrations on climate, and vice versa? What is the effect of changing climatic (or chemical conditions) on the aerosol-initiated stratospheric ozone depletion in the Arctic and Antarctic?

-What impact does the close coupling between tropospheric CH_4, CO, OH, NO_x, and O_3 have on projections of climate change, and how might the distributions of these species change? What is the role of anthropogenic emissions on such effects?

-How might the exchange of water vapor, and other gases, between the troposphere and stratosphere change in a changing climate? What effect do changes in stratospheric water vapor have on stratospheric cloud occurrences?

Of key importance is the possibility of depletion of stratospheric ozone caused by possible fleets of supersonic aircraft. The ozone abundance in the stratosphere is important for three primary reasons. First, ozone is one of the most important species in the atmosphere regulating the amount of ultraviolet radiation reaching the Earth surface. As stratospheric ozone is depleted, more and more radiation reaches the surface, and it is believed this increases the possibility of additional cases of skin cancer in humans. Second, too much ultraviolet radiation reaching the Earth's oceans can have negative impacts on the production of oceanic plankton, which plays a key role in the marine food chains. And thirdly, ozone is one of many greenhouse gases that plays a role in the overall radiative balance of the atmosphere. Human alterations in the radiative balance may affect climate.

C. Description

Overview/Statement of problem

Supersonic aircraft would dramatically shorten the flight times of intercontinental air traffic if they could be shown to be economically and environmentally feasible. For example, flight times for long over-water flights could be reduced by a factor of

2-3. Supersonic aircraft would fly in the stratosphere (e.g., flight altitudes of 18-20 kilometers for a Mach 2.4 aircraft). These flight altitudes are near the maximum of stratospheric ozone concentrations and concerns have been raised that emissions of oxides of nitrogen and water vapor from supersonic aircraft could destroy ozone.

Since a ground rule for the development of a supersonic commercial transport is that it must not cause any significant ozone impact, it is important to be able to accurately assess the effect of projected future fleets. These assessments could then help define the technical requirements for such aircraft (e.g., the required NOx emission levels and thus combustor requirements). Experiments to analyze this impact are difficult to envision since the aircraft have not even been designed. Thus, numerical atmospheric chemistry models will play a key role in this analysis. However, these numerical models are extremely large and require huge amounts of computer time to complete meaningful simulations.

Project Objectives

The objective of this project is to improve the understanding of the atmospheric chemical and climatic impacts, particularly on ozone in the troposphere and stratosphere, that may occur from future projected fleets of supersonic aircraft. This effort involved a close collaboration between LLNL and The Boeing Company. The primary tool to be used in these atmospheric chemistry transport studies was the LLNL IMPACT three-dimensional chemical-transport model of the troposphere and stratosphere. A significant fraction of this project was aimed at further development, testing, and validation of this model on the Cray T3D parallel computer to meet the needs for aircraft assessment.

Description of Application

The LLNL 3-D chemical-transport model, IMPACT (Integrated Massively Parallel Atmospheric Chemical Transport model), was designed and implemented based largely on the scientific need for coupled atmospheric chemistry/global climate simulations (Rotman, et al, 1993). When coupled, IMPACT will obtain its meteorological data directly from the concurrently running GCM. However, IMPACT is also capable of off-line (uncoupled) calculations using data assimilated meteorological fields (winds, temperature, etc.) such as those from the Data Assimilation Program at NASA-Goddard. Using assimilated data provides the advantage of allowing us to treat event-specific chemical phenomena as a technique for validating the processes treated in the model. IMPACT is based on an operator splitting method where each of the primary operators (advection, diffusion, convection, photolysis and chemistry) are dealt with in an independent fashion. Advection in all three dimensions is currently done using a variable order multidimensional flux form of the semi-Lagrangian method, an up-stream-biased monotonic grid point scheme (Lin and Rood, 1996). The upstream nature of this method reduces phase errors to a minimum and the monotonicity control eliminates the need for a filling algorithm and the severe problems that would arise with negative values of chemical species concentrations. This scheme also avoids the strict Courant stability problem at the poles, thus allowing large time steps to be used, resulting in a highly efficient advection operation. Diffusion is currently included using a constant coefficient multiplied by the spatial second derivative of the chemical species distribution. Species transport resulting from convective motion is implemented using the scheme of Lin (private communication), which for infinitely thin layers is essentially the apparent momentum transport of clouds (Schneider and Lindzen, 1976).

Photolysis implementation allows simulations using either complete diurnal calculations or calculating diurnally-averaged coefficients. The photolytic loss rate constants are calculated by integrating the product of absorption coefficient, quantum yield, and solar flux over wavelength, using temperature and pressure dependence where appropriate and available. A two-stream multiple-layer UV-visible model uses 126 wavelength bins to capture the spectral detail needed for photodissociation calculations. The scattering of energy from the direct solar beam is treated using the delta-Eddington algorithm (Joseph et al, 1976) while the scattering of diffuse radiation is modeled using the Sagan-Pollack algorithm (1967). Both algorithms allow inclusion of the bulk optical properties of clouds and aerosols.

Chemistry in IMPACT is solved with SMVGEAR II, a sparse-*m*atrix, *v*ectorized Gear code (Jacobson, 1995). The original SMVGEAR code (Jacobson, 1994; Jacobson and Turco, 1994) was derived from Gear's predictor/corrector, backward differentiation code (Gear, 1971). Gear's original code was extremely accurate but inefficient because it required decomposition and backsubstitution over a full matrix of partial derivatives many times. SMVGEAR gave exactly the same results as Gear's original code, but was about 120 times faster when both codes were run on a Cray C-90. The speedup in SMVGEAR was obtained from the implementation of sparse-matrix and vectorization techniques. The major sparse matrix technique was to reorder the matrix of partial derivatives and then to eliminate, in advance, all multiplies by zero that occurred during subsequent matrix decomposition and backsubstitution.

While the sparse matrix techniques accounted for about half the speedup, the other half resulted from vectorization. To vectorize, the grid domain was divided into blocks of grid cells, and the grid cell loop was made the inner loop throughout the code. In retrospect, this method was found to be useful for scalar and parallel machines as well as for vector machines. For scalar machines, the vectorized version of the code was useful since it minimized the number of outer loop array references. The vectorized version was also useful for parallel computing since several blocks of 500 grid cells could be placed directly on each individual scalar node, causing array references to be minimized.

However, a disadvantage of the original SMVGEAR code was that it required the same number of iterations for each grid cell in a block; thus iterations had to continue until the cell with the stiffest equations converged. To mitigate this problem, a method was developed to reorder grid cells each time interval by stiffness so that the stiffest cells could be solved together in the same blocks. The modified SMVGEAR code is known as SMVGEAR II.

How does the above application address the problem

The atmospheric impacts of supersonic aircraft have been under investigation for many years. Much of this work in the past has been accomplished through the use of a two-dimensional (latitude and altitude) model (zonal-averaged). While adequate for initial studies, the amount and level of uncertainties related to the zonal averaged fields required that complete global three-dimensional models be used for analysis and assessments. For example, the impact of aircraft is most clearly seen in the ozone depletion caused by the emission of oxides of nitrogen, i.e., NO_x emissions. These emissions of nitrogen obviously occur only where the aircraft fly; and, these so-called flight corridors are very much 3-D profiles -- that is, the emissions are not zonally averaged. Furthermore, the exchange of mass between the troposphere and stratosphere is highly unknown, non-zonal, and important to the analysis of emission deposition and chemical effects since the aircraft fly close to this dividing area called the tropopause.

Our general approach is to make use of the computing power of the Cray T3D by implementing our parallelized three-dimensional chemical transport model and adding the needed physics to further our understanding and analysis of the impacts of supersonic aircraft on the atmosphere.

D. Expected Economic Impact

The completion of this part of the CRADA with Boeing provided input to help guide the aerospace industry in developing an environmental analysis of possible future products through better understanding of the possible environmental factors.

E. Benefits to DOE

The Cray T3D located at LLNL was used for implementation and testing of new atmospheric chemistry capabilities. This application focused on aircraft emissions and their influence on the distribution of ozone, but the model can also be used for other studies, for example the influence of anthropogenic energy-use emissions on the distribution of ozone.

F. Industry Area

The completion of this part of the CRADA with Boeing provided input to help guide the aerospace industry in developing an environmental analysis of possible future products through better understanding of the possible environmental factors.

G. Project Status

As discussed in the report, the milestones were not completed. Computer issues played a small role in this issue, but the overwhelming cause of not attaining the goals was an under estimate of the effort required to complete the tasks. However, while the complete chemical transport model was not implemented, a tracer transport model (a subset of the chemistry model) was implemented and used for analysis.

H. LLNL Point of Contact for Project Information

Douglas Rotman
Lawrence Livermore National Laboratory
PO Box 808, L-103
Livermore, CA 94550
925/422-7746

Company Size and Point(s) of Contact

The Boeing Company has 238,000 employees. Primary contact for this project was Steve Baughcum.

J. Project Examples

K. Release of Information

I certify that all information contained in this report is accurate and releasable to the best of my knowledge.

[signature] 9/30/99

Karena McKinley, Director
Industrial Partnerships and Commercialization
Date

Release of Information

I have reviewed the attached Project Accomplishment Summary prepared by Lawrence Livermore National Laboratory and agree that the information about our CRADA may be released for external distribution.

[signature] 4/12/99

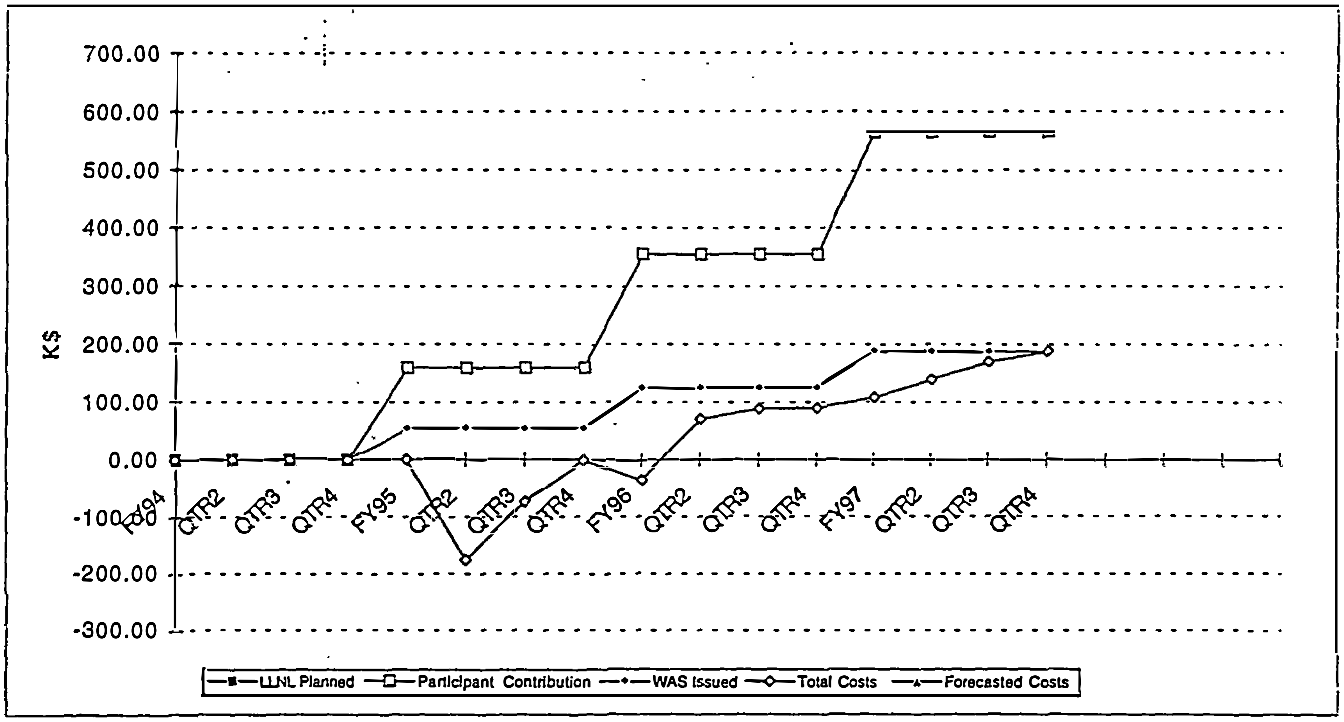
Steve Baughcum
Boeing Company
Date

Lawrence Livermore National Laboratory

Title:	HPPP Global Atmospheric Chemistry Models	Reporting Period:	07/01/95 - 09/30/96
Participant:	Boeing Company	Date CRADA Executed:	4/14/95
DOE TTI No.:	94-MULT-003-XX-1	DOE Approval Date:	4/17/95
CRADA No.:	TC-0824-94-(D)	Scheduled Ending Date:	5/1/98
Account Numbers:	4745-75, 85	Project Completion Date	N/A
Accounts Closed:	N/A	B & R Code (S):	DP0301, YN01000

Approved Funding Profile ($K)

	FY94	FY95	FY96	FY97	FYOUT	Total
LLNL Planned	0	162	195	209	0	566
Participant In-Kind	0	162	195	209	0	566
Paticipant Funds-In	0	0	0	0	0	0
WAS DP0301	0	55	70	63	0	188
LDRD Funds	0	0	0	0	0	0
Total Costs	0	-1	92	97	0	188



DP0301	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD	
														284
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0	
FY95	0	0	0	0	0	-174	0	63	40	25	26	19	-1	
FY96	-62	15	13	17	46	44	35	-21	4	1	0	0	92	
FY97	97	9	9	0	9	10	12	9	10	11	8	9	192	
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0	

YN01000	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD	
														0
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0	
FY95	0	0	0	0	0	0	0	0	0	0	0	0	0	
FY96	0	0	0	0	0	0	0	0	0	0	0	0	0	
FY97	0	0	0	0	0	0	0	0	0	0	0	0	0	
FYOUT	0	0	0	0	0	0	0	0	0	0	0	0	0	

STAFF w/phone:

Lab PI: Doug Rotman — Participant: Dr. Steven Lee (206) 965-0426

Resource Manager: Steve Stinson (510) 423-2888

DOE OAK: Jerry Scheinberg (510) 637-1653 — DOE HQ: A. Larzelere (202) 586-1101

Reporting Period : 07/01/95 - 09/30/96
DOE TTI No.: 94-MULT-003-XX-1
CRADA No.: TC-0824-94-(D)

Milestones and Deliverables:

List the complete set of milestones for all phases of the CRADA. Continue on a separate page if necessary.
Report any changes from the original CRADA or previous quarterly report on the CRADA Change Form.

Completion Date:
Scheduled Actual

See attached report

Verification of participants' in-kind contribution was made in accordance with LLNL policy. Explain basis of verification:

Please initial: YES X NO ______

List any subject inventions by either party (include IL# for LLNL inventions), additional background intellectual property, patents applied for, software copyrights, publications, awards, licenses granted or reportable economic impacts

Accomplishments

Describe Technical/Non-Technical lessons learned (address and be specific about milestones, participant contributions)
Summarize causes/justification of deviations from original scope of work. Continue on a separate page if necessary.

See attached report

Reviewed by CRADA project Program Manager: ______________ Date: ______

Reviewed by Karena McKinley, Director, LLNL/IP&C: Karena McKinley Date: 9/30/99

Direct questions regarding this Report to IP&C Resource Manager, Carol Asher, at (925) 422-7618